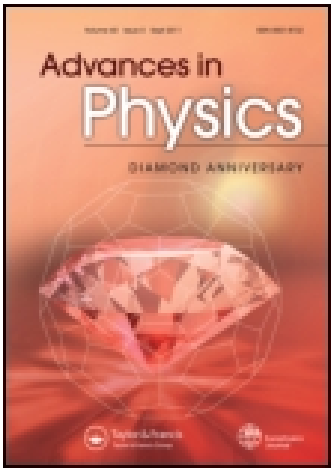
This article was downloaded by: [University of Chicago Library]
On: 18 August 2015, At: 18:11
Publisher: Taylor & Francis
Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: 5 Howick Place, London, SW1P 1WG




Advances in Physics
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/tadp20

# Exact results in the theory of magnetic alloys

A.M. Tsvelick [a] & P.B. Wiegmann [a]
[a] Landau Institute for Theoretical Physics , Vorobievskoye shosse 2, Moscow, 117334, U.S.S.R.
Published online: 02 Jun 2006.

To cite this article: A.M. Tsvelick & P.B. Wiegmann (1983) Exact results in the theory of magnetic alloys, Advances in Physics, 32:4, 453-713, DOI: 10.1080/00018738300101581

To link to this article: http://dx.doi.org/10.1080/00018738300101581

PLEASE SCROLL DOWN FOR ARTICLE

Taylor & Francis makes every effort to ensure the accuracy of all the information (the "Content") contained in the publications on our platform. However, Taylor & Francis, our agents, and our licensors make no representations or warranties whatsoever as to the accuracy, completeness, or suitability for any purpose of the Content. Any opinions and views expressed in this publication are the opinions and views of the authors, and are not the views of or endorsed by Taylor & Francis. The accuracy of the Content should not be relied upon and should be independently verified with primary sources of information. Taylor and Francis shall not be liable for any losses, actions, claims, proceedings, demands, costs, expenses, damages, and other liabilities whatsoever or howsoever caused arising directly or indirectly in connection with, in relation to or arising out of the use of the Content.

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden. Terms & Conditions of access and use can be found at http://www.tandfonline.com/page/terms-and-conditions

ADVANCES IN PHYSICS, 1983, VOL. 32, NO. 4, 453–713

# Exact results in the theory of magnetic alloys

By A. M. TSVELICK and P. B. WIEGMANN
Landau Institute for Theoretical Physics,
Vorobievskoye shosse 2, Moscow 117334, U.S.S.R.

[Received 16 July 1983]

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

ABSTRACT

Recently it has been shown that many traditional models used for a description of dilute magnetic alloys are completely integrable and may be solved exactly without any approximation. In this article we summarize the results which have been obtained in this way.

The main part of the article is devoted to the consistent and detailed account of the Bethe-Ansatz technique for the s–d exchange (Kondo) model with arbitrary impurity spin, s–d model with anisotropic exchange, degenerate exchange model and for the canonical Anderson model. The thermodynamic properties of a magnetic impurity in a non-magnetic metal host obtained by the Bethe method are considered in detail. Mainly attention is paid to the analysis of singularities associated with the formation of a localized moment, Kondo effect and mixed-valence phenomenon, which can be treated analytically.

In the introductory part of the article we discuss the applicability of the models which we study in the paper to the real alloys and consider some modern experimental data which give the evidence of the many-body effects in dilute magnetic alloys. A brief review of some theoretical results which have been obtained using alternative approaches is given. We think that these results illustrate some features of the exact solution.

This review was completed in June 1982.

CONTENTS

| | PAGE |
|---|---|
| INTRODUCTION. | 456 |
| §1. EXPERIMENTAL EVIDENCE FOR THE MANY-BODY EFFECTS IN DILUTE MAGNETIC ALLOYS. KONDO-LIKE BEHAVIOUR IN DILUTE LANTHANIDE IMPURITY SYSTEMS. | 465 |
| 1.1. Two typical examples: (La, Ce)$Al_2$ and (La, Ce)$B_6$. | 466 |
| §2. BASIC MODELS. | 480 |
| 2.1. The Anderson model. | 481 |
| 2.1.1. The general form of the Anderson model. | 481 |
| 2.1.2. The hierarchy of energies in the Anderson model. | 484 |
| 2.1.3. The Anderson model for the rare-earth alloys. | 486 |
| 2.2. Exchange hamiltonians. | 487 |
| 2.2.1. The general form of the exchange hamiltonians. | 487 |
| 2.2.2. Two simple exchange hamiltonians. | 489 |
| 2.2.3. Influence of the hyperfine coupling. | 491 |
| 2.2.4. Perturbation theory. | 492 |

§3. Recent theoretical developments. 495
3.1. The Kondo model. 495
3.1.1. The Coulomb gas and the resonant-level model. 495
3.1.2. Numerical renormalization group approach to the Kondo problem. 501
3.1.3. Nozières' Fermi-liquid theory. 504
3.2. The Anderson model. 507
3.2.1. Introduction. 507
3.2.2. The symmetric Anderson model. 509
3.2.3. The Fermi-liquid approach, based on the perturbation theory in the Anderson model. 511
3.2.4. Properties of the asymmetric Anderson model. 515

§4. Bethe method. 523
4.1. General. 524
4.2. The Bethe Ansatz for the s–d exchange model. 541
4.2.1. The effective hamiltonian. 541
4.2.2. The coordinate Bethe Ansatz. 542
4.2.3. Periodic boundary conditions. 546
4.2.4. The set of commuting operators. 547
4.2.5. Factorization equations. 549
4.2.6. Diagonalization of the trace of the monodromy matrix. 550
4.3. The Bethe Ansatz for the anisotropic exchange model. 553
4.3.1. The two-particle scattering matrix and the Bethe-Ansatz equations. 553
4.4. The Bethe Ansatz for the degenerate exchange model. 555
4.4.1. The coordinate Bethe Ansatz. 555
4.4.2. Bethe-Ansatz hierarchy. 557
4.5. The Bethe Ansatz for the Anderson model. 561
4.5.1. The effective hamiltonian. 562
4.5.2. The two-particle scattering matrix. 562
4.5.3. The coordinate Bethe Ansatz. 565
4.6. The Bethe Ansatz for the degenerate Anderson model. 566
4.7. General remarks. 568
Appendix to §4.3.1. Solution of the factorization equations. 572

§5. Exact solution of the s–d exchange model at $T=0$. 574
5.1. Isotropic s–d exchange model with an arbitrary impurity spin. 574
5.1.1. The continuous limit. 574
5.1.2. The ground state and magnetic susceptibility at zero magnetic field $H=0$. 577
5.1.3. Impurity magnetic susceptibility at arbitrary magnetic fields. 580
5.1.4. The scattering phase. 583
5.1.5. Scales in the Kondo phenomenon. 590
5.2. The anisotropic exchange model. 593
5.2.1. Scaling picture. 593
5.2.2. The ground state of the anisotropic exchange model at $I_\perp < I_\parallel$. 595
5.2.3. Magnetic susceptibility. 597
Appendix to §5.1.3. The Wiener–Hopf method. 600

§6. Thermodynamics of the exchange models. 602
6.1. Thermodynamics of the s–d exchange model. 602
6.1.1. Solutions with complex rapidities. 602
6.1.2. Thermodynamic limit. 604

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

6.1.3. Equilibrium distribution. 606
6.1.4. Non-interacting electron gas and the Bethe-Ansatz technique. 608
6.1.5. Universality. 611
6.1.6. The limits of strong and weak coupling. 612
6.1.7. The Fermi-liquid picture. 613
6.1.8. Thermodynamics of the impurity. 614
6.1.9. Zero-temperature limit. 617
6.1.10. Low-temperature expansion at $\mu_B H \gg k_B T$. 618
6.1.11. High-temperature expansion (perturbation theory). 619
6.1.12. Numerical solution of the non-linear integral equations. 622
6.2. The anisotropic s–d exchange model at finite temperatures. 627
6.2.1. Classification of states and basic equations for $I_\perp < I_\parallel < \pi$. 628
6.2.2 Impurity thermodynamics at $I_\perp < I_\parallel < \pi$. 631
6.2.3. Impurity thermodynamics at $\pi < I_\parallel < 2\pi$. 633
Appendix A to §6.2.1. The proof of the 'string' hypothesis. 635
Appendix B to §6.2.1. Thermodynamics equations for the arbitrary exchange anisotropy. 639
Appendix to §6.2.2. The proof of the identity (6.2.24). 640

§7. Introduction to thermodynamics of the degenerate exchange model. 641
7.1. Basic equations. 641
7.2. Low-temperature thermodynamics. 643
7.3. Magnetic susceptibility. 644
7.4. Discussion. 646

§8. Exact solution of the Anderson model. 646
8.1. Introduction. 646
8.2. Physical properties at zero temperature. 647
8.2.1. The Bethe-Ansatz equations for a large number of particles. 647
8.2.2. The continuous limit. 649
8.2.3. The particle–hole symmetry. 651
8.2.4. Ground state of the symmetric Anderson model. 653
8.2.5. Basic equations. 654
8.2.6. Valency of an impurity ion. 654
8.2.7. Magnetic susceptibility of the symmetric Anderson model in an arbitrary magnetic field. 658
8.2.8. Magnetic susceptibility at $H=0$ and arbitrary $\varepsilon_d + U/2$. 665
8.2.9. Magnetic susceptibility of the asymmetric Anderson model. 667
8.2.10. Localized-moment regime. 669
8.3. Thermodynamic properties of the Anderson model at finite temperatures. 670
8.3.1. The theory of a finite but large system. 670
8.3.2. Integral equations. 671
8.3.3. Thermodynamic equilibrium. 672
8.3.4. Symmetries of charge and spin excitations. 674
8.3.5. Low-temperature thermodynamics. 675
8.3.6. The Kondo limit. 676
8.3.7. Specific heat at $T \ll \epsilon_d + U/2$, $\Gamma$, $U$. 677
8.3.8. The specific heat of the symmetric Anderson model. 680
Appendix to §8.2.1. Solutions with complex rapidities for the Bethe-Ansatz equation for the Anderson model. 680

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Appendix to §8.2.6. Evaluation of the magnetic susceptibility and occupation number in the mixed-valence region ($|\epsilon_d^*| \ll \Gamma$). 681
Appendix A to §8.2.7. Proof of the relations (8.2.71) and (8.2.72). 682
Appendix B to §8.2.7. Expansion in inverse powers of the magnetic field at $H \gg (U\Gamma)^{1/2}$. 683
Appendix A to §8.3.3. High-temperature limit ($T \gg \Gamma$). 684
Appendix B to §8.3.3. Low-temperature limit ($T \ll \Gamma, H, \epsilon_d + U/2$). 685
Appendix to §8.3.7. Thermodynamics of the asymmetric Anderson model. 685

§9. Introduction to the exact solution of the degenerate Anderson model. 687
9.1. Basic equations. 687
9.2. Universality. 693
9.3. The occupation number. 695
9.4. Magnetic susceptibility and the Kondo limit. 696

SUPPLEMENT. 699

CONCLUSION. 703

ACKNOWLEDGMENTS. 705

REFERENCES. 708

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

## INTRODUCTION

In the last two decades theoretical physicists have frequently encountered quantum many-body problems characterized by the growth of an effective coupling at low energies. The principal difficulty in solving these problems, which attracts a great deal of attention from both condensed matter and particle physicists, is that the relevant low-energy phenomena cannot be treated in the framework of conventional perturbation theory. This implies that the genuine ground state of the system is radically different from that of the perturbation theory. Sometimes this can be understood intuitively and one can employ a suitable phenomenological theory. Even so, there remains the difficult problem—how to treat the crossover between the infrared and ultraviolet regions of the spectrum. A widespread opinion is that one can learn about the crossover only via numerical analysis.

The third approach, and an alternative method of avoiding perturbation theory, in which active development and growing popularity has recently been witnessed, is *integrability*. We have now had half a century since the work of Hans Bethe (1931) in which the integrability concept was discovered and foundations of the theory of integrable systems were laid. Remarkably, integrability was discovered only $6\frac{1}{2}$ years after Schrödinger's 'Erste Mitteilung' had been published; however, the subsequent

development of the theory had to wait until the 1960s. The growing interest of recent years in the integrability approach is a peculiar revelation of the 'retro'. Indeed, starting simple-mindedly with conventional quantum field theory one immediately encounters mathematical difficulties. The presence of many particles brings in a broad range of physical effects which have made the solution of the many-body problem a more elusive goal. On the other hand, the integrability property is not directly related to features of the many-body behaviour. Rather it is a consequence of specific, so-called 'hidden symmetries', which show up already at the two-particle level. All the properties of the many-particle system are already built-in in the two-particle system: one has to start from two particles, then add the next ones.

The subject of this paper is a microscopic theory of dilute magnetic alloys. As is well known, a small amount of magnetic impurities dissolved in a non-magnetic metal drastically affect its properties. The problem encountered in the theory of this phenomenon is that the perturbation theory in the impurity–conduction electron exchange interaction is not applicable at low temperatures.

The exchange interaction between the magnetic impurity and the electrons, which is responsible for those striking effects in the above alloys, can be described by a simple model hamiltonian. It is the so-called s–d exchange model of the Kondo hamiltonian, which is apparently one of the first and, perhaps, simplest quantum field theories with a growth of coupling at low energies. It is this model which has been successfully treated in the strong coupling limit in the framework of the phenomenological and numerical approaches mentioned above. A phenomenological description of the low-temperature limit was given by Nozières (1974, 1975), whereas a numerical treatment of the crossover was given by Wilson (1974, 1975).

It has been shown recently that many of the models, which for more than two decades have been applied to the description of dilute magnetic alloys, are completely integrable and the relevant solutions have been produced. These include the s–d exchange (Kondo) model, the degenerate exchange model, the Anderson model and the degenerate Anderson model.

The subject of this review is a Bethe-Ansatz approach to the above-mentioned models and a discussion of physical results which can be obtained using exact solutions. Our treatment differs from that of a conventional review article. Our goal is to present a self-contained microscopic theory of the dilute magnetic alloys based on a systematic use of the Bethe-Ansatz technique. The theory of dilute magnetic alloys and quantum integrable systems are interwoven to such an extent that we have tried to make our review an introduction to the theory of integrable systems also; though our principal subject is the physics of the magnetic alloys. To preserve the self-contained character we have in places recapitulated some details we have given elsewhere.

The subject *Magnetic impurities in nonmagnetic metals* is rather wide. The first experimental data on this subject belong to the early days of quantum metal physics when a striking phenomenon, the resistance minimum, was found in certain, supposed to be pure, metals at low temperatures. Later it was realized that the effect is due to transition element impurities and is proportional to their concentration. Experimental data on transition impurities in simple metals obtained in the course of extensive researches of the 1960s–1970s can be found in numerous reviews, for instance: van den Berg (1964), Heeger (1969), Narath (1970, 1973), Fisher (1970) and Daybell (1973). The most complete reviews are those by Rizzuto (1974) and Grüner (1974), which cover more than 800 papers published from 1962 to 1975.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Detailed studies of dilute magnetic alloys have shown that in all alloys below a certain temperature $T_K$, called the Kondo temperature, the impurity part of the magnetic susceptibility becomes temperature independent and remains finite at $T=0$. One may say the effective magnetic moment of the impurity vanishes as the temperature is lowered. The peculiar anomalies of thermal and transport properties of magnetic alloys are due to the smooth transition into the non-magnetic state. The Kondo temperature may change by orders in magnitude from impurity to impurity and/or from the matrix metal to metal—from milliKelvins to $10^2$ K; for instance, from 1 K for LaCe alloy (Sugawara and Eguichi 1966) to 40 K for YCe alloys (Maple and Wittig 1971), from 0·8 K for AuFe (Daybell 1973) to 300 K for AuV (van Dam *et al.* 1972). Hence the Kondo effect is not always a low-temperature phenomenon, it can be observed at room temperatures.

The properties of dilute alloys with localized moments are basically determined by the exchange interaction between the conduction electrons of the metal and the impurity magnetic moment. A conventional description of this interaction is based on the so-called s–d exchange (Kondo) model. It is the simplest model in which the impurity is represented by the localized magnetic moment $\mathbf{S}=(S_x, S_y, S_z)$. The origin of this model goes back to the early 1950s (Zener 1951, Vonsovskii 1946). In 1964 Jun Kondo applied perturbation theory to this model and explained the logarithmic growth of the resistivity at low temperatures. His paper gave rise to an enormous amount of theoretical activity in this area, which continued up to the mid-1970s.

The hamiltonian of the s–d exchange model is

$$\mathscr{H}_{\text{s-d}}=\sum_{k,\sigma}\epsilon_k c^+_{k\sigma}c_{k\sigma}+I\sum_{\substack{k,k'\\ \sigma,\sigma'}}c^+_{k\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}c_{k'\sigma'}\mathbf{S}, \tag{I}$$

where $c^+_{k\sigma}$, $c_{k\sigma}$ are the conduction electron creation and annihilation operators, $\epsilon_k$ is the electron's kinetic energy and $\sigma$ is the Pauli matrices.

As far as the linear effects in the impurity concentration are concerned we can confine ourselves to a single-impurity problem, the impurity being located at $X=0$, as was supposed when writing down (I).

In real alloys the exchange interaction is always antiferromagnetic: $I>0$, with a small dimensionless coupling $\rho(\epsilon_F)I\ll 1(\rho(\epsilon_F)$ is the density of states at the Fermi surface).

Kondo observed that the spin–flip scattering effective amplitude, computed to second order of perturbation theory, rises as energy and temperature decreases:

$$\rho I(\varepsilon)=\rho I+(\rho I)^2\ln D/\varepsilon+O((\rho I)^3),\quad (\rho=\rho(\epsilon_F)), \tag{II}$$

where $D$ is the cut-off of the order of the Fermi energy.

The resistivity due to the magnetic impurity is proportional to the scattering amplitude squared:

$$R_i\sim cI^2(T)\simeq c[I+\rho I^2\ln D/T+O(\rho^2 I^3)]^2, \tag{III}$$

where $c$ is a concentration of magnetic impurities. It increases with decreasing $T$, in contrast with the phonon part of resistivity $R_{ph}$, which rapidly decreases. Hence the total, phonon- and impurity-induced, resistivity should have a minimum at $R_i\sim R_{ph}$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

When the temperature is of the order of the Kondo temperature

$$T_K \sim D \exp(-1/\rho I) \tag{IV}$$

all the terms of the perturbation expansion are of the same order in magnitude and, despite the weak bare coupling, perturbation theory no longer holds.

Soon after Kondo's paper Abrikosov in his pioneering work (Abrikosov 1965) summed the most divergent terms in perturbation theory expansion (the so-called leading-log terms):

$$I(T) = \frac{I}{1 - \rho I \ln D/T}. \tag{V}$$

The same result was derived by Suhl (1965) who used the unitarity equation in the two-particle scattering approximation. Besides summing the leading-logs, Abrikosov proved that the exchange hamiltonian (I) is renormalizable. This implies that for the antiferromagnetic interaction at $\rho I \ll 1$ and $D \to \infty$ all the physical quantities are universal functions of the temperature, magnetic field, etc. For instance, the temperature dependence of the resistivity is of the form:

$$R_i = \text{const} f(T/T_K).$$

Formula ($V$) is but a leading approximation at $T \gg T_K$:

$$I(T) = \frac{1}{\rho \ln T/T_K} + O\left(\frac{1}{\rho \ln^2 T/T_K}\right). \tag{VI}$$

In the case of a ferromagnetic exchange interaction eqn. (V) gives a complete solution since the effective amplitude is small at all temperatures and the higher-order perturbation terms are irrelevant. For example, the impurity part of the magnetic susceptibility differs from that given by Curie law by logarithmic terms which are small at all temperatures and, moreover, vanish at $T \to 0$

$$\chi_i = \frac{S(S+1)}{3T}(\mu_B g)^2 \left(1 + \frac{1}{\ln D/T} + \dots\right). \tag{VII}$$

One encounters a distinct situation at $I > 0$. In this case the effective interaction amplitude increases as temperature decreases. The next-to-leading-log terms do not alter the situation. For instance, the magnetic susceptibility which at this order is proportional to the scattering amplitude, equals

$$\chi_i = \frac{S(S+1)}{3T}(\mu_B g)^2 \left(1 - \frac{1}{\ln T/T_K} - \frac{\ln \ln T/T_K}{2 \ln^2 T/T_K} + \dots\right).$$

It is quite obvious that such a divergence is rather an artefact of the approximation used. The perturbation expansion parameter is $(\ln T/T_K)^{-1}$ hence perturbation theory breaks down at $T \sim T_K$ and has nothing to tell us about the ground state of magnetic impurity in a non-magnetic metal. This problem is called the *Kondo problem*.

The exceptional simplicity of the s–d exchange model (I), combined with giant effects easily observed experimentally made the Kondo problem rather popular. Simple though it is, the physical and mathematical features of the phenomena described by this hamiltonian proved to be not so simple. There have been many

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

attempts to go beyond perturbation theory. Most of the theories, put forward in the 1960s, are but unsuccessful attempts to develop an approximate approach to the ground state of the impurity. However, the lack of any parameter at $T \lesssim T_K$ leads inevitably to uncontrolled approximations resulting frequently in wrong results.

It would be impossible to survey the 'jungle' of more than $1{\cdot}5 \times 10^3$ papers on the Kondo problem, though a critical and valuable survey may well prove instructive as a contribution into the sociology of science†. In the course of this section we shall mention the main lines of thought which have been explored during the 1960s. More than 20 review articles, some of which are cited below, on the magnetic alloys problem have appeared since 1962; early theoretical works have been reviewed by Abrikosov (1969), Kondo (1969), Grüner and Zawadowski (1974, 1978), Fischer (1970), and also by Yosida and Yoshimori (1973), Brenig and Zittartz (1973) and Anderson and Yuval (1973) collected in the book *Magnetism*, Vol. V, edited by H. Suhl. For a more exhaustive bibliography we refer the reader to these articles.

Although a consistent theoretical study of the low-temperature properties of magnetic alloys was lacking, in 1965 Nagaoka had already made a correct conjecture on the nature of the ground state of the impurity (Nagaoka 1965, 1969). He constructed the special mean field theory using the decoupling scheme, which resulted in complex singular integral equations. Then Nagaoka solved these equations 'approximately' and obtained the desired result: namely, the ground state of the 1/2-spin impurity is a singlet one. As a result he found the simple power laws at low temperature. Other approximate methods (dispersion theory of Suhl (1965 a, b, 1966) and Maleev (1966, 1967), perturbation expansions of Brenig and Götze (1968), etc.) proved to be equivalent to the equations of motion of Nagaoka. Furthermore, it turned out that these approximate equations can be solved exactly (Bloomfield and Hamann 1967, Zittarz and Müller-Hartmann 1968). This exact solution of the Suhl–Nagaoka equations is drastically different from Nagaoka's approximate solution, and results in physically meaningless behaviour when $T \to 0$. In particular, instead of Nagaoka's powers one again finds, as at $T \gg T_K$, the inverse logs of the temperature‡.

Factually, the starting approximation in all of these theories is poor at low temperatures. It was sensible only at $T \gg T_K$ and only in the leading-log approximation. Hence, nothing comes out except formulae such as (VI) and (VII). Since Abrikosov's approach was more consistent, it explicitly stated what was neglected, one has never been tempted to go beyond the perturbation-theory approach.

Of all the works of the 1960s one can single out that of Mattis (1967), in which it has rightly been conjectured that (i) the ground state of the $S$-spin impurity is $2S$-fold degenerate, (ii) for $S > 1/2$ the impurity remains magnetic even at $T = 0$, but the spin becomes $S - 1/2$.

A qualitative understanding of the phenomenon dates back to the early 1970s and is due to remarkable papers by Anderson and Yuval (1969) and Anderson *et al.* (1970 a) (see also, Anderson 1970, 1971, Yuval and Anderson 1970, Anderson *et al.* 1970 b, a review of this approach is given by Anderson and Yuval (1973)), and by Wilson (1974, 1975) and Nozières (1974, 1975). As was stated, they produced

† A study of this kind on the specialized topic 'The formation of the localized moment in metals' was made by Morandi *et al.* (1981).

‡ Interestingly enough, there exists the logarithmic situation as $T \to 0$, but only for $S \neq 1/2$ (see § 5).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$(100-\varepsilon)\%$ proof that as the temperature decreases the effective coupling increases unboundedly, which implies the complete compensation of the impurity magnetic moment by the conduction electrons. As a result the ground state of the impurity is a singlet one, the magnetic susceptibility is finite at $T=0$ and all physical quantities have a simple power law behaviour at $T \ll T_K$. Moreover, the Fermi-liquid-like relationships have been proven between the lowest-order coefficients of the temperature expansions for the specific heat and magnetic susceptibility (Wilson 1974, 1975, Nozières 1974, 1975) and resistivity (Nozières 1974, 1975).

$$\left.\begin{aligned} \chi_i &= \frac{(g\mu_B)^2}{2\pi T_K}\left(1+O\left(\frac{T^2}{T_K^2}\right)\right), \\ C_i &= \frac{\pi}{3}\frac{k_B T}{T_K}\left(1+O\left(\frac{T^2}{T_K^2}\right)\right), \\ \frac{R_i-R_0}{R_0} &= \frac{(k_B T)^3}{T_k^2}\left(-\pi^2+O\left(\frac{T^2}{T_K^2}\right)\right), \end{aligned}\right\} \qquad \text{(VIII)}$$

where $R_0 = 3/(\pi(\rho V_F e)^2)$ is the unitary limit.

When the temperature goes through $T_K$, the qualitative physical Fermi-liquid-like picture changes—only perturbative logarithmic terms make the impurity unlike the free spin. These limits $T \gg T_K$ and $T \ll T_K$ are both conceptually rather simple.

The well-known anomalies in the specific heat, magnetic susceptibility, resistance, thermopower, etc., can be qualitatively understood in terms of the concept of a many-body resonance at the Fermi level. The phase shift $\eta(\omega)$, defined as

$$\eta(\omega) = \tan^{-1}\left[\frac{\operatorname{Im} T(\omega)}{\operatorname{Re} T(\omega)}\right],$$

where $T(\omega)$ is a $T$-scattering matrix, reaches its unitary limit at $\omega \to 0$ and can be expanded in integer powers of $\omega/T_K \ll 1$:

$$\eta(\omega) = \pi/2 - (\omega/2T_K)^2 + O((\omega/T_K)^4).$$

Far away from the Fermi level the tail of the resonance has a perturbative logarithmic behaviour. This so-called Abrikosov–Suhl narrow many-body resonance is evidence of formation of the complex many-body bound state.

One can justify all the theoretical efforts and theoretical games devoted to this fairly limited problem not only by the strong correlation of theory and experiments in this particular field of solid-state physics, but also by referring to the fact that many of the methods developed to attack it proved to be universal ones and productive in other branches of theoretical physics as well. For instance, the recursion procedure, the basic ingredient of the renormalization group approach, was first employed by Anderson *et al.* (1970). The bosonic representation of the fermion operators, so effective in one-dimensional quantum and two-dimensional classical physics was developed in the remarkable papers by Schotte and Schotte (1969) and Schotte (1970) (for a review see Wiegmann 1980 b). This list can easily be continued.

The first half of this paper is devoted to the solution of the Kondo problem. In the second half (§§ 4.5, 8 and 9) we discuss the solution of the model which describes the

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

electronic mechanism of the formation of the magnetic moment of an ion with an incomplete inner shell placed in a metal.

As is well known the behaviours of different impurities with incomplete inner shells in different metals are quite different. For instance, Mn, Cr and Fe in Cu, Au and Ag matrices, like Ce in La, possess well-defined magnetic moments: the impurity susceptibility follows the Curie law at high temperatures. On the other hand, Ni and Ti in the same Cu, Au and Ag samples prove to be non-magnetic: rather weak Pauli paramagnetism is observed. Transition ions which proved to be magnetic in Cu, Au or Ag samples, lose this property in Al (see, for example, Rizzutto 1974). Similarly, Ce in La ceases to be magnetic after Th and/or Y is introduced, or under a pressure of $\sim 6$ kbar (see Maple *et al.* 1978 and Steglich 1977 for a review).

Whether the impurity is magnetic or non-magnetic, depends on the properties of both the impurity ion and the host metal. A free $3d$ or $4f$ ion is obviously magnetic. However, the metal overlap of the $3d$ or $4f$ electron wave function with that of the conduction electron band of the host metal leads to delocalization of the impurity electron states and can destroy the magnetic moment, a situation first recognized by Friedel (1958). A conventional approach to the formation of the localized magnetic moments in metals is based on the Anderson model (Anderson 1961, see also Anderson 1978)

$$\mathscr{H}_{\mathrm{A}} = \sum_{k,\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + V \sum_{k,\sigma} (c^+_{k\sigma} d_\sigma + d^+_\sigma c_{k\sigma}) + \sum_\sigma \epsilon_d n_{d\sigma} + U n_\uparrow n_\downarrow . \tag{IX}$$

It is the so-called non-degenerate Anderson model where orbital degeneracy of the impurity shell is neglected. It is supposed that no more than two electrons with spins $\sigma = \uparrow, \downarrow$ can simultaneously occupy the impurity level $\epsilon_d$. The intratomic Coulomb interaction is given by the term $U$, and $V$ is the admixture of the $d$ level with conduction band states.

The mixing of $d$ and $s$ states leads to broadening of the $d$ level. If $U \to 0$ the resonance level has the width $\Gamma = \pi\rho(\epsilon_{\mathrm{F}})V^2$ and is centred at $\epsilon_d$. If, after adding or removing one electron to and from the impurity shell, the respective energy variation $-\epsilon_d$ and $\epsilon_d + U$ exceeds the resonance width, the shell can be considered as singly-occupied and the impurity would possess a magnetic moment. The virtual processes, which change the number of particles by $\pm 1$, induce the exchange interaction between the conduction electrons and the localized moment (Anderson and Clogston 1962). Schrieffer and Wolf (1966) produced the formal proof of the equivalence of the $S = 1/2$ Kondo model and the Anderson model in the limit

$$\Gamma \ll -\epsilon_d, \epsilon_d + U, \tag{X}$$

with the antiferromagnetic exchange

$$\rho(\epsilon_{\mathrm{F}}) I = \frac{\Gamma}{\pi}\left( -\frac{1}{\epsilon_d} + \frac{1}{\epsilon_d + U} \right) > 0.$$

In the opposite case, when a broad resonance level is formed near the Fermi level $|\epsilon_d| \ll \Gamma$ and the Coulomb energy is relatively small compared with $\Gamma (U \lesssim \Gamma)$ the impurity is partially occupied with spin-up and spin-down electrons. This state is non-magnetic, only the fluctuation of the occupation numbers for different spins can result in magnetic susceptibility. For this reason at temperatures below the level

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

width ($T \lesssim \Gamma$) all the physical quantities can be expanded in integer powers of $T$. For instance, for the symmetric Anderson model ($U = -2\epsilon_d$), the magnetic susceptibility is

$$\chi_i = \frac{\alpha(U/\Gamma)}{\Gamma}\left(1 + \left(\frac{T}{\Gamma}\right)^2 \beta(U/\Gamma) + \ldots\right),$$

where dimensionless coefficients $\alpha$ and $\beta$ can be calculated in perturbation theory in $U/\Gamma$.

If we change the relative values of $U$, $\epsilon_d$ and $\Gamma$ the non-magnetic regime goes over continuously to the magnetic regime, but, simultaneously, the impurity magnetic moment is compensated by the conduction electrons due to the Kondo effect. Hence, the Anderson model, being the microscopic justification of the exchange hamiltonian (I), provides, simultaneously, a unified description of the narrow many-body and the broad single-particle resonances. With regard to the Anderson model the theoretical part of the problem has not been developed in a satisfactory manner and has lagged behind the advances in the theory of the exchange model.

The Hartree–Fock approach to the description of transition between the magnetic and non-magnetic regimes was proposed by Anderson (1961). It is a fairly rough approximation which leads to the sharp transition at $U = \pi\Gamma$ and, frankly, has no region of applicability. None the less, it provides the qualitatively correct description of the tendency of the formation of the localized moment, i.e. splitting of the peak in the impurity density of states, and is confirmed by the available optical data (for a review see Grüner 1974). Early theoretical works based on the Hartree–Fock approximation are reviewed by Blandin (1973). Correlation effects, due to the Coulomb repulsion, were treated in a large number of papers; the reader can find a detailed analysis of these in Mills *et al.* (1973) and Grüner and Zawadowski (1974). In the early 1970s great hopes were related to the functional integral method, reviewed by Hamann and Schrieffer (1973) and Morandi *et al.* (1974). We refer also to the book by Morandi *et al.* (1981) for analysis of all theoretical papers on the formation of local magnetic moment in metals published between 1952 and 1973. This volume contains an interesting study of the sociology of this area of creative activity.

Of all the approaches to the Anderson model, as well as the exchange model, the most reliable and productive ones proved to be the Fermi-liquid approach by Yosida and Yamada (1970, 1975) and Yamada (1975) for the symmetric Anderson model, the scaling approach by Haldane (1978) for the asymmetric Anderson model and Wilson's numerical renormalization group approach by Krishna-Murthy *et al.* (1975, 1980 a, b) for both the symmetrical and asymmetrical cases.

Yamada and Yosida gave the closed mathematical form for the perturbation theory in $U$ and used it to prove the Fermi-liquid like general relations between different physical quantities, particularly, relation (VIII) in the Kondo limit $U \to \infty$.

Recently, interest has been aroused in the asymmetric Anderson model in view of the mixed valence problem. In the asymmetric limit $|\epsilon_d|$, $\Gamma \ll U$ the state with double occupation may only be a virtual one, whereas in the states with $n_d = 0$ and 1 the impurity ion may be stable for a long time. In the mixed valence regime $|\epsilon_d| \sim \Gamma$, which is apparently the most interesting one, there appear new features due to the average occupation number being essentially non-integer, thus leading to strong renormalization of the effective level: $\epsilon_d^* = \epsilon_d + \Gamma/\pi \ln U/\Gamma$. Haldane (1978) for-

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

mulated the scaling approach to this case and showed that all the physical quantities are universal functions of $\Gamma/\epsilon_d^*$, the latter being the real expansion parameter. For example, the average occupation number $n_d$ has the form

$$n_d = \begin{cases} 1+\Gamma/\pi\epsilon_d^* + O(\Gamma^2/\epsilon_d^{*2}\ln\Gamma/|\epsilon_d^*|) & (\epsilon_d^*<0), \\ 2\Gamma/\pi\epsilon_d^* + O(\Gamma^2/\epsilon_d^{*2}\ln\Gamma/\epsilon_d^*) & (\epsilon_d^*>0). \end{cases}$$

Thus, one encounters a situation reminiscent of that in the Kondo problem: despite the bare coupling being arbitrarily small, $\Gamma \ll U$, when the level approaches the Fermi surface the effective mixing increases and in the most interesting region $|\epsilon_d^*| \lesssim \Gamma$ perturbation theory no longer holds. (A much closer analogy exists between the Kondo and mixed valence problem for the single impurity, see below.)

Krishna-Murthy *et al.* (1975, 1980a, b) extended Wilson's numerical renormalization group technique to the general Anderson model. Their results, though being only numerical, provide a comprehensive temperature dependence of the magnetic susceptibility in all the possible regimes and enable one to follow the smooth crossovers from one to another regime as the parameters are varied.

The bulk of this review is devoted to the exact solution of the s–d exchange model (§§ 4.2, 4.3, 5, 6) and the Anderson model (§§ 4.5, 8). The crossover between the low- and high-energy regimes in the Kondo model will be described in an analytical way. For the Anderson model we give a similar analytic description of the crossovers between non-magnetic and local moment regimes and between local moment and mixed-valence regimes. The theory to be exposed below restores our naive perception of hamiltonians (I, XI) as simple ones. Their simplicity reveals itself, however, not in the many-body dynamics, but rather at a quite different level—in the dynamics of the two-particle scattering. Readers familiar with the history of studies in the Kondo and Anderson models could not miss noticing what a frightening mathematical debris one is trapped in, while attacking by inadequate methods the phenomena which were eventually described by such simple mathematics.

Despite the considerable contributions of the theory of integrable systems to mathematical physics in one-dimension, the elegant methods of this algebraic theory are not that wide-spread. For this reason we have tried to make our presentation of the Bethe-Ansatz technique as applied to the s–d exchange (Kondo) model (§ 4.2), the exchange model with anisotropic exchange (§ 4.3), the degenerate exchange model (§ 4.4), the Anderson model (§ 4.5), the degenerate Anderson model (§ 4.6) and the resonant level (RL) model (supplement) as self-contained as possible, so that one should not need to consult the original papers. In our presentation we employ the recently discovered quantum inverse scattering method (for a review, see Faddeev 1980).

The Bethe-Ansatz technique enables one to parametrize the spectrum of the hamiltonian in terms of the so-called rapidities which characterize the state of the many-body system. These rapidities obey the system of algebraic transcendental equations, the so-called Bethe-Ansatz equations. To find that the system is integrable is not the same as to solve it. In order to get certain results, one has to construct the equilibrium state of the system at the given temperature and solve the relevant Bethe-Ansatz equations. The relevant mathematical technique is exposed in detail on an example of the s–d exchange model (§ 5.1, 6.1) and applied afterwards to other models (§ 5.2, 6.2, 7).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Once the Bethe-Ansatz equations are solved, one can comprehensively describe the magnetic and thermal properties of the impurity in the non-magnetic metal.

We conclude with a discussion of the thermodynamic properties of the non-degenerate and degenerate Anderson model in §§ 8 and 9. In these sections the relation between the Anderson model and the s–d exchange model in terms of the exact solutions will also be discussed. Particular attention is paid to the asymmetric Anderson model for the mixed-valence states.

The detailed presentation and discussion of exact solutions follows the three introductory review sections (§§ 1–3). Some recent theoretical developments will be briefly reviewed in § 3. We have selected only those papers which are the most instructive in that the ideas developed are related to the mathematical structure of the solutions and shed light on the physical meaning of the latter. On the other hand, an exact solution enables us to justify and visualize the physical approximations and hypotheses of these works. This is most relevant in the phenomenological Fermi-liquid picture which played an important heuristic role in the construction of exact solutions.

Reviews of Nozières' phenomenological Fermi-liquid approach to the Kondo model and Yamada–Yosida's approach to the Anderson model are given in §§ 3.1.2 and 3.2.1. In § 3.1.1 we discuss the Anderson *et al.* (1970 a, b) approach to the triad of Kondo hamiltonian, Coulomb gas partition function and resonant level model equivalences. Also in §§ 3.1.2 and 3.2.4 we give a brief review of Wilson's numerical renormalization group approach to the Kondo and Anderson models. The perturbation theory motivated scaling approaches to the exchange models and asymmetric Anderson model are discussed in §§ 2.2.4 and 3.2.4 respectively.

Theoretical activity on magnetic alloys was based mainly on the simple exchange Kondo hamiltonian, although until recently there were no known magnetic impurities to which application of this model in its present over-simplified form was justified without ignoring qualitatively important features. Now such substances are found among La-based compounds, two of which are discussed in § 1.1.1. Hence, it seemed worthwhile to present the microscopic derivation of realistic hamiltonians with allowance for the orbital structure of the impurity ion, the crystal field effects, fine and hyperfine structure, etc., and to discuss the limits of applicability of the traditional models to real metal (§ 2).

## § 1. Experimental evidence for the many-body effects in dilute magnetic alloys. Kondo-like behaviour in dilute lanthanide impurity systems

In the 1960s considerable efforts were made in experimental investigation of the properties of dilute alloys in the Kondo state.

One of the results of this effort is that even in classical Kondo transition alloys there are always traces of interimpurity correlation. To avoid impurity–impurity interaction effects it is required that the impurity concentration be in the p.p.m. region, which makes it difficult to extract the single-impurity effect from the measured signal. For instance, in the case of the traditional CuMn alloy the estimate of the RKKY-interaction energy proves that at temperatures near and below $T_K$ the alloy can be regarded as dilute only if the concentration is less than 5 p.p.m. Such pure substances are not in fact available (Hirshkoff *et al.* 1971).

The situation is contrary in Kondo systems containing rare-earth ions such as Ce and Yb. In these systems the interaction between rare-earth ions is believed to be

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

negligible. In rare-earth alloys the impurity can be considered as isolated for amounts up to 1%†. Moreover, the concentrated lanthanide systems exhibit anomalies strongly resembling those of the dilute transitional alloys.

In 1965 Sugawara observed the first resistance minimum phenomenon due to a lanthanide solution in the dilute alloy system YCe. Following this discovery of the Kondo effect in the YCe system numerous dilute and concentrated lanthanide metallic systems have been investigated. Of the thirteen lanthanide ions with a partially-filled $4f$ shell only Ce, Sm, Tu and Yb have Kondo-like behaviour. We shall confine the discussion below mainly to Ce as the most explicit example of an ambivalent rare-earth element.

Recent developments confirm that RE-alloys have great advantages over similar transition metal systems. First, as we have mentioned above, the single-impurity effects can probably be studied not only in the extremely low-concentration range. The second reason is that the structure of the moment in the magnetic state is well defined and rather simple.

The Hund correlations between the $4f$ electrons and the spin-orbit coupling result in a ground state of the $4f$ shell which exhibits a magnetic momentum of the $4f$ shell. Further simplification is due to a strong crystal field. The Kramers ion $Ce^{3+}$ ($^2F_{5/2}$) in a crystal environment of the cubic La-based compounds splits into a $\Gamma^7$ doublet ground state and a $\Gamma^8$ quartet separated by $\Delta_{CF} \sim 150$–$200$ K. Therefore, at sufficiently low temperatures only the doublet is important and the orbital structure of the shell is maximally simplified.

To have a sufficiently wide temperature range above and below $T_K$ to observe the low-temperature properties as well as high-temperature properties of the Kondo state, the Kondo temperature of such systems should be of the order of degrees. At the same time $T_K$ is sufficiently small in comparison with the crystal electric field (CEF) splitting and the Ce alloys may be perfect examples of substances adequately described by the s–d exchange model (I) with the 1/2 spin. Such an arrangement of the magnetic CEF levels enables one to observe simultaneously the *Kondo, and CEF effects*. Both these effects are characteristic of the single Ce impurity in lanthanide systems.

Finally, there are important phenomena relevant to the Kondo effect of Ce dilutely dissolved in La-based compounds, namely, a strong increase of the Kondo temperature and, as a result, destruction of the local-moment state under pressure or under the so-called 'chemical pressure'.

### 1.1. *Two typical examples: (La, Ce)$Al_2$ and (La, Ce)$B_6$*

Recently, great attention has been drawn to the matrix-lanthanide impurity systems, where the metallic matrix is a compound. Today, such systems exhibiting Kondo-like anomalies have been observed. Of all these, the system (La, Ce)$Al_2$ has been by far the most extensively investigated and, therefore, we discuss properties of

† The reason that the RKKY interaction displays itself so weakly is not quite clear since the exchange integral in the RE-alloys is of the same order as that for the transition alloys; however, numerous experiments have consistently indicated that the result of the RKKY polarization of the conduction electrons must be weak and does not lead to any appreciable modification of the local moment.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

this example in some detail. The Kondo effect of (La, Ce)$Al_2$ was first discovered by Maple and Fisk (1968). Kondo anomalies were observed in

(i) resistivity (Winzer 1973),
(ii) magnetic resistivity (Felsch and Winzer 1973),
(iii) specific heat (Deenades *et al.* 1971, Armbrüster *et al.* 1974, Steglich and Ambrüster 1972, Bader *et al.* 1975, Steglich 1976),
(iv) thermoelectric power (Moeser *et al.* 1974),
(v) magnetic susceptibility (Felsch *et al.* 1975) and in addition
(vi) (La, Ce)$Al_2$ is a classical example of the 're-entrant' superconductivity phenomenon (Maple *et al.* 1972).

Unfortunately the investigations of these Kondo anomalies in (La, Ce)$Al_2$ are restricted to Ce concentrations $\gtrsim 0{\cdot}7$ at.% because for smaller concentrations the system becomes superconducting in the temperature range of interest.

Another typical La-based compound exhibiting Kondo-like anomalies but not showing superconductivity was found in the borides. It is (La, Ce)$B_6$ whose conductive and magnetic properties were investigated in the remarkable experiments by Winzer (1975), Samwer and Winzer (1976) and Felsch (1978).

As is known, the most characteristic behaviours of the many-body effects are:

(i) Fermi-liquid simple power behaviour at low temperatures ($T \ll T_K$);
(ii) logarithmic behaviour at high temperatures ($T \gg T_K$).

Experiments in a magnetic field also testify to the appearance of the characteristic scale: unlike a free ion, dimensionless physical quantities are not determined by the ratio $\mu_B H/k_B T$ only—they change with variation of, for instance, $H$ with $\mu_B H/k_B T$ constant. Note that the observation of pure many-body effects is rather delicate: at low temperatures the interimpurity interaction becomes involved, at high temperatures in magnetic experiments a strong influence of the crystal field is observed and separation of the logarithmic behaviour is a difficult task. For some measured quantities, for instance for the specific heat, the logarithmic behaviour displays itself at extremely high temperatures: $\ln T/T_K \sim 6$–$7$.

More clear-cut evidence of the logarithmic behaviour is given by the temperature dependence of the impurity resistivity. Note that the simple power low-temperature behaviour above cannot be considered as evidence of the many-body effects. The case is that due to the broad one-body resonance the Fermi-liquid like behaviour is demonstrated also by the non-magnetic alloys for which the criterion of the local-moment state and the Kondo effect, defined as $U \gg \Gamma$, is not fulfilled. Only the change of the regime from logarithmic to simple power laws is the characteristic feature of the Kondo effect.

We shall give below certain experimental data for magnetic susceptibility, magnetization, specific heat, resistivity, magnetoresistivity, lattice pressure effects and re-entrant superconductivity effect for (La, Ce)$Al_2$ and (La, Ce)$B_6$ testifying to the many-body effects.

(a) *The crystal field effects*

The $^6F_{5/2}$ term of $Ce^{3+}$ ion is usually believed to be split by the cubic crystal field into the doublet $\Gamma_7$ and quartet $\Gamma_8$. In recent neutron scattering experiments on (La, Ce)$Al_2$ Loewenhaupt *et al.* (1979) studied the energetic level scheme of the $Ce^{3+}$ ion. A well-resolved inelastic peak was observed at an energy transfer 100 K in

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

the energy-gain spectrum. In addition, extra scattering intensity was observed at 180 K. The first peak is attributed to the CEF transition between $\Gamma_7$ and $\Gamma_8$, while the second is considered to be due to a dynamic strain which couples the states inside the excited $\Gamma_8$ quartet.

Thus at $T \ll 100$ K only the doublet $\Gamma_7$ is significantly populated. According to Murao and Matsubara (1957) this $\Gamma_7$ state may be described by a spin with the magnitude $S=1/2$ and a modified Lande factor $g'=-(5/3)g$ with $g=6/7$ for the free $Ce^{3+}$ ion. Therefore, the CEF theory gives $g'=-5/3\times 6/7 \simeq -1{\cdot}43$ for the ground state of cerium impurities in the La-based compounds†. The effective magnetic moment $\mu_{\text{eff}}=g'(S(S+1))^{1/2}$ is $1{\cdot}24\mu_B$. Then the exchange interaction with the conduction electrons will be described by the effective s–d exchange hamiltonian (I) with an impurity spin $S=1/2$ and $g=1{\cdot}43$. Note, that although the splitting of the $\Gamma_8$ quartet may appear sufficiently large, it is evident that the matrix elements of the quadrupole operator are also large and lead to a large Van Vleck contribution to the magnetic susceptibility (Loewenhaupt *et al.* 1979).

(b) *Magnetic susceptibility and magnetization*

Felsch (1977, 1978) measured the low-field magnetic susceptibility of the rare-earth (RE) Kondo system (La, Ce)$B_6$ for low and moderate Ce concentrations in the temperature range between 30 mK and 300 K as well as low-temperature magnetization extending to high magnetic fields. He studied the single impurity behaviour of Ce ions subjected to the Kondo effect and found out how the impurity interaction and crystal field effects interfere with the Kondo effect. In fig. 1.1 the data for the inverse low-field impurity susceptibility are represented as $\chi^{-1}$, for two (La, Ce)$B_6$ alloys with 0·072 and 0·13 at.% Ce as a function of the temperature in the regime below 10 K.

The data scale well with the concentration, indicating that $\chi$ originates from isolated Ce ions. In a wide temperature range the solute susceptibility can be described by the Curie–Weiss law

$$\chi=\frac{C}{T+\theta}$$

with the Curie temperature $\theta=(2{\cdot}8\pm 0{\cdot}1)$ K which is independent of the Ce concentration, and the Curie constant $C=1/3\mu_{\text{eff}}^2$ yielding the effective magnetic moment $\mu_{\text{eff}}=(1{\cdot}13\pm 0{\cdot}02)\mu_B$ (remember that the theory gives $\mu_{\text{eff}}=1{\cdot}24\mu_B$).

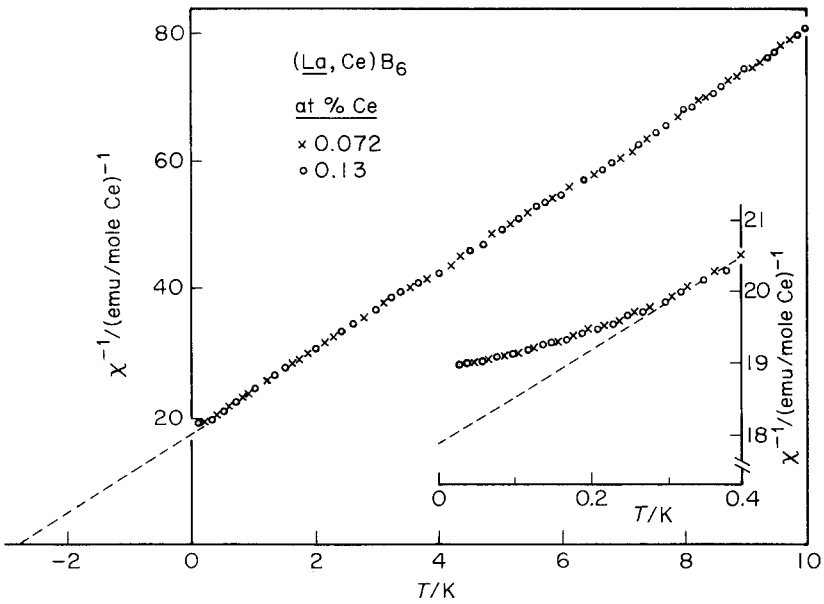
However, the behaviour of the susceptibility even at high temperatures could not be described in terms of the crystal field effects alone as is illustrated in fig. 1.2. Alongside these effects one should take into account the logarithmic corrections due to the Kondo effect.

At temperatures below $\sim 0{\cdot}3$ K $\chi^{-1}$ decreases more slowly with temperature decrease than according to the Curie–Weiss law. This is demonstrated by the insert in fig. 1.1. For (La, Ce)$Al_2$ the accord between experimental and theoretical values of $\mu_{\text{eff}}$ is still better, $\mu_{\text{eff}}=(1{\cdot}25\pm 0{\cdot}03)\mu_B$. The Curie temperature is equal to $(0{\cdot}40\pm 0{\cdot}05)$ K (Felsch *et al.* 1975). The inverse low-field susceptibility per mole Ce

† One can expect similar orders of magnitude of the crystal fields for all cerium compounds.

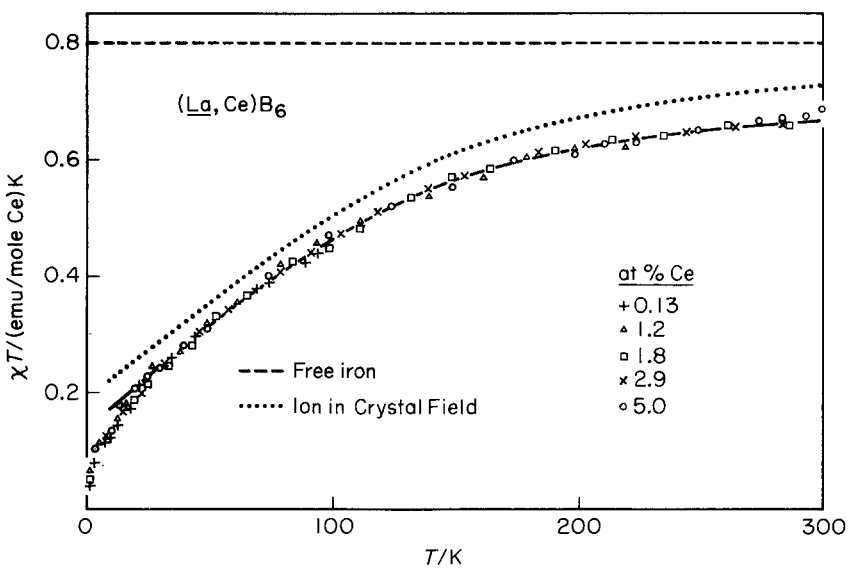
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.1




Inverse impurity susceptibility per mole Ce, $1/\chi$ of (La, Ce)$B_6$ alloys with 0·072 and 0·13 at.% Ce as a function of temperature $T$. The insert shows the behaviour at low temperature on an expanded scale. The dashed line is an extrapolation of the Curie–Weiss law fitted to the data (after Felsch 1978).

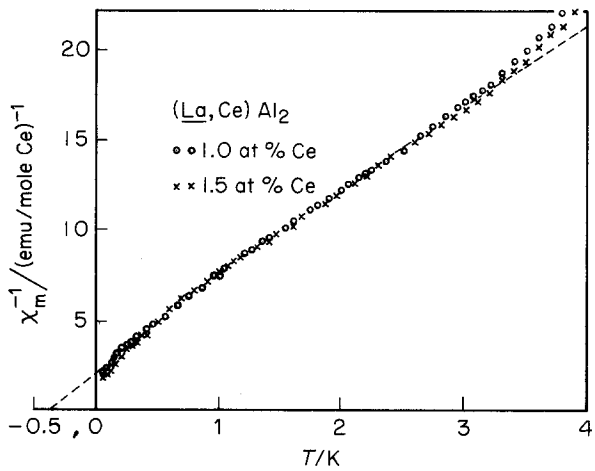
Fig. 1.2




$\chi T$ versus temperature $T$ for (La, Ce)$B_6$ alloys. The dashed line is the behaviour of free $Ce^{3+}$ ions. The dotted line is the behaviour of $Ce^{3+}$ ions in the cubic crystal field of $LaB_6$ (after Felsch 1978).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.3




Inverse impurity susceptibility per mole Ce, $1/\chi$ of (La, Ce)$Al_2$ alloys with 1·0 and 1·5 at.% Ce as a function of temperature $T$. The full line is a fit of eqn. (I) to the data (after Felsch *et al.* 1975).

is plotted in fig. 1.3. At temperatures sufficiently below the Kondo temperature in (La, Ce)$B_6$ the leading temperature correction to $\chi(0)$ can be considered as quadratic:

$$\chi(T)=\chi(0)(1-(T/\theta_0)^2),$$

where $\theta_0=(1{\cdot}20\pm0{\cdot}08)$ K. This can be seen in fig. 1.4, where $\chi$ is plotted versus $T^2$. In the case of (La, Ce)$Al_2$ this simple power law could not be detected up to 1 at.%. At this concentration the impurity–impurity interaction becomes noticeable at 0·15 K (Felsch *et al.* 1975).

The influence of the Kondo effect on the magnetic properties of (La, Ce)$B_6$ and (La, Ce)$Al_2$ is particularly apparent in the low-temperature magnetization data. Typical results of the magnetization curves of the alloys are given in figs. 1.5 and 1.6, where the magnetization per Ce impurity, $M$, is shown as a function of $H/T$ in a logarithmic plot for several constant magnetic fields $H$ (Felsch *et al.* 1975, Felsch 1978). As a result of the interaction of the Ce-ion local moment with the conduction electrons, magnetization is no longer a unique function of $H/T$. The observed behaviour reflects the conception that at temperatures $T<T_K$ spin polarization in an external magnetic field is achieved by polarization of the Kondo ground state. The impurity magnetization depends on $H/T_K$ rather than on $H/T$ as it would for a free spin.

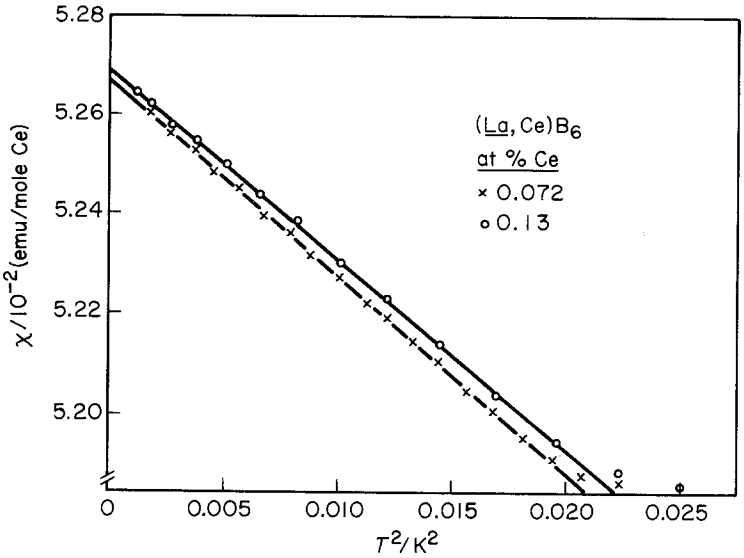
Figure 1.7 shows the field dependence of magnetization per Ce impurity at 50 mk for (La, Ce)$B_6$ with 0·072 at.% Ce (Felsch 1978). Even at 60 kOe the Kondo effect is not suppressed completely: $M(H)$ still increases with $H$ and does not reach the saturation value $M=g'S\mu_B=0{\cdot}71\mu_B$ of the free ion.

(c) *Specific heat*

The Kondo anomaly in the specific heat is a broad peak. Thorough experiments for various values of the magnetic field $H\leqslant 2$ kOe performed by Bader *et al.* (1975) in

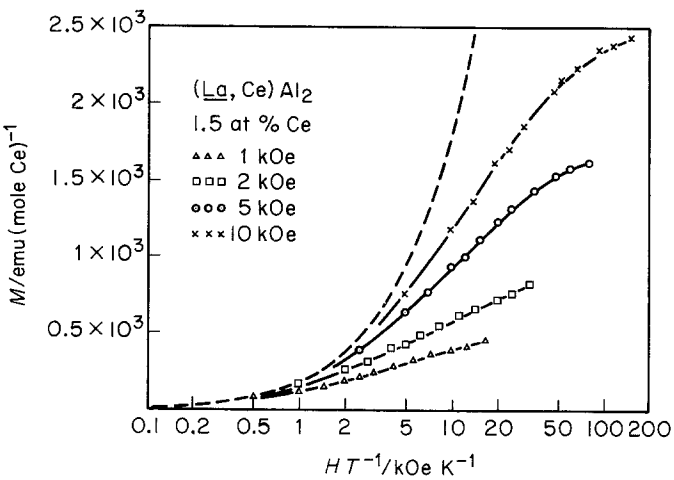
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.4




Impurity susceptibility per mole Ce, $\chi$ of (La, Ce)$B_6$ with 0·072 and 0·13 at.% Ce as a function of $T^2$ in the low-temperature region (after Felsch 1978).

Fig. 1.5

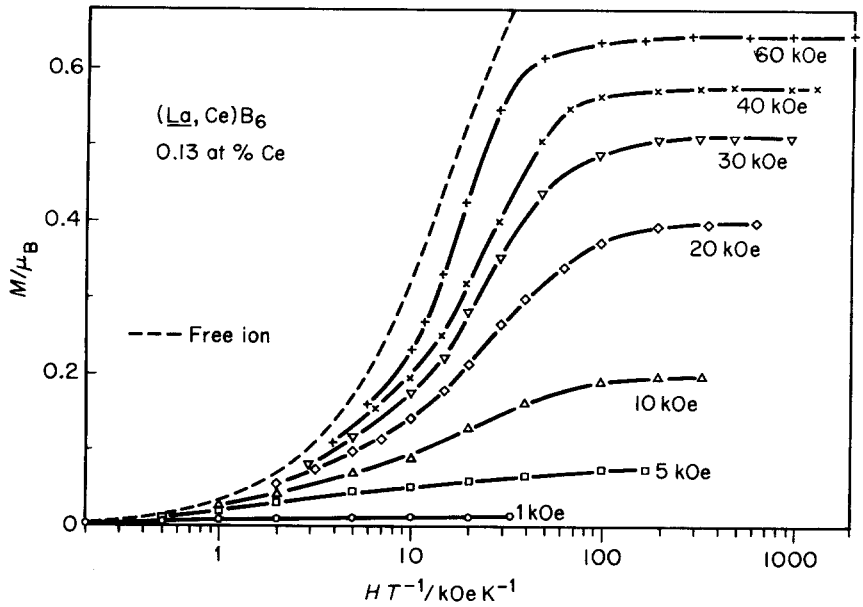



Magnetic moment per Ce impurity, $M_i$, of (La, Ce)$Al_2$ as a function of $H/T$ for different applied magnetic fields $H$. The dashed line is the free $Ce^{3+}$ ion paramagnetism (after Felsch *et al.* 1975).

(La, Ce)$Al_2$ alloys of composition 0·64 at.% in the logarithmic scale are shown in fig. 1·8. These curves correspond to the entropy ln 2. This shows unambiguously that the Ce ground state at $T \gg T_K$ is indeed a doublet in accord with the magnetic susceptibility measurements. At $H < 2$ kOe the superconductivity transition occurs at $T \sim 1$ K.

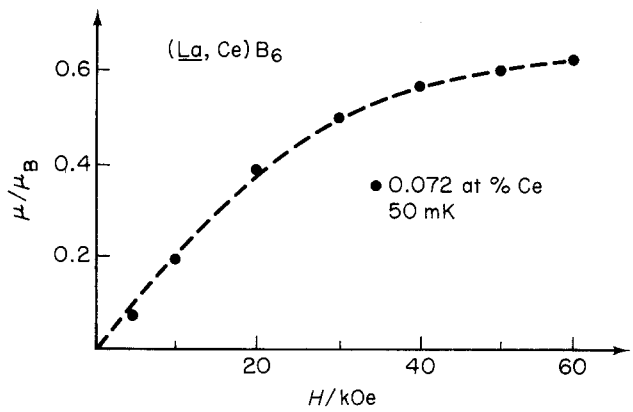
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.6




The same as fig. 1.5 for (La, Ce)$B_6$ (after Felsch 1978).

Fig. 1.7.



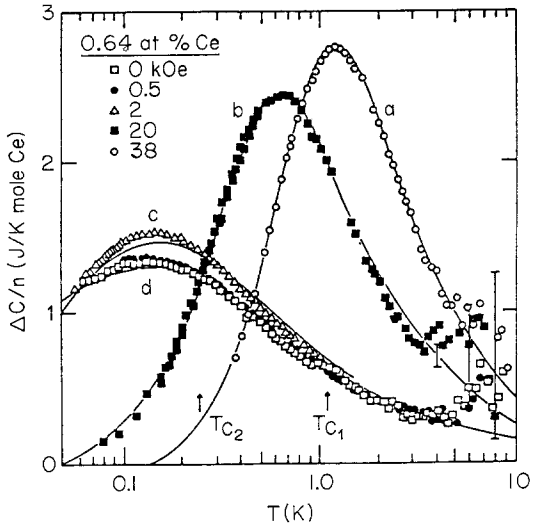

Magnetic moment per Ce impurity, $M$, of (La, Ce)$B_6$ with 0·072 at.% Ce at $T = 50$ mK as a function of the external magnetic field $H$ (after Felsch 1978).

(d) *Resistivity*

The minimum temperature dependence of the resistivity, which has been experimentally known for 40 years, is the most easily verified evidence of the Kondo effect. Moreover, as has been already mentioned, a clear-cut logarithmic behaviour at $T \gg T_K$ is experimentally noticeable exclusively for the resistivity measurements. This makes the resistivity measurements a principal test for the presence of a local moment in the system.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.8




Heat capacity per mole Ce of an (La, Ce)$Al_2$ alloy of composition 0·64 at.% Ce versus temperature in various magnetic fields up to 38 kOe. Curves (a)–(c) correspond to an entropy of a $k_B \ln 2$ ion, showing that $Ce^{3+}$ is Kramer's doublet. The zero field superconducting transition temperatures are indicated (after Bader *et al.* 1975).

Resistivity and magnetoresistivity measurements on (La, Ce)$Al_2$ and (La, Ce)$B_6$ were carried out by Winzer (1973, 1975), Felsch and Winzer (1973), Samwer and Winzer (1976). The results of Winzer (1973, 1975) are given in figs. 1.9–1.11. The clear logarithmic character of the impurity part of the resistivity of both systems at $T \gg T_K$ is evident from figs. 1.10 and 1.11, where the electric resistivity is given in the logarithmic scale at two concentrations: 0·78 at.% and 0·63 at.% Ce in $LaAl_2$ and 0·61 at.% and 1·20 at.% Ce in $LaB_6$. In fig. 1.12 the normalized resistivity is given as a function of $T^2$ for (La, Ce)$B_6$ (Winzer 1975). It can be seen from the figure that the $T^2$ dependence is fulfilled up to 0·15 K. For the concentration 1 at.% the impurity–impurity interaction becomes notable.

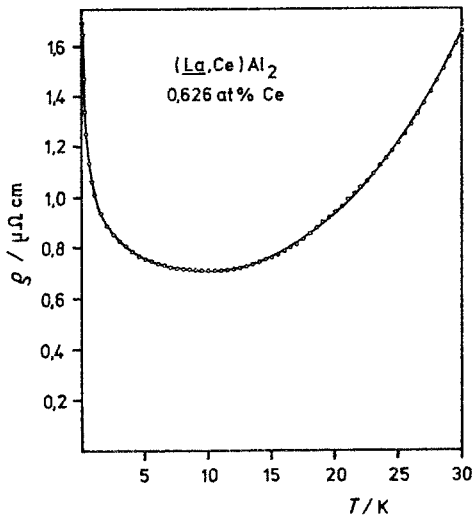
Samwer and Winzer (1976) measured the magnetoresistivity of (La, Ce)$B_6$ in the temperature range 0·04–20 K in magnetic fields up to 6 T.

The zero field electric resistivity in a pure $LaB_6$ sample and in four (La, Ce)$B_6$ alloys containing up to 2·9 at.% Ce is given as a function of the temperature in fig. 1.13. The alloys show the Kondo minimum at about 20 K and a strong increase of the resistivity with a tendency of saturation below 0·1 K at a temperature decrease.

For finite magnetic fields the resistivity is given as a function of the temperature in fig. 1.14. The resistivity of the sample is reduced to about 0·12 of the zero field resistivity by a magnetic field of 6 T at low temperatures. In the presence of the magnetic field several features immediately become apparent. The Kondo effect is suppressed by the magnetic field and the resistivity curves flatten out with increasing field and a maximum is observed for $B \gtrsim 1{\cdot}2\ T$. At low temperatures and in a constant field, the resistivity saturates at a temperature-independent value, being a function of the magnetic field only. A similar behaviour was found for an (La, Ce)$Al_2$ (Felsch and Winzer 1973) alloy with a concentration of Ce 0·63 at.% (fig. 1.15). In fig. 1.16

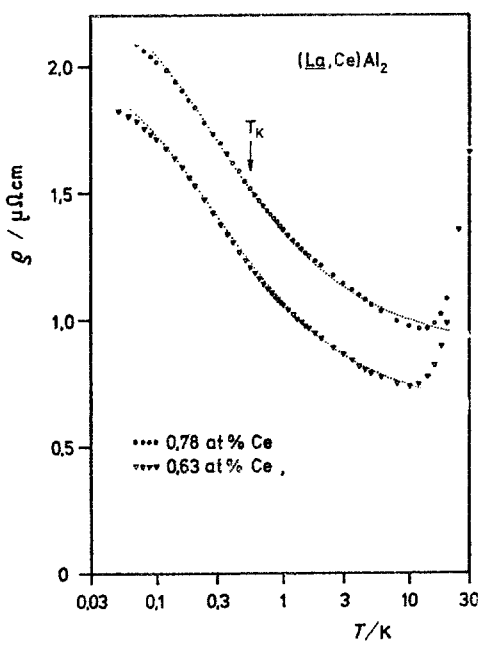
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.9




Electrical resistivity of an (La, Ce)$Al_2$ sample with 0·626 at.% Ce versus temperature (after Winzer 1973).

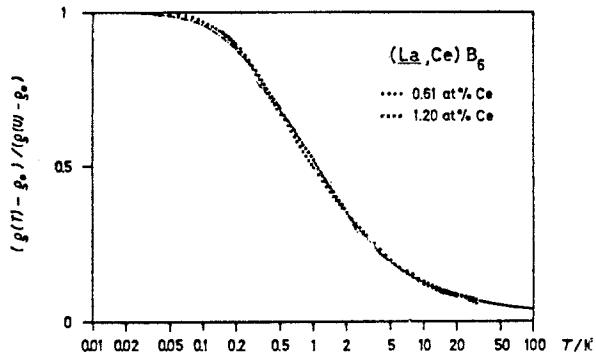
Fig. 1.10




Electrical resistivity versus log $T$ for two (La, Ce)$Al_2$ samples (after Winzer 1973).

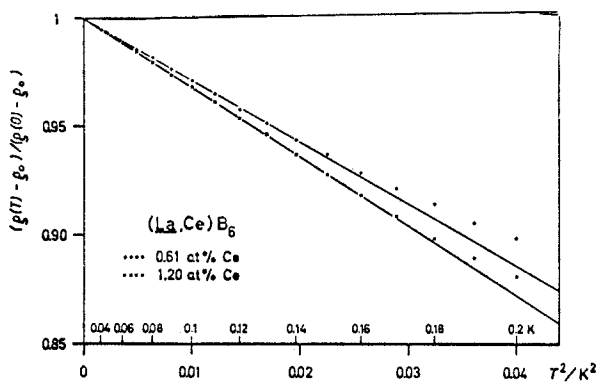
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.11




Normalized temperature-dependent part of the resistivity $[\rho(T)-\rho_0]/[\rho(0)-\rho_0]$ versus temperature of (La, Ce)$B_6$ (after Winzer 1975).

Fig. 1.12




Normalized resistivity $[\rho(T)-\rho_0]/[\rho(0)-\rho_0]$ of (La Ce)$B_6$ as a function of $T^2$ in the low-temperature region (after Winzer 1975).

the magnetoresistivity, divided by the Ce concentration, is shown as a function of the magnetic field at two different temperatures for (La, Ce)$Al_2$. The initial field dependence of $\Delta\rho_m$ follows the $H^2$ law for $H \leqslant 4{\cdot}5$ kOe at $T = 0{\cdot}06$ K and for $H \leqslant 22$ kOe at $T = 1{\cdot}36$ K. At $T = 0{\cdot}06$ K $\Delta\rho_m$ appears nearly saturated for $H = 50$ kOe. The dependence of the impurity part of the resistivity on the magnetic field for (La, Ce)$B_6$ is shown in fig. 1.17.

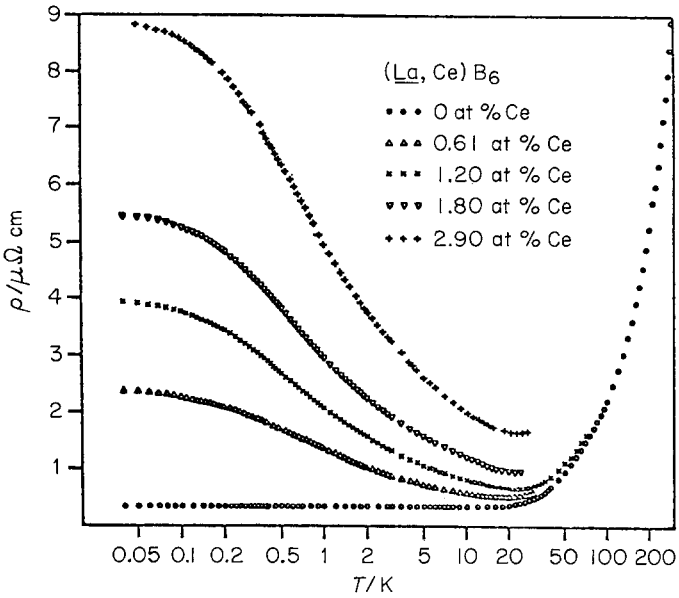
For a magnetic field decrease, as for a temperature decrease, the effective exchange interaction increases. This results in an increase of the resistivity which reaches its unitary limit at $T = H = 0$. Thus, the magnetic field breaks the Kondo state and enhances conductivity.

(e) *Lattice pressure effects*

We have mentioned above that the La-based alloys are sensitive to the lattice pressure. Below we briefly discuss the recent experiments by Steglich *et al.* (1977) reflecting the effect of the 'chemical pressure' in the (La, Ce)$Al_2$ alloy.

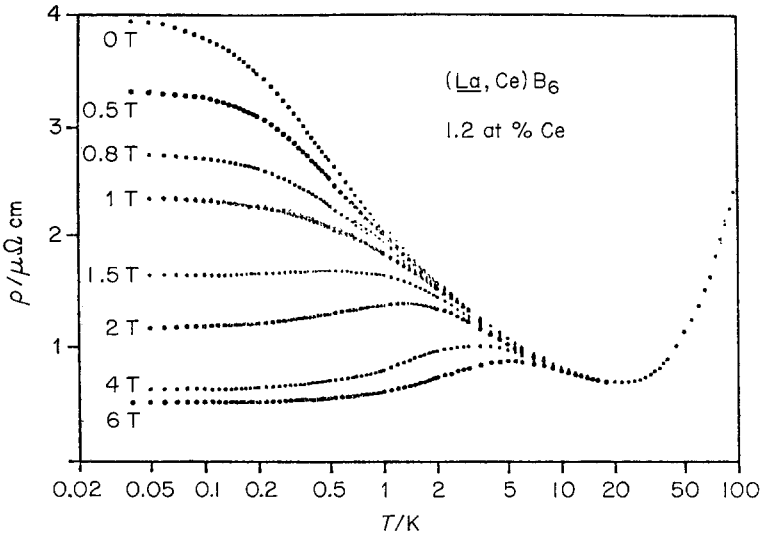
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.13




Electrical resistivity of $LaB_6$ and four $(La, Ce)B_6$ samples as a function of temperature (after Samwer and Winzer 1976).

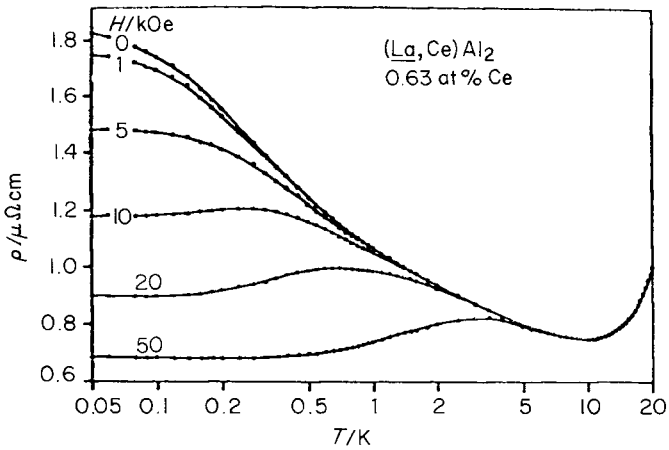
Fig. 1.14




Electrical resistivity of an $(La, Ce)B_6$ sample with 1·2 at.% Ce versus temperature for various magnetic fields (after Samwer and Winzer 1976).

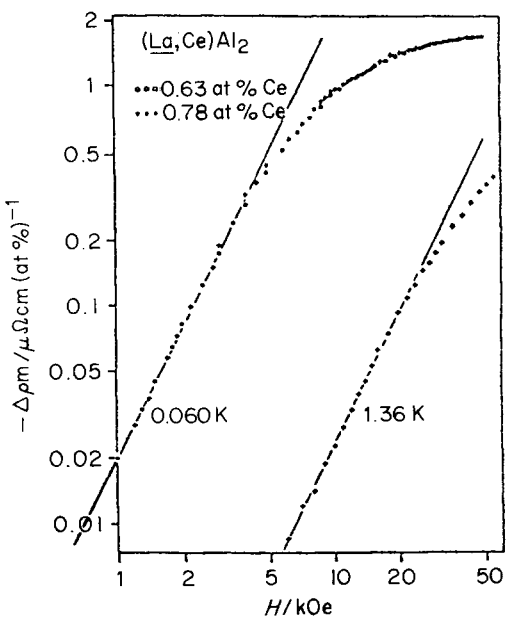
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.15




Electrical resistivity $\rho$ of $(La, Ce)Al_2$ with 0·63 at.% Ce substitution for La, versus temperature $T$ for various magnetic fields $H$ (after Felsch and Winzer 1973).

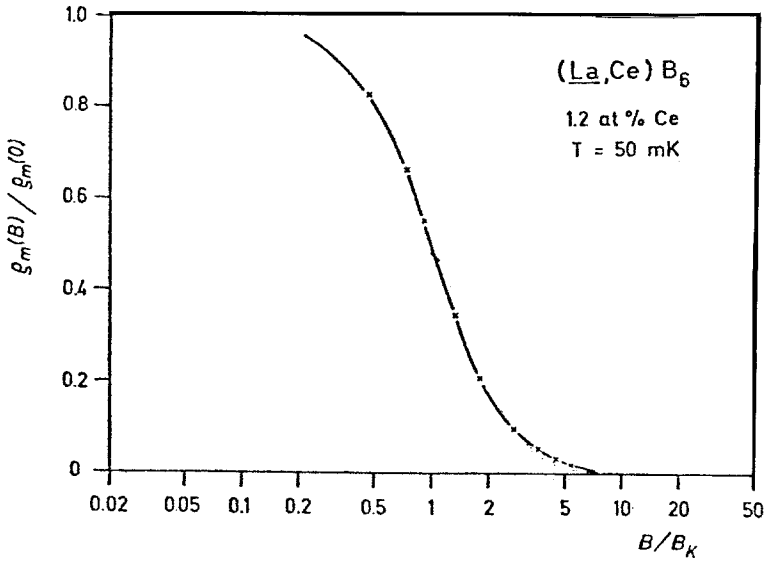
Fig. 1.16




Magnetic field dependence of the magnetoresistivity divided by the Ce substitution for La, $\Delta\rho_m/c$ of $(La, Ce)Al_2$ alloys at $T = 0{\cdot}06$ K and $T = 1{\cdot}36$ K. The lines of slope 2 show the initial variation of $\Delta\rho_m/c$ with $H^2$ for both temperatures (after Winzer 1975).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.17




Normalized spin-dependent part of the resistivity $\rho_m(B)/\rho_m(0)$ of (La, Ce)$B_6$ versus normalized magnetic field $B/B_k$. $B_k = 1{\cdot}1\ T$ (after Samwer and Winzer 1976).

The resistivity of homogeneous $[(La_{1-z}, Y_z)_{1-x}Ce_x]Al_2$ alloys was measured. In fig. 1.18 the resistivity of $[(La_{1-z}, Y_z)_{0,85}Ce_{0,15}]Al_2$ samples at $z = 0$, 0·3, 0·5, 0·75 and 1 is given as a function of temperature on the logarithmic scale.

The resistivity minimum shifts to higher temperatures with the Y-concentration increase displaying a marked enhancement of the Kondo temperature caused by the contraction of the lattice. Whereas $T_K \lesssim 1$ K for dilute (La, Ce)$Al_2$, $T_K$ reaches $\sim 15$ K for $z = 0{\cdot}5$. The Y-concentration increase brings about a linear decrease of the lattice parameter of the matrix and an increase of the energy of the atomic level $\epsilon_f$. Thus the effect may be attributed to the initial increase of the Kondo temperature with a decrease of $\epsilon_f$ and the subsequent destruction of the local moment when $\epsilon_f$ passes through the Fermi level. When $\epsilon_f$ passes through the Fermi level the system passes into the mixed-valence regime which is characterized by an essentially non-integer occupation number of the $4f$ shell.

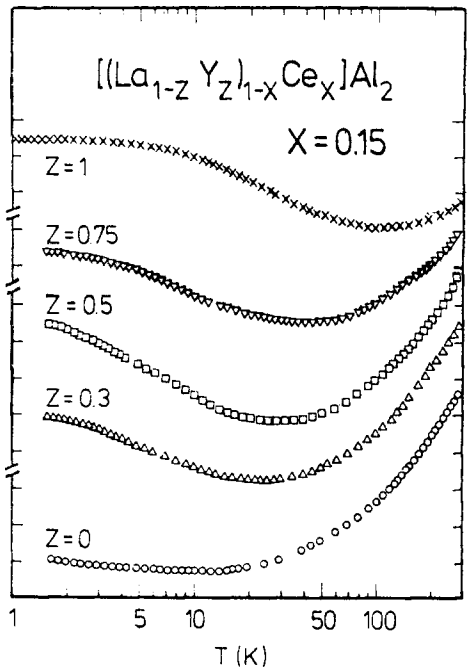
The behaviour described is also well known for the $(La_{1-z}Th_z)_{1-x}Ce_x$ alloys (Luengo *et al.* 1974) and for the LaCe and YCe alloys under pressure (for a review see Maple 1976).

(f) *Kondo effect in superconductors*

We end this section with a mention of the striking manifestations of the Kondo effect in the superconducting state for the case when the superconducting transition temperature of the matrix is $T_{c0} \gg T_K$. There is a vast literature concerning the Kondo effect in superconductors (for a review see Maple 1973, 1976). Below we shall deal only with the so-called 're-entrant' superconductivity phenomenon which was first observed by Riblet and Winzer (1971) for the (La, Ce)$Al_2$ system. The condition $T_{c0} \gg T_K$ is satisfied in this system ($T_{c0} = 3{\cdot}3$ K) and it exhibits the 're-entrant' curve

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 1.18




Resistivity as a function of temperature for several $[(La_{1-z}, Y_z)_{1-x}Ce_x]Al_2$ alloys with constant Ce concentration of 15 a/o, but with varying Y concentrations (after Steglich 1977).

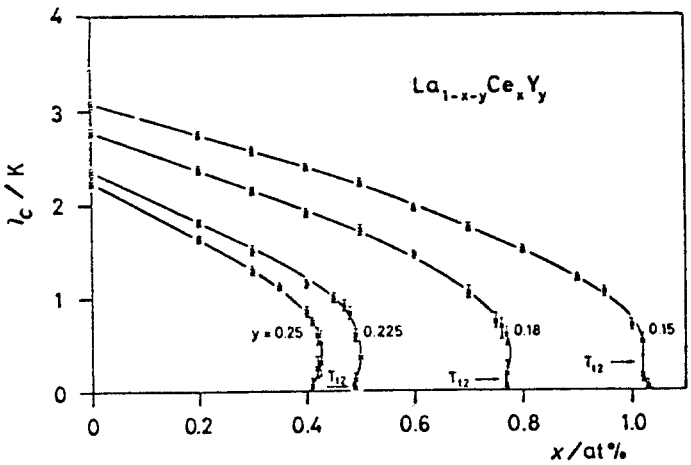
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$T_c$ versus the Ce concentration, i.e. the 'phase boundary' which separates the normal metal from the superconductor: within a certain concentration range the superconducting state exists only in the temperature range $T_{c_2} < T < T_{c_1}$ and at $T < T_{c_2}$ the sample returns to the normal state. Moreover, in a narrow concentration range the alloy is again back in the superconducting state at $T < T_{c_3}$. The results of the recent experiments by Dreyer *et al.* (1982) for (La, Y)Ce are given in fig. 1.19.

We have not aimed at surveying the up-to-date state of experiments in the field of rare-earth alloys. Such a survey would not be appropriate since the physics and chemistry of rare-earth alloys are fields of immense activity and our understanding of lanthanide systems is far from complete. We have given only certain data accumulated for the (La, Ce)$B_6$ and (La, Ce)$Al_2$ systems, which, on the one hand, can serve as a reliable test of theories, and, on the other, demonstrate the many-body effects. More detailed reviews on the Kondo effect with rare-earth ions have been given by Maple *et al.* (1978) and Steglich (1977).

We believe that the models for which solutions are derived below have to do with the substances and phenomena discussed in this section. We shall refrain from a numerical comparison of theoretical results with experimental data and confine ourselves to the qualitative agreement of theory and experiment.

Fig. 1.19




Superconducting normal phase boundaries of (La, Y)Ce between 15 and 25 at.% Y (after Dreyer *et al.* 1982).

## § 2. Basic models

The phenomenon associated with local moments in metals may roughly be classified as

(i) one-body local effects, related to the structure of the impurity atomic shell and crystalline surrounding, studied by various kinds of magnetic measurements, and

(ii) many-body effects due to the broad conduction band of a metal. Thermal and transport properties proved a very sensitive source of information on the many-body effects.

The majority of theoretical investigations concerning dilute magnetic alloys have been devoted to many-body effects and therefore are based on the most simple models: s–d exchange model (Kondo model) or non-degenerate Anderson model. The impurity is supposed to be pointlike and to possess only spin degrees of freedom. The orbital nature of impurities (usually rare earth or transition element atoms), the non-sphericity of the crystalline surrounding, spin–orbit and nuclear spin effects, are normally ignored. This makes the theory much simpler, while retaining its basic features and all the important difficulties. In fact, this simple theory has met with some success in qualitative interpretation of the many-body effects. As to the quantitative merging of theory and experiment this theory, as noted in § 1, provides an appropriate model for special classes of real alloys.

There have been many attempts to construct hamiltonians describing real impurities in real metals†, yet this work is far from being completed. Of many papers on the subject there are very few good ones. Most extensive treatment was given by

† The local density type calculations of Zeller and Diedrich (1971) give an interesting guide to the occurrence of magnetic moments but yield moments that persist at $T=0$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Nozières and Blandin (1980), Coqblin and Schrieffer (1969) and Schrieffer (1967). We follow these authors in our presentation.

Though the detailed analysis of concrete alloys and applications of theoretical results to the experimental data is a matter for the future, one may single out a few generalized hamiltonians which may be regarded as a starting point on the pathway to real substances.

## 2.1. *The Anderson model*

### 2.1.1. *The general form of the Anderson model*

The experimental evidence is that various impurities in different hosts display widely different behaviours. The magnetic properties of the impurity depend both on the host matrix and on the presence of $3d(4f)$ elements. The behaviour of the impurity is basically affected by two interactions: atomic Coulomb and exchange forces in a free atom and the admixture of the wavefunctions with the conduction electron band of the host (Friedel 1958). The development of the theory started with two questions: 'Under what circumstances does a localized moment exist in a metal?' and 'What are the consequences of the interaction between a localized moment and the conduction electrons?

The Anderson model (Anderson 1961) can answer both these questions. To be definite, consider the impurity transition ion embedded into the metallic matrix. The general form of the metal–impurity interaction is

$$\mathscr{H}=\mathscr{H}_0+\sum_{j=1}^{N} V_{\text{imp}}(r_j)+\frac{1}{2}\sum_{i\neq j}\frac{e^2}{r_{ij}}+\sum_{j=1}^{N}\frac{1}{mcr_j}\frac{dV_{\text{imp}}(r_j)}{dr_j}\times(\mathbf{L}_j\cdot\boldsymbol{\sigma}_j). \tag{2.1.1}$$

Here $\mathscr{H}_0$ is a hamiltonian of electrons placed in the potential of the crystal lattice; $m, \mathbf{L}$ and $\boldsymbol{\sigma}, N$ are the mass, orbital moment, spin and the number of electrons, respectively; and $V_{\text{imp}}(r)$ is a potential of the impurity stripped of all the electrons of the outer shell. With good accuracy one may suppose $V_{\text{imp}}(r)$ to be spherically symmetric. The third term in (2.1.1) is a Coulomb interaction, whilst the fourth term described the spin–orbit coupling caused by the impurity potential.

The crucial observation in deriving the Anderson model is that the $l=2$ levels of $V_{\text{imp}}$ are very close to the Fermi surface, thus forming the narrow resonance. Its small width is due to the difference between the interatomic distance $k_{\text{F}}^{-1}$ and the Bohr radius $r_{\text{B}}$ of the $d$ shell: $k_{\text{F}}r_{\text{B}}\ll 1$. This greatly simplifies the hamiltonian (2.1.1). Indeed, the wavefunction of electrons with near-to-Fermi-surface energy contains both localized and delocalized components. Hence, the eigenfunctions of (2.1.1) can be expanded using as a basis the orbital and band wavefunctions. For the latter it is convenient to choose a spherical wave with the centre at the impurity site. In the second quantization formalism one has

$$\Psi^+(\mathbf{r})=\sum_{\substack{k<r_{\text{B}}^{-1}\\ l,m,\sigma}}\Psi_{lm}(k,\mathbf{r})a^+_{klm\sigma}+\sum_{m,\sigma}\Psi_d(\mathbf{r})\,d^+_{m\sigma}, \tag{2.1.2}$$

where $a^+_{klm\sigma}$ is a creation operator for the spherical wave with the centre at the impurity point:

$$\Psi_{lm}(k,\mathbf{r})=r_l(kr)\,Y_{lm}\left(\frac{\mathbf{r}}{r}\right). \tag{2.1.3}$$

The operator $d^+_{m\sigma}$ corresponds to the localized components of the state with $l=2$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\Psi_d(\mathbf{r}) = R_{l_0}(r/r_B)\, Y_{l_0 m}(\mathbf{r}/r), \tag{2.1.4}$$

where $l_0 = 2$ and 3 for the transition and rare-earth impurities, $m$ is a $z$-component of the angular momentum: $m = -l_0, \ldots, l_0$.

The set of functions so chosen is not orthogonal. However, in view of greatly differing scales $r_B$ and $k_F^{-1}$ the corresponding overlap integral

$$\alpha = \int_0^\infty r_{l_0}(kr) R_{l_0}(r/r_B) r^2 dz \tag{2.1.5}$$

is small and within this accuracy the non-orthogonality can be neglected. An estimation for the overlap $\alpha$ will be presented at the end of this section.

When rewritten in terms of $a^+, a$ and $d^+, d$ the hamiltonian

$$\mathscr{H} = \int \Psi^+(r)\left(\mathscr{H}_0(r) + V_{\text{imp}}(r) + \frac{1}{mcz}\frac{dV_{\text{imp}}(r)}{dr}\mathbf{L}\cdot\boldsymbol{\sigma}\right)\Psi(r) d^3r$$
$$+ \int \Psi^+(r)\Psi^+(r')\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\Psi(r')\Psi(r) d^3r d^3z'$$

contains a rather large number of terms. Let us discuss them in due turn.

($i$) Start with terms containing only $a$ and $a^+$. Put together they form the hamiltonian of the host metal. We neglect the many particle corrections to the band spectrum. Usually this approximation is good enough for a description of the conduction band. We also assume that the spectrum of electrons near the Fermi surface is spherically symmetric. Note that the energy of the conduction electrons is diagonal in the spherical-wave representation if the impurity point is chosen for the centre.

$$\mathscr{H}_0 = \sum_{k,l,m,\sigma} \varepsilon(k) a^+_{klm\sigma} a_{klm\sigma}. \tag{2.1.6}$$

($ii$) The terms with only $d$ operators represent the hamiltonian of a $3d(4f)$ ion in a crystal field:

$$\mathscr{H}_{\text{atom}} = \sum_{m,m',\sigma} \varepsilon_{mm'} d^+_{m\sigma} d_{m'\sigma} + \sum_{m_i,\sigma_i} \Gamma^{m_3\sigma_3;m_4\sigma_4}_{m_1\sigma_1;m_2\sigma_2} d^+_{m_1\sigma_1} d^+_{m_2\sigma_2} d_{m_3\sigma_3} d_{m_4\sigma_4} - A\mathbf{L}_d\cdot\mathbf{S}_d. \tag{2.1.7}$$

Here

$$\varepsilon_{mm'} = \delta_{mm'} \int \Big[ R^2_{l_0}(r/r_B)(V_{\text{imp}}(r) + l_0(l_0+1)/2mr^2)$$
$$- \frac{1}{2mr} R_{l_0}(r/r_B) \frac{\partial^2}{\partial r^2}(rR_{l_0}(r/r_B)) \Big] r^2 dr + (\text{crystal field})$$

is the one-electron atomic energy (measured from the Fermi energy which we choose as the origin). The second term in (2.1.7) is the non-relativistic part of interaction between $d(f)$ electrons. It is invariant under rotations in both real and spin space and therefore matrix $\Gamma$ obeys the following constraints:

$$m_1 + m_2 = m_3 + m_4$$
$$\sigma_1 + \sigma_2 = \sigma_3 + \sigma_4.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Thus matrix $\Gamma$ is described by $l+1$ Slater coefficients†. The last term in (2.1.7) represents the spin–orbit coupling:

$$\mathbf{L}_d = \sum_{m,m',\sigma} d^+_{m\sigma} \mathbf{l}_{mm'} d_{m'\sigma}$$

is the angular momentum of $d(f)$ shell and

$$\mathbf{S}_d = \sum_{m,\sigma,\sigma'} d^+_{m\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} d_{m\sigma'}$$

is a total spin of the $d(f)$ shell.

(*iii*) The one-electron mixing interaction is the part of $\mathscr{H}_0$ which is off-diagonal in the number of $3d(4f)$ electrons

$$\mathscr{H}_{\text{mix}} = \sum_{l,m,m',\sigma} v^{l_0 m}_{lm'} (a^+_{klm'\sigma} d_{m\sigma} + \text{h.c.}), \tag{2.1.8}$$

where

$$v^{l_0 m}_{lm'}(k) = \int r_l(kr)\, Y^*_{lm'}\left(\frac{\mathbf{r}}{r}\right)(\mathscr{H}_0(r) + V_{\text{imp}}(r)) R_{l_0}(r/r_{\text{B}})\, Y_{l_0 m}\left(\frac{\mathbf{r}}{r}\right) d^3 r.$$

One can always neglect the crystal field and spin–orbit effects while evaluating the hybridization matrix element. Therefore, one can retain in (2.1.8) only terms invariant under rotation in the coordinate space. Spherical symmetry implies that this interaction can involve only conduction electrons in the partial wave $l = l_0$ and requires it to have the following form, which conserves the angular momentum as well as spin (Schrieffer 1967):

$$\mathscr{H}_{\text{mix}} = \sum_{k,m,\sigma} v_k (a^+_{kl_0 m\sigma} d_{m\sigma} + \text{h.c.})$$

$$v^{l_0 m}_{lm'} = v_k \delta_{ll_0} \delta_{mm'}.$$

(*iv*) Finally, there are terms containing both $d$ and $a$ operators:

(1) $$a^+ d^+ a d,$$

(2) $$a^+ a^+ d d,\ d^+ d^+ a a,$$

(3) $$a^+ a^+ a d,\ d^+ d^+ d a.$$

In the following we neglect all these terms. Term (1) describes the contact exchange coupling. Usually the sign of this coupling is ferromagnetic and it competes with virtual-mixing coupling. For $3d$ impurities strong Kondo effect suggests that the virtual-mixing mechanism is dominant. For $4f$ ions we must distinguish between normal ions and ions near a valence instability. It is well known

† Until recent Nozières and Blandin (1980) and Mihaly and Zawadowski (1978) papers appeared it was customary to use without much ado a truncated $\Gamma$-matrix which contained only two interaction parameters, a 'Coulomb energy' $U$ and an 'exchange energy' $I$:

$$(U/2 - I/4) d^+_{m\sigma} d^+_{m'\sigma'} d_{m'\sigma'} d_{m\sigma} - I \boldsymbol{\sigma}_{\sigma\tau} \cdot \boldsymbol{\sigma}_{\sigma'\tau'} d^+_{m\sigma} d^+_{m'\sigma'} d_{m'\tau'} d_{m\tau}$$

(see, for example, Grüner and Zawadowski 1974).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

that such instabilities occur often for Ce, Sm, Eu, Tm and Yb (see, for example, Varma 1976). The fact that no Kondo effect is observed for other $4f$ ions can be explained by the ferromagnetic sign of the dominant contact exchange contribution. As a $4f$ ion approaches a valence instability, the virtual-mixing coupling becomes large by virtue of a small energy denominator. As we are only interested in alloys exhibiting the Kondo effect we can neglect the contact exchange coupling.

Usually the states with $(n_{d_0} \pm 2)$ (corresponding to two additional orbital electrons or holes) lie sufficiently high and the processes described by (2) may only be virtual and result in renormalization of the Coulomb interaction.

Finally, term (3) gives only trivial renormalization of virtual-mixing coupling (Hirst 1978).

Thus, in the spirit of Fermi-liquid theory, the behaviour of a magnetic impurity in a metal may be described by the semiphenomenological Anderson hamiltonian:

$$\mathscr{H}_A = \sum_{k,\sigma=\uparrow,\downarrow} \sum_{m=-l_0}^{l_0} \varepsilon(k) a^+_{km\sigma} a_{km\sigma} + \frac{1}{N} \sum_{k,m,\sigma} v_k (a^+_{km\sigma} d_{m\sigma} + d^+_{m\sigma} a_{km\sigma}) + \mathscr{H}_{\text{atom}}, \quad (2.1.9)$$

where $\mathscr{H}_{\text{atom}}$ is given by (2.1.7). Here we write only conduction electrons in partial waves with $l = l_0$:

$$a_{kl_0m\sigma} \equiv a_{km\sigma}.$$

The essence of (2.1.9) is that it describes the one-dimensional system. All quantities entering (2.1.9) depend only on the modulus of $\mathbf{k}$: $|\mathbf{k}| = k$. This one-dimensionality follows from the hypothesis about a spherical Fermi surface and impurity-ion potential. Obviously, one-dimensionality is held only until one can consider impurities as independent scatterers.

Now let us estimate the quantity $\alpha$ (2.1.5). The magnitude of $\alpha$ for $3d$ and Ce impurities and other $4f$ impurities is quite different. For $4f$ impurities it is well known (see, for example, Varma 1976) that $\rho v^2 \sim 0{\cdot}02$ eV. Comparing the expressions for $v$ (2.1.8) and $\alpha$ (2.1.5) one obtains the estimate $v \sim \alpha\epsilon_F$ and $\rho(\epsilon_F)v^2 \sim \alpha^2\epsilon_F$. Taking $\epsilon_F \sim 5$ eV we obtain $\alpha_{4f} \sim 0{\cdot}05$. Analogous estimation for Ce and $3d$ impurities gives $\rho v^2 \sim 0{\cdot}2$ eV and $\alpha_{3d} \sim 0{\cdot}2$† (Croft *et al.* 1981, Allen *et al.* 1981, Myers *et al.* 1968).

### 2.1.2. *The hierarchy of energies in the Anderson model*

Most interesting cases correspond to distinct energy scales of parameters of the Anderson model (2.13). This circumstance leads to great simplifications.

Let us first discuss the energy scales of atomic hamiltonian (2.1.9), ignoring the hybridization term.

Let $n_d^{(0)}$ be the occupation number in the ground state of $\mathscr{H}_{\text{atomic}}$, $|n_d^{(0)}\rangle$ being the subspace of atomic states with that occupation number. The hybridization term in (2.13) couples $|n_d^{(0)}\rangle$ to the subspaces $|n_d^{(0)} \pm 1\rangle$ with occupation numbers $n_d^{(0)} \pm 1$. Since the conduction band acts as a reservoir, one-electron energies corresponding to transitions from $|n_d^{(0)}\rangle$ to $|n_d^{(0)} \pm 1\rangle$ should be measured from the Fermi level. Typical ionization energy for $3d$ and Ce ions is $\sim$2–3 eV (see Allen *et al.* 1981, Croft *et al.* 1981, Myers *et al.* 1968). Conversely, in some $4f$ compounds, one of these

† We do not compute $\alpha$ straightforwardly from (2.1.5), since, strictly speaking, the function $R_{l_0}$ is not purely atomic.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

ionization energies may be sufficiently small, while the other is large (for a review see Varma 1976).

Within a given valency subspace, the various terms are split according to Hund's rule. The ground state of $\mathscr{H}_{\text{atom}}$ is obtained by first maximizing the total spin $S$, and then the total orbital momentum $L$. Typical splitting may be of the order of 1 eV.

It is possible that Hund's ground state is an orbital singlet $L=0$ and there is no further splitting. This situation takes place for $Mn(n_d^{(0)}=5)$. The influence of the crystal field is very small ($\sim 0{\cdot}1$ K) and spin–orbit coupling is negligible.

If Hund's ground state has non-zero orbital momentum $L \neq 0$, then one should consider the crystal electric field (CEF) and spin–orbit splitting.

For $3d$ impurities the next step after the Hund's splitting is CEF-splitting—typically a fraction of an eV†. An orbital multiplet ($L \neq 0$) will split into irreducible representations of the impurity point group. The resulting lowest component may itself be either orbital singlet or multiplet. If the ground state is multiplet, it will eventually be split by the spin–orbit coupling.

For the rare-earth impurity the order of spin–orbit coupling is 0·2–0·3 eV and the crystal field energy is $\sim 100$ K. Thus, the spin–orbit splitting occurs first, the (LS) multiplet is split into states of different total angular momentum $J$, and then every multiplet with given $J$ is split by the crystal field.

In transition impurities all the above-mentioned energies exceed the possible temperature interval. Therefore, one should consider in hamiltonian (2.1.9) only virtual transitions between *the ground state* of multiplet $|n_d^{(0)}\rangle$ and the states of multiplets $|n_d^{(0)} \pm 1\rangle$. The typical energy differences corresponding to these transitions are denoted as $E\pm$.

The hybridization mixes the states with different occupation numbers and may break the localized moment. Resonances with adjacent occupation numbers acquire the width $\Gamma \sim \pi\rho(\epsilon_F)v^2$. The real processes with change of occupation number can be neglected provided that

$$\frac{\Gamma}{E\pm} \ll 1. \tag{2.1.10}$$

Hence, at temperatures exceeding the Kondo temperature one may speak about the local moment state with the magnetic moment, calculated according to Hund's rule and crystal field. Generally speaking, in the majority of transition ions the inequality (2.1.10) is not strong. For example, for the AuMn alloys the corresponding amplitudes are estimated as $\Gamma \sim 0{\cdot}5$ eV, $E_+, E_- \sim 2{\cdot}5$ eV.

For rare-earth alloys the situation may be simplified further. In most of the rare earths the $4f$-electron level lies so deep under the Fermi level that many-body effects do not play any role and the simple ionic model holds. Conversely, in Sm, Tm and Yb alloys one of the ionization energies may be extremely small ($\lesssim 0{\cdot}1$ eV). As this energy is much smaller than all the splittings (except crystal field) the impurity behaviour is determined only by transitions between *the ground state* of $|n_d^{(0)}\rangle$ *multiplet* split by CEF and the *ground state* of one of either $|n_d^{(0)} \pm 1\rangle$ or $|n_d^{(0)} - 1\rangle$ multiplets. In Sm, Yb and Tm alloys this corresponds to the transitions $4f^5\,{}^6H_{5/2} \rightleftarrows 4f^6\,{}^7F_0$; $4f^{13}\,{}^2F_{7/2} \rightleftarrows 4f^{14}\,{}^1S_0$ and $4f^{12}\,{}^3H_6 \rightleftarrows 4f^{13}\,{}^2F_{7/2}$, respectively.

† Unfortunately, the ground states of $3d$ ions dissolved in simple metals are poorly investigated.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The energy gap between these terms (we denote it $\varepsilon_f$) is sensitive to pressure and may vary in a wide interval. Depending on whether condition (2.2.1) holds or not the system may be either in the local moment regime or in the mixed-valence state. As a rule the Sm and Yb compounds show mixed-valence behaviour (for a review, see Varma 1976 and Khomski 1979); however in the dilute (La, Sm)$Sn_3$ alloy, the $Sm^{3+}$ ion has a well-established magnetic moment and Kondo effect was observed (Bakanowski *et al.* 1977. The AuYb and MgYb alloys are also excellent examples of the Kondo effect (Baberschke and Tsang 1980, Floquet 1978, Tselfes *et al.* 1980).

In Sm and Yb alloys the hybridization mixes a magnetic state with a non-magnetic one, thus breaking the magnetic moment in the mixed-valence state. Conversely, in Tm alloys the transition takes place between the magnetic configurations. In this interesting case the Kondo effect is present alongside the mixed-valence state (Berger *et al.* 1979).

The next interesting objects are Ce alloys. They occupy a place intermediate between the transition alloys and the rare-earth alloys with Sm, Tm and Yb. The recent experiments on Ce compounds have found the sufficiently high one-electron energy level corresponding to the transition $4f^1\,{}^2F_{5/2} \rightleftarrows 4f^0\,{}^1S_0$ with large width $\Gamma$. For example, in $CeAl_2$ one finds $\varepsilon_f \simeq -2{\cdot}5$ eV, $\Gamma \simeq 0{\cdot}55$ eV (Croft *et al.* 1981, Allen *et al.* 1981). On the other side the ground state of the $Ce^{3+}$ ion is formed by spin–orbit coupling and CEF which have the same order of magnitude as in the other rare earths. According to recent measurements of susceptibility $\chi(T)$ for $CeAl_2$, performed up to 1000 K, $\chi(T)$ can be fitted well by the $J=5/2$ and $7/2$ terms of $Ce^{3+}$ with multiplet separation of $2500 \pm 500$ K. In dilute alloy (La, Ce)$Al_2$ the cubic crystal field splits the term ${}^2F_{5/2}$ into the doublet $\Gamma_7$ and quartet $\Gamma_8$, which is further split due to the Jan–Teller effect. The magnitudes of corresponding splittings are of the order of 100 K (Loewenhaupt *et al.* 1979).

In the above discussion the hyperfine coupling of the localized impurity moment with the nuclear spin has been neglected. The energy of the hyperfine coupling is of the order of 100 mK. It may only be essential for alloys with low Kondo temperature, for example, for AuYb alloys (for references see Floquet 1978).

### 2.1.3. *The Anderson model for the rare-earth alloys*

In rare-earth alloys showing the valence instability, the energies $E_\pm$ and $\Gamma$ have different orders of magnitude. As we mentioned in the previous subsection, only mixing between the ground states of the $|n_d^{(0)}\rangle$ multiplet and one of the $|n_d^{(0)} \pm 1\rangle$ multiplets is essential. In Ce, Sm and Yb ions one of these states is non-magnetic. We denote this state by $|0\rangle$. Due to the strong spin–orbital coupling, the magnetic state is characterized by the value of total angular momentum $J$ and its projection $j$. The hybridization operator conserves the total angular momentum. Therefore it is convenient to expand the plane electronic wave using the eigenfunctions of the total angular momentum operator (Coqblin and Schrieffer 1969):

$$a_{kJj} = (-1)^{l+J-1/2}(2J+1)^{1/2}\left\{\begin{pmatrix} l & 1/2 & J \\ j+1/2 & -1/2 & -j \end{pmatrix} a_{kl,\,j+1/2,\,-1/2} + \begin{pmatrix} l & 1/2 & J \\ j-1/2 & 1/2 & -j \end{pmatrix} a_{kl,\,j-1/2,\,1/2}\right\}, \qquad (2.1.11)$$

where the brackets are corresponding Clebsch–Gordon coefficients.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

As far as the state $|0\rangle$ is non-magnetic ($J=0$), the matrix element of hybridization

$$\langle Jj|\mathscr{H}_{\text{mix}}|0\rangle = v(j)$$

is diagonal with respect to $J$ and $j$.

Let us define the operators $\mathbf{X}_{0j}$, $\mathbf{X}_{j0}$ changing the configuration of the impurity shell as follows:

$$\left.\begin{aligned} |0\rangle &= \mathbf{X}_{0j}|j\rangle \\ |j\rangle &= \mathbf{X}_{j0}|0\rangle. \end{aligned}\right\} \tag{2.1.12}$$

The other matrix elements of these operators are set to zero. These $\mathbf{X}$ operators satisfy the following parastatistics (Hubbard 1965):

$$\mathbf{X}_{jk}\mathbf{X}_{pq} = \delta_{kp}\mathbf{X}_{jq} \tag{2.1.13}$$

and have matrix representation $\mathbf{X}_{jk}^{\alpha\beta} = \delta_{\alpha k}\delta_{\beta j}$. In terms of $\mathbf{X}$ the Anderson hamiltonian takes the form:

$$\mathscr{H}_{\text{A}} = \sum_{k,j} \varepsilon(k) a_{kj}^{+} a_{kj} + \sum_{k} \sum_{j=-J}^{J} v(|j|)(a_{kj}^{+}\mathbf{X}_{0j} + \mathbf{X}_{j0}a_{kj}) + \sum_{j=-J}^{J} \varepsilon_f \mathbf{X}_{jj} + (\text{crystal field}). \tag{2.1.14}$$

Hereafter we omit the subscript $J$ in $a_{kJj}$, $a_{kJj}^{+}$. Now the total interaction of electrons in the $f$ shell is hidden in the $\mathbf{X}$-operator algebra (2.1.13).

A further simplification takes place for Ce and Yb ions. In $Ce^{4+}$ or $Yb^{2+}$ ions the state $|0\rangle$ corresponds to either the empty or full shell, respectively. In these states the impurity potential is spherically symmetric. Therefore, the hybridization matrix element does not depend on the momentum projection $j$. There is no simplification of this kind for Sm ions where the state $|0\rangle - {}^7F_0$ has non-zero orbital momentum and spin. In this state, obviously, the impurity potential is not spherically symmetric.

Finally, in Tm ions the states with non-zero total angular momentum are mixed. This results in the very complex dependence of hybridization amplitudes on initial and finite states of the impurity shell and the Anderson hamiltonian cannot be written down in such a simple form as (2.1.14).

The crystal field splits the $f$-electron level. The crystal field effects are essential in mixed-valence state if the magnitude of CEF-splitting is of the order of the effective resonance width $(2J+1)\pi\rho(\epsilon_{\text{F}})v^2$ (Barabanov and Tsvelick 1979). Usually the latter is much larger than the crystal field. Thus CEF-effects seem to be negligible in the mixed-valence region, so that the degeneracy of the $f$-electron level is essential. In § 9 we present the exact solution of the degenerate Anderson model (eqn. (2.2.4)) for Ce and Yb impurities.

## 2.2. *Exchange hamiltonians*

### 2.2.1. *The general form of the exchange hamiltonians*

When we study processes in which the variation of $n_d$ is virtual, an exchange hamiltonian emerges as a result of projecting the Anderson hamiltonian into a sector with a fixed number of particles $n_d^{(0)}$ (Anderson and Clogston 1962, de Gennes 1962, Kondo 1962, Schrieffer and Wolf 1966).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

In second-order perturbation theory in $v_k$ the effective exchange hamiltonian in the most general form can be written as

$$\mathscr{H}_{\text{ex}} = \mathscr{H}^{0}_{\text{atom}} + \sum_{k,k'} T_{m\sigma,m'\sigma'}(k,k') a^{+}_{km\sigma} a_{k'm'\sigma'}. \tag{2.2.1}$$

Here $\mathscr{H}^{0}_{\text{atom}}$ is the projection of $\mathscr{H}_{\text{atom}}$ on to the subspace with a given $n_d$, and matrix $T$ in the same subspace is written as

$$T = v_k v_{k'} \left( d_{m\sigma} \frac{1}{\epsilon_k - \mathscr{H}_{\text{atom}}} d^{+}_{m'\sigma'} - d^{+}_{m\sigma} \frac{1}{\epsilon_{k'} - \mathscr{H}_{\text{atom}}} d_{m'\sigma'} \right). \tag{2.2.2}$$

These formulae express virtual transitions from a sector with $n_d = n_d^{(0)}$ to a sector with $n_d^{(0)} \pm 1$, and vice versa. In the process of such transition the momentum, projection of angular momentum and spin of the electronic partial wave $(k', m', \sigma')$ change to $(k, m, \sigma)$.

As the energy splitting of the ionic shell is very large, $\mathscr{H}^{0}_{\text{atom}}$ should be considered as the projection operator on the ground state of the impurity atom. Apart from some special cases the exchange operator $T$ projected on to this subspace has a rather complex structure.

Until the spin–orbit coupling may be neglected, the form of the exchange hamiltonian is restricted only by invariance under rotations in the spin and coordinate spaces and may be written thus:

$$\mathscr{H}_{\text{ex}} = \sum_{p,q=0}^{1,\min(l,L)} I_{pq} (\mathbf{S}\boldsymbol{\sigma}_{\sigma\sigma'})^{p} (\mathbf{L}\mathbf{l}_{mm'})^{q} a^{+}_{km\sigma} a_{k'm'\sigma'}, \tag{2.2.3}$$

where $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices, and $l$ is the operator of orbital angular momentum of the electronic partial wave that interacts with the impurity.

To this hamiltonian we must add the spin–orbit coupling and the crystal field. For rare-earth impurities the large spin–orbit coupling immediately projects the hamiltonian (2.2.2) on to the state of the shell with total angular momentum $J$, which is $L+S$ for $n_f^{(0)} > 7$ and $|L-S|$ for $n_f^{(0)} \leqslant 7$. In this case the general form of the exchange hamiltonian is

$$\mathscr{H}_{\text{ex}} = \sum_{p,q=0}^{1,\min(l,J)+1} I_{pq} (\mathbf{J}\boldsymbol{\sigma}_{\sigma\sigma'})^{p} (\mathbf{J}\mathbf{l}_{mm'})^{q} a^{+}_{km\sigma} a_{k'm'\sigma'}. \tag{2.2.4}$$

Further splitting of the multiplet is caused by the crystal field.

The quantities $I_{pq}$ in eqns. (2.2.3) and (2.2.4) are the amplitudes of the exchange interaction. To estimate their values we neglect the energy splitting within one valence in comparison with the energies $E_{\pm}$ (that estimate is good enough for transition and Ce ions). Then the energy denominators in (2.2.2) do not depend on $(m, \sigma)$ and $(m', \sigma')$, and matrix $T$ contains only one parameter:

$$T_{m\sigma,m'\sigma'} = \left( v_k v_{k'} \frac{\delta_{mm'} \delta_{\sigma\sigma'}}{\epsilon_k - E_+} + I_{kk'} \right) d^{+}_{m\sigma} d_{m'\sigma'}, \tag{2.2.5}$$

where

$$I_{kk'} = v_k v_{k'} \left( \frac{1}{\epsilon_k - E_+} + \frac{1}{\epsilon_{k'} - E_-} \right).$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

This formula provides for the upper estimate of $I_{pq}$. It is important that $I_{kk'}$ never changes sign and corresponds to antiferromagnetic interaction. Although $\rho(\epsilon_F)I_{pq} \ll 1$, in view of the resonance nature of the superexchange it considerably exceeds the contact exchange coupling, which is caused by the Coulomb interaction of orbital and band electrons, and usually has a sign corresponding to ferromagnetic interaction.

The hamiltonian (2.2.3) and (2.2.4) may be assumed to be the first terms in a series expansion in $v^2$, which can be obtained from (2.1.9) as a result of a canonical Schrieffer–Wolf transformation (Schrieffer and Wolf 1966). Higher-order terms are small if

$$\rho(\epsilon_F)v^2\left(\frac{n_d^{(0)}}{E_-}+\frac{(2l+1)-n_d^{(0)}}{E_+}\right)\ll 1. \tag{2.2.6}$$

2.2.2. *Two simple exchange hamiltonians*

We shall consider below two simple cases, important from a practical standpoint.

(i) *Impurities with orbital singlet local shell.* If the atomic shell of the impurity ion is half-filled, Hund's rule states that the ion ground state is an orbital singlet with spin $S=l+1/2$. This is the case with Mn, which has $n_d^{(0)}=5$ and whose $d$ shell has the configuration $^6S_{5/2}$. Here scattering involves only exchange of spins, while the projection of the orbital angular momentum of the electronic wave remains unchanged. As a result the exchange hamiltonian simplifies considerably. If, in the general formula (2.2.3), we put $L=0$ (Schrieffer 1967) we have

$$\mathscr{H}_{\text{ex}}=\sum_{\substack{\sigma,\sigma'\\ k,k'}}\left[(V_{\sigma\sigma'}+I\mathbf{S}\boldsymbol{\sigma}_{\sigma\sigma'})\sum_{m=1}^{n}a^{+}_{km\sigma}a_{k'm\sigma'}\right]. \tag{2.2.7}$$

Since the ground state of the ion is spherically symmetric, the influence of the crystal field is negligible. It manifests itself in the exchange hamiltonian only in virtual states with $n_d=n_d^{(0)}\pm 1$, which leads to a weak dependence of $I$ on $m$.

An orbital singlet may also appear as the result of the combined action of the Hund rule and the crystal field. This is the case with impurities of vanadium ($n_d^{(0)}=3$) and cobalt ($n_d^{(0)}=8$) in a cubic crystal field (Nozières and Blandin 1980). In this field the five orbital states split into a doublet ($E$) and a triplet ($T$), with the triplet lying below the doublet on the energy scale. Then at $n_d^{(0)}=3$ the triplet is half-filled and, according to Hund's rule, an orbital singlet state with spin $S=3/2$ forms. The situation is similar for $n_d^{(0)}=8$—the triplet is filled completely but the doublet is half-filled; for this reason $L=0$ again, but $S=1$. In these cases the exchange hamiltonian again has the form (2.2.7). The plane wave corresponding to the conduction electrons must be expanded according to the irreducible representations of the cubic symmetry point group. The splitting of atomic levels leads to a situation in which the electrons belonging to the doublet and triplet are scattered by the impurity with markedly different amplitudes, e.g. for $n_d^{(0)}=3$ we have $I_T \gg I_E$, and the discrepancy is greater the higher the strength of the crystal field.

In studying the renormalization group equations for such a doubly-charged model, Nozières and Blandin (1980) demonstrated that the amplitude $I_E$, being bare (and therefore small), vanishes completely as the energy decreases. Hence, ignoring $I_E$ we return to the hamiltonian (2.2.7) but with spin $S=3/2$ and three values of $m$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

($n=3$). The case $n_d^{(0)}=8$ is described by the same hamiltonian but with $S=1$ and $n=2$.

In previous examples the multiplicity of the impurity appears to be equal to that of conduction electrons. This property results in the *total compensation* of the impurity magnetic moment at low temperatures, so that the impurity ground state is *orbital and spin singlet.*

At the end of this topic we argue that for alloys with extremely low Kondo temperatures the hyperfine coupling is essential and the case $n \neq 2S$ may be realized. The case will be studied below (§§ 5.1 and 6.1) using the exact solution. In this case the effective coupling increases with decreasing energy scale, however, the impurity ground state is still magnetic with effective spin $S-1/2$.

A very interesting case is that with $n>2S$. According to the Nozières and Blandin (1980) point of view, as well as the numerical study by Cragg and Lloyd (1979), the scaling trajectory has a fixed point at finite $I=I^*$. It means that all physical quantities have power temperature dependence.

(ii) *Degenerate exchange model.* (Impurities with one electron or hole in the local shell.) Another simple and important hamiltonian comes into play when there is either an electron or a hole in the $d$ or $f$ shell. Hund's rule does not work any more in this case. Such impurities would be found at the beginning and at the end of a transition series, and are Ce and Yb among the rare earths. All other magnetic impurities apparently have more than one electron (or hole) in the shell. Unfortunately, none of the transition metals mentioned so far have been found to be magnetic in high dilution (see, for example, the experiments with CuNi alloys (Drew and Doezema 1972)). They become magnetic only at high concentrations. The only impurities in the one-electron (hole) class which show magnetic moments in dilute alloys are Ce and Yb.

Go back to the Anderson hamiltonian in form (2.1.14). After the Schrieffer–Wolf transformation the exchange operator takes the form (Coqblin and Schrieffer 1969):

$$T_{jj'}=V^2\mathbf{X}_{j0}[(\epsilon_k-\epsilon_f)+E]^{-1}_{jj'}\mathbf{X}_{0j'}$$

and according to the algebra (2.1.13) we obtain

$$\mathscr{H}=\sum_{k,j}\epsilon_k a^+_{kj}a_{kj}+\sum_{\substack{j,j'\\k,k'}} I a^+_{kj}\mathbf{X}_{j'j}a_{k'j'}+\sum_{j,j'}E_{jj'}\mathbf{X}_{jj'}, \tag{2.2.8}$$

where $E_{jj'}$ is the crystal field splitting.

Often, even in the presence of a crystal field, we can assume that $I_{jj'}$ is isotropic since, as a rule, $-\epsilon_f \gg \max E_{jj'}$. Then we have

$$I=\frac{V^2}{\epsilon_k-\epsilon_f} \tag{2.2.9}$$

and only the last term in (2.2.8) describes the effect of the crystal field.

At $E_{jj'}=0$ the hamiltonian (2.2.8) is invariant under transformations of the $SU(n)$ group, where $n=2J+1$. In these conditions we shall speak of an *n-fold degenerate model.*

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The Kondo temperature in such a model depends strongly on the value of $n$ (Coqblin and Schrieffer 1969):

$$T_K \sim \epsilon_F \exp(-1/I_n). \tag{2.2.10}$$

In alloys with rare-earth impurities the crystal field is comparable to the possible temperature interval. Hence, as the temperature rises, more and more degrees of freedom may take part in the scattering processes. On the other hand, an increase in $n$ leads, according to (2.2.10), to an increase in $T_K$, and we may once more have the Kondo effect. The region of $T \sim T_K$ is well delayed in this case. The possibility of such a 'sequence' of Kondo effects was pointed out by Cornut and Coqblin (1972). Indeed, suppose that the crystal field splits the multiplet into $n_0$, $n_1$, ... multiplets with energies 0, $E_1$, .... At $T \ll E_1$ the particular alloy is described by the $n_0$-fold degenerate model (2.2.8) with a Kondo temperature $T_K(n_0)$ given by (2.2.10). Let us assume that $T_K(n_0) \ll E_1$. Then the system, after reaching the weak-coupling regime at $T \ll T_K(n_0)$ with a further increase in temperature reaches the region where $T \gg E_1$ and is again in the strong coupling regime; but now its effective multiplicity is $n_1 + n_0$. As a result $T_K(n_0 + n_1)$ may prove to be higher than $E_1$. This process repeats as the temperature increases. If $n_0 = 2$, *then the traditional s–d exchange model with spin* $S = 1/2$ (1.1.1) *is realized at* $T \ll E_1$. This situation is typical for rare-earth magnetic alloys. The Kondo temperature for Ce alloys is found to be of the order of one degree. For YbAu and YbMg it is even smaller. The two characteristic examples of Ce alloys exhibiting clear Kondo effect have been discussed in § 1.2.

The exact solution of the degenerate model is expounded in §§ 4.4 and 7.

### 2.2.3. *Influence of the hyperfine coupling*

The model with $n \neq 2S$ does not seem to be only academic. One must look for such impurities among the isotopes of heavy metals having a sizeable hyperfine coupling of the localized moment with their nuclear spin:

$$\mathscr{H}_{hf} = B\mathbf{I} : \mathbf{S},$$

where $\mathbf{I}$ is nuclear spin.

At low temperature $T \ll |B|$ the local moment is strongly coupled to the nuclear spin. If the hyperfine coupling is such that a well-isolated ground state $\mathbf{F} = \mathbf{I} + \mathbf{S}$ can be defined, the hamiltonian (2.2.7) can be reduced to

$$\mathscr{H}_{int} = I \sum_n \boldsymbol{\sigma}_n \cdot \mathbf{F}.$$

If the exchange coupling changes its spin, the Kondo effect disappears. This is the case with the antiferromagnetic spin–nuclear coupling when $S < \mathscr{I}$ (Benoit and Floquet 1976). In the opposite case we arrive at the hamiltonian (2.2.7) in which the electron multiplicity $n$ is determined by the structure of the shell, whilst the magnitude of $S$ is determined by properties of the nucleus. For the Kondo effect to persist under the strong hyperfine interaction the Kondo temperature must be lower than the splitting between states with different $F$: $T_K \ll |B|$. Influence of the hyperfine coupling may be substantial in alloys with Mn such as, for instance, $^{54}$Mn, in which $\mathscr{I} = 3$; $S = 5/2$ and the relative splitting between successive levels for different $F$ change from 10 to 35 mK (for a review, see Floquet 1978). In AuMn and CuMn this splitting is comparable with $T_K$, though at such a low $T_K$ the impurity–impurity interaction might prove important (Hirshkoff *et al.* 1971).

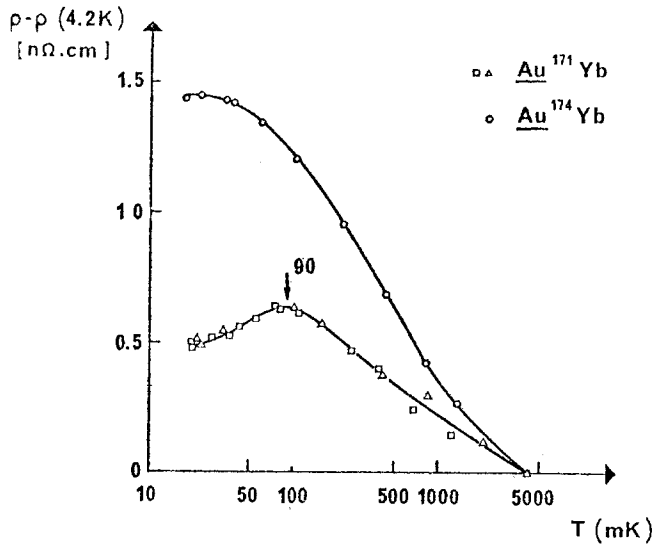
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

A nice example of the Kondo effect under the strong hyperfine coupling $|B| \gg T_K$ is provided by AuYb alloys. The element Yb has a number of radioisotopes, some of which (for instance $^{174}$Yb) lack a nuclear moment. The ground state of the Yb impurities dissolved in gold is the $\Gamma_7$ crystal field doublet which can effectively be described as a spin $\frac{1}{2}$ system with $g = 10/7$ appropriate for the $\Gamma_7$ ground state. The isotopes $^{173}$Yb and $^{171}$Yb have nuclear moments of opposite sign. For $^{171}$Yb $B = 128$ mK and $\mathscr{I} = 1/2$, while for $^{173}$Yb $B = 35$ mK and $\mathscr{I} = 5/2$.

Furthermore, for the $^{171}$Yb isotope the conditions for electron–nuclear singlet coupling hold, whereas the $^{173}$Yb electron–nuclear ground state is an $F = 3$ multiplet. In the latter case at temperatures well below the energy splitting between the electron–nuclear ground state $F = 3$ and the first excited level, which is equal to 105 mK, the Au$^{173}$Yb alloy must be described by hamiltonian (2.2.7) with $S = 3$. The measurements of conductivity of Au$^{174}$Yb and Au$^{171}$Yb alloys give perfect evidence for the role of hyperfine coupling (see, for example, Floquet 1978).

The isotope $^{174}$Yb with $\mathscr{I} = 0$, dissolved in Au, shows a perfect Kondo behaviour. Au$^{171}$Yb alloy shows the Kondo effect tendency. However, in the $\sim 100$ mK range the nuclear and electron shell spins couple and form a singlet, the Kondo effect disappears and below 90 mK the impurity resistance decreases (see fig. 2.1). Regretfully, we know of no similar experiments with a $^{173}$Yb isotope.

Fig. 2.1




The resistivity of Au$^{171}$Yb and Au$^{174}$Yb alloys (Hebral *et al.* 1976) versus log $T$. The $^{174}$Yb without hyperfine interaction shows up a Kondo behaviour. Increase in resistivity stops near 90 K for Au$^{171}$Yb, where the singlet electron-nuclear state becomes isolated from the triplet excited level (see ref. in Floquet 1978).

### 2.2.4. *Perturbation theory*

Just as in the case of the non-degenerate s–d exchange model (I), at low energies perturbation-theory series in the strength of the exchange interaction leads to logarithmic singularities. The Kondo temperature is the characteristic that divides the regions of weak and strong coupling. If the physically possible temperature

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

interval is commensurable with the size of the level splitting in the $d$ (or $f$) shell (since the latter cannot be considered infinite and, therefore, it is impossible to take only the ground state of the atom), there will be other characteristic parameters in the system besides $T_K$. Practically, this is the case only for rare-earth impurities. Now we shall assume, although this is not always true, that there is a temperature region between two energy levels of the ion, $E_\alpha \ll T \ll E_{\alpha+1}$, so that inside this region we can ignore all transitions to levels higher than $E_{\alpha+1}$ and assume all levels below $E_\alpha$ degenerate. Then in the system there is only one energy scale, $E_\alpha \ll T_K \ll E_{\alpha+1}$, and scaling can be employed.

The condition for renormalization implies that as the ultraviolet cut-off $D$, equal in this case to $E_{\alpha+1}$, changes, accompanied by a respective variation in the coupling constants $I_{pq}$, physical quantities are multiplied by a constant that is not a function of the energy variables $\varepsilon$ (external frequency, temperature or magnetic field strength). This means that any physical quantity, as a function of, say, temperature, is expressed as

$$Q(T, I, D) = \tilde{Q}(D, I)\zeta(T/T_K). \tag{2.2.11}$$

If we assume, for simplicity, that there is only one interaction amplitude $I$ in the system, then mathematically the renormalization condition (2.2.11) can be expressed in the following manner.

Suppose that $z$ is a function of $I$, $D$ and $\varepsilon$ that is invariant under transformations of the renormalization group and chosen by convenience. Then another invariant quantity, $\zeta(\varepsilon/T_K)$, is a function of the *invariant charge* $z$:

$$\frac{d\ln\zeta}{d\ln\varepsilon} = \frac{d\ln Q}{d\ln\varepsilon} = \Psi(z). \tag{2.2.12}$$

As for $z$ it can be defined as the solution to

$$\frac{dz}{d\ln\varepsilon} = \beta(z), \tag{2.2.13}$$

where $\Psi(z)$, $\beta(z)$ are some functions.

To build a perturbation theory it is expedient to select $z$ in such a way that at $\varepsilon = D$ it coincides with the bare interaction amplitude at $I \ll 1$:

$$z_0 \equiv z(D) = I + O(I^2). \tag{2.2.14}$$

Then, knowing the terms in the perturbation theory series for $z(\varepsilon)$ and $Q(\varepsilon)$, we can easily find the expansions of $\beta(z)$ and $\Psi(z)$ in powers of $z$. Suppose that

$$z(\varepsilon) = I + cI^2 + dI^3 + aI^2\ln(\varepsilon/D) - a^2I^3\ln^2(\varepsilon/D) + \ldots + bI^3\ln(\varepsilon/D) + \ldots. \tag{2.2.15}$$

Then if we find the derivative of (2.2.15) with respect to $\ln(\varepsilon/D)$ and put $\varepsilon = D$, according to (2.2.14) we have

$$\beta(z) = az^2 + bz^3 + O(z^4). \tag{2.2.16}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Equation (2.2.13) defining the invariant charge $z$ can be rewritten thus:

$$\Phi(z) = \ln(\varepsilon/T_K) \tag{2.2.17}$$

with

$$\Phi(z) = \int^z \frac{dz'}{\beta(z')} = \frac{1}{az} - \frac{b}{a^2}\ln|z| + \alpha + O(z), \tag{2.2.18}$$

where $\alpha = \text{const}$ and the Kondo temperature defined as

$$T_K = D\exp[\Phi(I)] = \text{const}\, DI^{b/a^2}\exp(-1/aI)(1+O(I)). \tag{2.2.19}$$

The choice of the invariant charge is not unique. More than that, if we do choose the regularization of the theory at small distances and times, the functions $\Psi(z)$ and $\beta(z)$ may still change and, therefore, are not universal.

The pre-exponential dependence of $T_K$ in the constant $I$ is also non-universal. But the simultaneous solution of eqns. (2.2.12) and (2.2.13) leads to a universal dependence of all physical quantities on the ratios $\varepsilon/T_K$, $T/T_K$ and $H/T_K$:

$$Q = Q_0 \exp\left(\int_I^{z(\varepsilon/T_K)} \frac{\Psi(z')}{\beta(z')}dz'\right), \tag{2.2.20}$$

where $Q_0$ is the value of $Q$ at $\varepsilon = D$.

From the point of view of perturbation theory the most convenient form of the function $\Phi(z)$ is

$$\Phi(z) \equiv \frac{1}{az} - \frac{b}{a^2}\ln|z| = \ln\frac{\varepsilon}{T_K}. \tag{2.2.21}$$

(We retained the term $\ln|z|$ in the definition of $\Phi(z)$ so that all physical quantities at $0 < z \ll 1$, i.e. $\varepsilon \gg T_K$, could be expanded in a power series in $z$.) We note that eqn. (2.4.21) is valid only if the cut-off $D$ can be considered infinite when compared with $T_K$, while the separation between the atomic levels $\alpha$ and $\alpha+1$ is infinite as compared with $D$:

$$E_\alpha \ll T_K, \qquad T \ll D \ll E_{\alpha+1}.$$

In what follows we give the results obtained via perturbation theory for the impurity parts of the thermodynamic functions in the s–d exchange model discussed in detail in §§ 5 and 6.

The Gell–Mann–Low equation (2.2.21) in this case takes the form

$$\frac{1}{z(\varepsilon)} - \frac{1}{2}\ln z(\varepsilon) = \ln\frac{\varepsilon}{T_K} \tag{2.2.22}$$

and does not depend on the impurity spin $S$.

At $H=0$ the magnetic susceptibility as a function of temperature $T \gg T_K$ is expressed thus (Abrikosov and Migdal 1970, Fowler and Zawadowski 1971):

$$\chi_i(T) = (g_L\mu_B)^2\frac{S(S+1)}{3T}\left(1 - z\left(\frac{T}{T_K}\right) + O(z^2)\right) \tag{2.2.23}$$

or, if we do not employ (2.2.21)

$$\chi_i(T) = (g_L\mu_B)^2\frac{S(S+1)}{3T}\left(1 - \frac{1}{\ln T/T_K} - \frac{\ln\ln T/T_K}{2\ln^2 T/T_K} + \dots\right). \tag{2.2.24}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The impurity magnetic moment at $T=0$ and $H \gg T_K$ is (Abrikosov and Migdal 1979):

$$M_i(H)=S\left(1-\frac{1}{2}z\left(\frac{H}{T_K}\right)+O(z^2)\right). \tag{2.2.25}$$

Finally, the heat capacity at $H=0$ and $T \gg T_K$ is (Kondo 1969, Fateev and Wiegmann 1981 a)

$$C_i(T)=S(S+1)\pi^2 z^4(T/T_K)+\ldots \tag{2.2.26}$$

Here we also give the Gell–Mann–Low equations for the hamiltonians (2.2.7) and (2.2.8). In the first instance

$$\ln\frac{\varepsilon}{T_K}=\frac{1}{z}-n\ln|z| \tag{2.2.27}$$

while in the second

$$\ln\frac{\varepsilon}{T_K}=\frac{1}{nz}-\ln|z|. \tag{2.2.28}$$

We note that the perturbation theory series (2.2.23)–(2.2.26) are asymptotic. Therefore, even a large number of terms can hardly help in studying the low energy properties of a system.

In the following sections we shall derive the exact solution for the s–d exchange model with an arbitrary impurity spin (the hamiltonian (2.2.7) with $n=1$) and for the $n$-fold degenerate exchange model (2.2.8). On the basis of these solutions we shall establish the general nature of the ground state of the impurity and find the thermodynamical functions at finite temperatures and magnetic fields. At present there is no solution for the interesting and important, from the practical standpoint, problem (2.2.7) for arbitrary $n$ and $S$ (see Note added in proof).

## § 3. Recent theoretical developments

In this section we describe some interesting theoretical approaches which enable us to understand the behaviour of the s–d exchange and Anderson models. We think that the results derived by these approaches are a remarkable supplement to the exact solution.

### 3.1. *The Kondo model*

#### 3.1.1. *The Coulomb gas and the resonant-level model*

Despite considerable efforts the low-temperature behaviour of the s–d model was unknown until Anderson *et al.* (1970 a, b) obtained a qualitative solution of the problem. The mathematical technique which has been developed in these papers (Anderson and Yuval 1969, Yuval and Anderson 1970, Anderson 1970), as well as in the paper by Schotte (1970), proved very powerful and has had a great impact on the physics of one-dimensional systems.

In the first paper Anderson and Yuval (1969) demonstrated that the thermodynamics of a magnetic impurity can be reformulated as classical statistics of the gas

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

of alternating charged particles with the logarithmic interaction. It is convenient to attack the problem starting with the s–d model with the anisotropic exchange:

$$\mathscr{H}_{\text{int}} = \sum_{\substack{k,k'\\ \sigma,\sigma'}} c^{+}_{k\sigma}\left[\frac{1}{2} I_{\parallel}\sigma^{z}_{\sigma\sigma'}\mathbf{S}^{z} + \frac{1}{2} I_{\perp}(\sigma^{x}_{\sigma\sigma'}\mathbf{S}^{x} + \sigma^{y}_{\sigma\sigma'}\mathbf{S}^{y})\right] c_{k'\sigma'}. \tag{3.1.1}$$

The point is that at $I_{\perp}=0$ the hamiltonian (3.1.1) is diagonal, hence the perturbation expansion in $I_{\perp}$ can be developed at arbitrary $I_{\parallel}$. The s–d model partition function is equal to

$$Z = Z_0 Z_1, \tag{3.1.2}$$

where $Z_0$ is a partition function at $I_{\perp}=0$ which is free of singularities due to the Kondo effect. The latter quantity

$$Z_1 = 2\sum_{n=0}^{\infty}\left(\frac{I_{\perp}\cos^2\delta}{2\tau}\right)^{2n}\int_0^{\beta-\tau} d\tau_{2n}\ldots\int_0^{\tau_2-\tau} d\tau_1 P_{2n}(\tau_1,\ldots\tau_{2n}), \tag{3.1.3}$$

where

$$P_{2n} = \exp\left\{2\left(1-\frac{2\delta}{\pi}\right)^2 \sum_{\nu>\nu'}^{2n}(-1)^{\nu+\nu'}\ln\left[\frac{\sin(\pi T(\tau_\nu-\tau_{\nu'}))}{\pi T\tau}\right]\right\} \tag{3.1.4}$$

describes the grand partition function of the so-called 'Coulomb gas'. The cut-off $\tau$ regularized the theory at short times: $\tau^{-1}$ is of the order of the Fermi energy. The quantities $(I_{\perp}\cos^2\delta/2\tau)$ and $\sqrt{2}(1-2\delta/\pi)$ may be taken for the fugacity and charge of classical particles, $\delta(I)=\pi I_{\parallel}/8+O(I^2)$ is a scattering phase for the potential $I_{\parallel}/4$. The function $\delta(I)$ is non-universal and, apart from the linear term $I_{\parallel}$, depends on the regularization procedure, therefore we do not write it down in a complete form. The formulae hold only provided that only the near-Fermi-surface states contribute, so that the spectrum can be considered linear. Hence the s–d model–Coulomb-gas equivalence only holds in the 'long-time' approximation.

The next paper of Anderson *et al.* (1970) consists of two parts. In the first part the renormalization of the Coulomb-gas problem has been performed: enlarge the interparticle distance from $\tau$ to $\tau+d\tau$ and integrate over the degrees of freedom corresponding to the scales from $\tau$ to $\tau+d\tau$. The resulting dependence of the chemical potential and charge on the scale takes in terms in $I_{\parallel}$ and $I_{\perp}$ of the form (valid at $I\ll 1$):

$$\left.\begin{aligned} dI_{\parallel}/d\ln\tau &= I_{\perp}/2\pi,\\ dI_{\perp}/d\ln\tau &= I_{\perp}I_{\parallel}/2\pi \end{aligned}\right\} \tag{3.1.5}$$

(we put $\rho(\epsilon_F)=1/2\pi$).

The corresponding solutions, known as a 'poor man' scaling, are shown in fig. 5.4 alongside the exact solution trajectories (see below, § 5.2). The arrows are directed towards rising $\tau$. In the FM sector the interaction vanishes as $\tau$ increases, hence at low energies and/or temperatures the impurity is almost free.

Nothing of the sort is observed in sectors AFM and AN. Irrespective of the strength of the initial interaction it blows up at large time scales. Once the couplings are large eqn. (3.1.5) no longer holds. Anderson (1970) conjectured that this growth is bounded only by unitarity.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

An implicit assumption was that in one-dimensional systems there may be no singularity at finite couplings. Now we know of a few cases of one-dimensional systems with a fixed point at finite couplings (Nozières and Blandin 1980, Cragg *et al.* 1980), still for the s–d model Anderson's conjecture proved correct. This is made evident by an extensive numerical study of Wilson (1974, 1975) and was confirmed by the exact solution. In the second part of their paper the authors have shown that at a certain value of $I_{\|}=I_T$, such that $2(1-2\delta(I_\perp)/\pi)^2=1$ (the so-called Toulouse limit), the sum (3.1.3) is equivalent to the one for a certain simple quadratic model and can easily be calculated. The hamiltonian of this model has the form

$$\mathscr{H}_{\mathrm{T}}=\sum_k \varepsilon_k c_k^+ c_k + V\sum_k (d^+ c_k + c_k^+ d). \tag{3.1.6}$$

Here $c_k, d$ are the operators of spinless fermions.

One can easily check that the partition function of the model (3.1.6) is exactly equal to $Z_1$ in (3.1.2) for the case of classical charges $\pm 1$ (Toulouse 1969). In this case $V\sim I_\perp \tau^{-1}$ and the role of the magnetic field is played by the resonant level energy. The width $\Gamma=\pi V^2\rho(\epsilon_{\mathrm{F}})$ of the level determines the specific heat and susceptibility of the impurity at $T\to 0$:

$$c_{\mathrm{i}}\sim T/\Gamma, \qquad \chi_{\mathrm{i}}\sim 1/\Gamma. \tag{3.1.7}$$

Thus, at least for $I_{\|}=I_\perp$, the magnetic susceptibility proved finite at $T=0$.

Anderson *et al.* (1970) assumed that the effective coupling $I(\tau)$ rises from the initial small value as long as at a certain $\tau=\tau_T$ it becomes equal to $I_T$, so that the low-temperature behaviour of the s–d model at small $I$ is identical to that of model (3.1.6) with $\Gamma$ substituted by $T_{\mathrm{K}}$. This resulted in the correct answer:

$$\chi_{\mathrm{i}}\sim 1/T_{\mathrm{K}}. \tag{3.1.8}$$

However, the line of reasoning which led to (3.1.8) lacks rigour. First, the renormalized hamiltonian (3.1.1) does not retain its form; new vertices, which also rise as $\tau\to\tau_T$, are generated (Nozières 1975). Second, as the exact solution demonstrated, $I(\tau)$ reaches the Toulouse limit only at the fixed point $I(\infty)$. As seen in fig. 5.4 the Toulouse limit trajectory $\delta(I_{\mathrm{T}})=\pi/2(1-1/\sqrt{2})$ intercepts other trajectories only in the strong coupling limit, when the unitarity limit is saturated.

Another approach consists of using (3.1.6) as a zeroth-order approximation of an infrared-finite perturbation theory. To realize this approach Schlottmann (1978 a, b, 1981) and Wiegmann and Finkelstein (1978) proposed the so-called resonance-level model, generalizing $\mathscr{H}_{\mathrm{T}}$ (RL model):

$$\mathscr{H}_{\mathrm{RL}}=\mathscr{H}_{\mathrm{T}}+\frac{U}{2}\sum_{k,k'}(c_k^+ c_{k'}-c_{k'}c_k^+)(d^+ d-1/2). \tag{3.1.9}$$

The RL model is equivalent to the s–d exchange model at an arbitrary $I_{\|}$, provided

$$\left(1-\frac{2}{\pi}\delta(U)\right)^2=2\left(1-\frac{2}{\pi}\delta(I_{\|})\right)^2, \tag{3.1.10}$$

where $\delta(U)$ is the scattering phase for the potential $U/4$.

This equivalence holds in the so-called long-time approximation and the two models have common features at large time scales $t\gg\tau$. Despite criticisms (Wilson 1975) this approximation is not so bad: the universal characteristics of both models coincide.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The hamiltonian (3.1.9) can be easily diagonalized at both $V=0$ and $U=0$. The perturbation expansion in $V$, like the similar expansion in $I_\perp$ in the s–d model, does not enable us to study the low-temperature properties of the system: the zeroth-order ground state is orthogonal to that of the exact solution. Hence, the relevant divergences are but an artefact of the bad approximation. Rather, one should expand in $U$. In this case all the perturbation theory expansion terms are finite at $T=0$, since there is a finite scale—the level width—which is renormalized only by the interaction. Though small $\Gamma$'s correspond to large $U$, such a perturbation theory is more convenient.

The Coulomb-gas-to-RL-model equivalence can be checked by a straightforward order-by-order comparison of the relevant perturbation expansions. Below, we prove this equivalence using the bosonic representation of fermionic operators (Schotte 1970). As a by-product one gets the spin- and charge-density waves which will be extensively exploited below.

As is well known, the currents of one-dimensional fermions

$$b^+_{k\sigma}=\frac{1}{k}\sum_{p>0} c^+_{k+p,\sigma}c_{p\sigma} \tag{3.1.11}$$

are bosonic operators such that

$$[b^+_{k\sigma}, b_{k'\sigma'}]=k\delta_{kk'}\delta_{\sigma\sigma'}. \tag{3.1.12}$$

In the long-time approximation the inverse formulae read (Schotte 1969, 1970):

$$\sum_k c_{k\sigma}=\epsilon_F^{1/2}\exp\left[-\sum_{k>0}(b^+_{k\sigma}-b_{k\sigma})\right]. \tag{3.1.13}$$

It is important to note that the s–d model hamiltonian can be rewritten in terms of $b, b^+$. Introduce the spin and charge current operators

$$\sigma_k=\frac{b_{k\sigma}-b_{k,-\sigma}}{\sqrt{2}}, \qquad \rho_k=\frac{b_{k\sigma}+b_{k,-\sigma}}{\sqrt{2}}. \tag{3.1.14}$$

Then:

$$\left.\begin{aligned}
&\mathscr{H}=\mathscr{H}^{\mathrm{ch}}+\mathscr{H}^{\mathrm{sp}},\\
&\mathscr{H}^{\mathrm{ch}}=\sum_k k^2\rho^+_k\rho_k,\\
&\mathscr{H}^{\mathrm{sp}}=\sum_k k^2\sigma^+_k\sigma_k+\frac{I_\parallel}{\sqrt{2}}\sum_k S^z(\sigma^+_k+\sigma_k)k\\
&\qquad +I_\perp\epsilon_F\left[S^+\exp\left(-\sqrt{2}\sum_k\frac{1}{k}(\sigma^+_k+\sigma_k)\right)+\mathrm{h.c.}\right].
\end{aligned}\right\} \tag{3.1.15}$$

A corollary is that the *spin- and charge-density* waves do not interact. Moreover, the charge excitations are free particles. No wonder, the partition function of the s–d model is a simple product (3.1.2) of the partition functions $Z_0$ and $Z_1$ of the two hamiltonians.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

This will show up again in the exact solution. However, one has to bear in mind that this non-interaction of the charge and spin excitations takes place only in the linear spectrum approximation.

One can apply to the hamiltonian $\mathscr{H}^{\mathrm{sp}}$ one more canonical transformation such that the coefficient $\sqrt{2}$ in front of $\sigma_k$ becomes 1. The new electron operators will describe spinless particles. This transformation simply shifts equilibrium positions of the harmonic oscillators $\sigma$ and $\sigma^+$:

$$T\mathscr{H}T^+ = \sum_k k^2\sigma_k^+\sigma_k + US^z\sum_k k(\sigma_k^+ + \sigma_k) + \left[S^+\exp\left(-\sum_k \frac{1}{k}(\sigma_k^+ + \sigma_k)\right) + \text{h.c.}\right] I_\perp \epsilon_{\mathrm{F}}, \tag{3.1.16}$$

where

$$T = \exp\left[(\sqrt{2}-1)\sum_k S^z \frac{1}{k}(\sigma_k^+ - \sigma_k)\right] \tag{3.1.17}$$

and $U$ is related to $I$ via (3.1.10). Introduce now spinless fermions according to

$$\sum_k c_k^+ = \epsilon_{\mathrm{F}}^{1/2}\exp\left[-\sum_{k>0}(\sigma_k^+ - \sigma_k)\right] \tag{3.1.18}$$

replace the $S=1/2$ operators by the spinless localized fermion operators:

$$S^+ = d^+, \qquad S^- = d, \qquad S^z = d^+d - 1/2$$

and we get the RL model.

The RL model has been used to prove the relationship between the impurity specific heat and the magnetic susceptibility in the limit $T\to 0$ (Wiegmann and Finkelstein 1978):

$$C_{\mathrm{i}}/T\chi_{\mathrm{i}} = 2\pi^2/3. \tag{3.1.19}$$

Let us outline this proof. In the linear spectrum approximation the charge excitations do not contribute to the considered specific heat. Hence the specific heats of the RL model and s–d model coincide. To find the magnetic susceptibility add to the relevant hamiltonians the Zeeman terms:

$$-H\left(S^z + \sum_{\sigma,k}\frac{1}{2}\sigma^z c_{k\sigma}^+ c_{k\sigma}\right)$$

and

$$-2h\left\{\sum_k (c_k^+ c_k - 1/2) - (d^+d - 1/2)\right\}$$

for the s–d and RL model, respectively. The two Zeeman hamiltonians coincide if $h=\sqrt{2}H$. Hence $\chi_{\mathrm{sd}} = 1/2\chi_{\mathrm{RL}}$.

A further analysis of the perturbation theory in $U$ (Schlottmann 1978 a, b, Wiegmann and Finkelstein 1978), shows that

$$C_{\mathrm{RL}}/T\chi_{\mathrm{RL}} = \pi^2/3.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

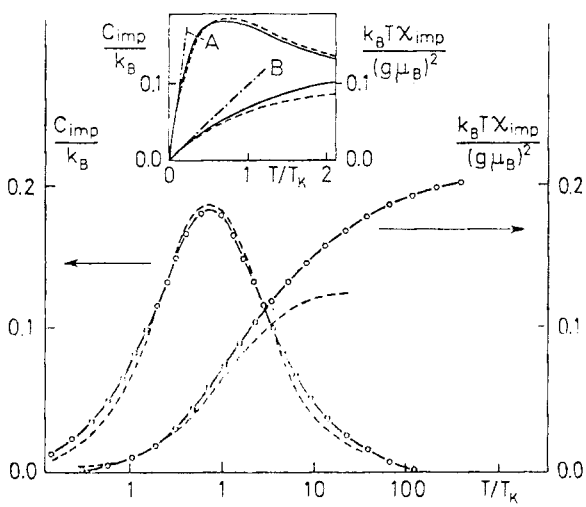
These results in (3.1.19) were first found numerically by Wilson (1975), and then proved analytically by Nozières (1975).

The analysis of the Coulomb gas statistics has led to a first numerical study of s–d model thermodynamics. Schotte and Schotte (1971) used the Monte-Carlo method to compute the temperature dependence of the magnetic susceptibility. They found it to be finite at $T=0$ and very close to the one given by the Curie–Weiss law.

Recently Oliveira and Wilkins (1981) studied the RL model numerically using the Wilson renormalization group approach. The results for the heat capacity and the magnetic susceptibility of the RL model are shown in fig. 3.1. It has been shown that the mapping between the RL model and Kondo model does exist. It has been found numerically by means of the Wilson (1975) numerical solution of the Kondo model (see § 3.1.2). The RL model is found to be more convenient for a numerical investigation. As for the Kondo hamiltonian, a calculation utilizing the RL hamiltonian brings about a hundred-fold reduction in computation time (Oliveira and Wilkins 1981). Note that the specific heat and magnetic susceptibility curves are in excellent agreement with the Toulouse limit (see fig. 3.1). This phenomenon also takes place for the straight calculations of the heat capacity for the Kondo model (Melnicov 1982, Rajan *et al.* 1982, Desgranges and Schotte 1982) and accounts for the success of the attempts by Schotte and Schotte (1975). They have used the generalized Toulouse hamiltonian for interpretation of some Kondo experiments.

The RL model was the first problem associated with magnetic impurities in a metal to which the Bethe Ansatz was applied (Filyov and Wiegmann 1980). The Bethe Ansatz used in this case is the most simple. The diagonalization procedure of the RL-model hamiltonian is discussed in the supplement section.

Fig. 3.1




The universal curves for the impurity specific heat $C_i$ and the susceptibility $\chi_i$ for the resonant-level model. The dashed lines are the Toulouse limit specific heat and susceptibility for a resonance width chosen to make the zero-temperature Kondo Toulouse limit susceptibilities equal. The inset shows the same plots on a linear temperature scale (after Oliveira and Wilkins 1981)

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

3.1.2. *Numerical renormalization group approach to the Kondo problem*

Wilson (1974, 1975) developed a new formulation of the renormalization group theory which is not based on perturbation theory but requires a computer. Using the modern numerical renormalization approach he treated numerically the crossover between the high-temperature and low-temperature regions. His method has been applied recently to the numerical investigation of other models:

The Anderson model (Krisna-Murthy *et al.* 1975, 1980 a, b).
The orbital degenerative exchange hamiltonian (Cragg *et al.* 1980, Cragg and Lloyd 1979).
The resonance-level model (Oliveira and Wilkins 1981).
Two-impurity problem (Jayaprakash *et al.* 1981).

Without going into details of the computation and accuracy, we confine ourselves only to the conclusions of Wilson.

The reader is referred to the original papers (Wilson 1975), Krishna-Murthy 1980 a, b) for a complete account of the theory. Interesting discussion of Wilson's treatment can be found in Noziéres (1975).

(i) The renormalized spectrum calculated by the renormalization procedure was compared with one corresponding to a similar hamiltonian but without the impurity and a particle in the impurity site. It turns out that these two spectra coincide with great accuracy for the lowest states. This result can be interpreted as follows: the impurity and electron on the impurity site are glued together with the infinite coupling $I_{\text{eff}}=\infty$ to form a singlet. The other electrons behave like a free gas. Thus we have made sure that the strong-coupling limit $I=\infty$ is indeed a fixed point of the Kondo hamiltonian. Having used the numerical procedure Wilson showed that for temperatures much lower than the band edge, and for small antiferromagnetic exchange coupling $I$ the functional dependence of the magnetic susceptibility $\chi_i(T)$ on the temperature and on $I$ can be expressed (see eqn. 2.4.18) as the Gell–Mann–Low equation

$$\Phi(4T\chi_i(T)-1)=\ln(T/T_W(I)), \tag{3.1.20}$$

where $\Phi(y)$ is the universal function of its argument $y$ (i.e. its functional form is independent of $I$, band-edge effects, etc.). The Kondo temperature $T_W$ is defined in terms of the same universal function by

$$T_W(I)=D(I)\exp(-\Phi(I)), \tag{3.1.21}$$

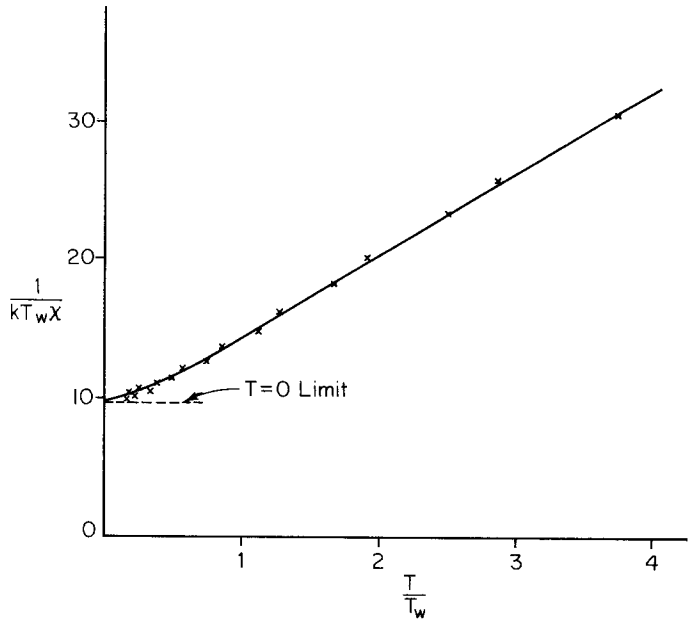
where $D(I)$ is an effective band width $D(I)=\epsilon_F\,\text{const}\,(1+O(I))$ and has a non-universal power-series expansion in $I$. For the small values of argument, $\Phi(y)$ can be obtained from the perturbation theory and is given by

$$\Phi(y)=y^{-1}-\frac{1}{2}\ln|y|+1{\cdot}58\,y+O(y^2). \tag{3.1.22}$$

The first two terms in that formula were known (Abrikosov and Migdal 1970, Fowler and Zawadowski 1971), the last term was computed numerically by Wilson.

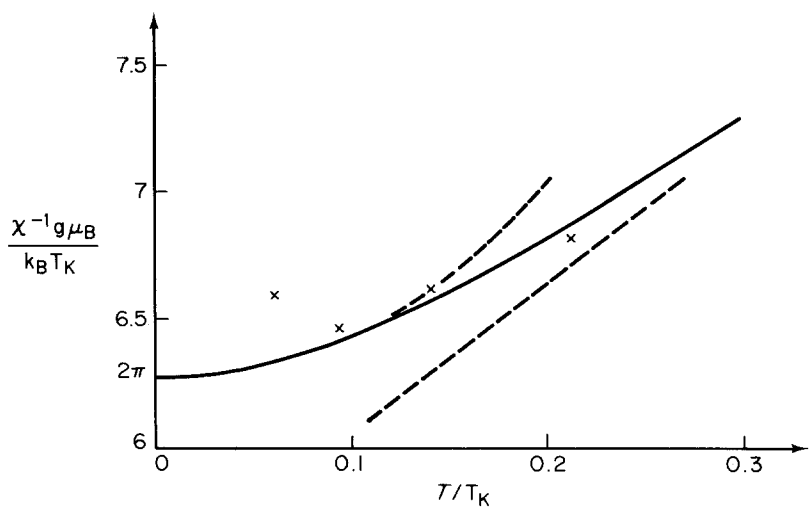
(ii) The magnetic susceptibility has been obtained from rather accurate numerical calculation and is represented in figs. 3.2–3.4. (The full curve in fig. 3.3. is the numerical result obtained by Melnicov (1982 a) from the exact solution (see §6.1.11).

Fig. 3.2




Universal inverse magnetic susceptibility $\chi_i^{-1}(T)$ versus $T$ plot from Wilson's (1975) computer calculations.

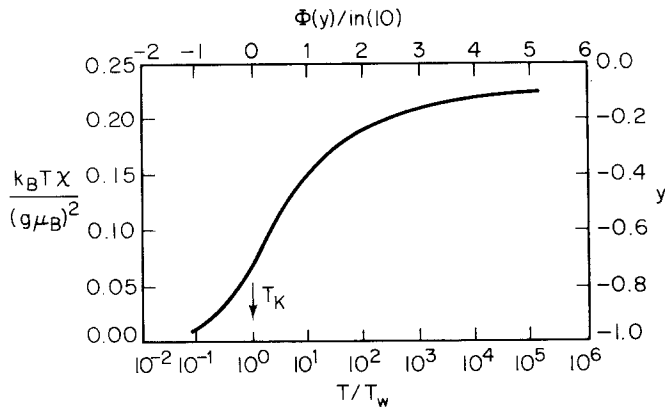
Fig. 3.3




Universal inverse magnetic susceptibility $(g\mu_B)^2 * \chi_i^{-1}(T)$ versus $T$ plot at $T \lesssim T_K$. Crosses correspond to the Wilson (1975) renormalization group results; the full curve is the numerical result obtained on the basis of the exact solution; dashed curves are the asymptotic behaviour of the susceptibility at (see eqn. (6.1.115) or the footnote on p. 503) and the Curie–Weiss interpolation at $0{\cdot}3T_K < T < 10T_K$ (see eqn. (3.1.23)) (after Melnicov 1982 a).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 3.4




Universal $k_B T\chi_i(T)/(g\mu_B)^2$ versus $\ln T/T_W$ plot from Wilson's (1975) computer calculations. At $T=T_W$, $T\chi=0{\cdot}701$. The same plot also served as a graph of the universal function $\Phi(y)$ (see eqn. (3.1.20)) (after Krishna-Murthy *et al.* 1980 a).

(iii) When $T \gtrsim 16\ T_W$ the function $\Phi(y)$ may be determined from its asymptotics (2.2.3). For $0{\cdot}5\ T_W < T < 16\ T_W$ the universal curve fits the Curie–Weiss law

$$\chi_i(T) = 0{\cdot}17(T+\sqrt{2}T_W)^{-1}. \tag{3.1.23}$$

Melnicov (1982 a) noted the fact that in the original paper this formula is written with an error (Wilson 1975), eqn. IX.99); there is a factor 2 in front of $T_W$. This error has been repeated in all the papers known to the authors containing the formula (3.1.23). Applying a ruler to fig. 3.2 one immediately makes sure that the factor in front of $T_W$ must be equal to 1·46. Following the Pythagorean spirit of Wilson's paper we write down $\sqrt{2}$ instead of 1·46 in (3.1.23).

(iv) The susceptibility for $T < T_W$ approaches a constant†

$$\chi_i(T=0) = \frac{0{\cdot}1032}{T_W}. \tag{3.1.24}$$

(v) The ratio of the coefficients of the linear terms in the specific heat and of the susceptibility can be very well fitted by

$$\frac{3}{4\pi^2} \lim_{T\to 0} \frac{C_i(T)}{T\chi_i(T)} = 0{\cdot}5. \tag{3.1.25}$$

The renormalization group calculation of the impurity specific heat for the entire temperature range took a considerably longer computational time than that for the susceptibility. Therefore, to calculate the specific heat of the Kondo model Oliveira

† It is worth showing that the coefficient at $T^2$ in the temperature dependence of magnetic susceptibility computed by Melnicov (1982 a) on the basis of the exact solution is:

$$\chi_i(T<T_K) = \frac{0{\cdot}1032}{T_W}\left(1 - 1{\cdot}14\left(\frac{T}{T_W}\right)^2 + \ldots\right).$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

and Wilkins (1981) employed the renormalization group approach in the resonant-level model (3.1.9) whose partition function maps on to the partition function for the Kondo hamiltonian.

The specific heat shown in fig. 3.1 is a universal function of $T/T_W$ where $T_W$ depends on $V$ and $U$ parameters of the RL model. The specific heat is peaked at $T \simeq 0{\cdot}6\, T_W$.

The numerical procedure relating the RL parameters to the isotropic Kondo-model parameter $I$ used by Oliveira and Wilkins consists of mapping the magnetic Kondo susceptibility on the charge RL susceptibility. Their results are in a good agreement with the straightforward numerical calculations based on the exact solution (Desgranges and Schotte 1982, Melnicov 1982 a, Rajan *et al.* 1982, see § 6.1.11 for a review).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

### 3.1.3. *Nozières' Fermi-liquid theory*

Using the fact that a singlet ground state is formed and in the low-temperature limit the s–d exchange hamiltonian evolves towards a fixed point in which the effective exchange coupling of the impurity and conduction electrons is infinitely strong, Nozières (1974, 1975) proposed an elegant phenomenological theory in the same spirit as the Landau theory of Fermi liquids. On the basis of this theory the low-temperature properties of the specific heat, spin susceptibility and resistivity are derived in a simple way. Having been constructed for the s–d exchange model this theory proved to be very powerful. Later it was generalized for degenerate exchange models with hamiltonians (2.4.7) and (2.4.8) (Nozières and Blandin 1980, Mihaly and Zawadowski 1978).

As we discussed in § 3.1.2, Wilson's results may be interpreted in such a way that in the low-energy limit the interaction tends to infinity and therefore an electron is frozen near the impurity forming a singlet ground state. Other $N-1$ electrons scatter on this composite and polarize it in a virtual way. This polarization leads to the local interaction between trapped electrons.

When $T \ll T_K$ the probability of breaking the singlet is very small and one has the Fermi liquid with interaction concentrated in a point.

In the spirit of the ordinary Landau theory of Fermi liquids one may suppose that the spectrum of the system for the low-temperature region differs slightly from the spectrum of the non-interacting system so that there is a simple correspondence between the eigenstates of the hamiltonian in the fixed point ($I^* = \infty$) and near it.

The most fundamental quantity of Nozières' theory is an elastic-scattering phase. As there is the fixed marked point in the system so the quasiparticles may be characterized by an energy and phase shift $\eta_\sigma$. This quantity depends on the energy of quasiparticle $z$ and the distribution of quasiparticles with a given spin:

$$\eta_\sigma = \eta(z, n_{\sigma'}).$$

Assuming that a spin polarization is along the $\hat{z}$ axis, one may write the phase shift as an expansion:

$$\eta_\sigma(z, \sigma n_{\sigma'}) = \eta_0 - \alpha z + \Phi \delta n_{-\sigma}, \tag{3.1.26}$$

(where $\delta n_\sigma$ is the departure from the ground-state distribution and $z$ is measured from the Fermi level in zero magnetic field). The term with $\delta n_\sigma$ in the expansion (3.1.26) is absent due to the Pauli exclusion principle. From $\eta$, one infers the scattering-state energy, hence the specific heat and the spin susceptibility.

Moreover, $\eta$ yields the resistivity right away. Low-temperature physics thus depends on three parameters only: $\eta_0, \alpha$ and $\Phi$.

These parameters are not independent. Primarily the well-known *Friedel sum rule* says that a scattering phase depends on an impurity spin:

$$\eta_\sigma(z=\delta H)=\pi/2-\sigma\pi M_\sigma \tag{3.1.27}$$

(we shall derive this formula rigorously in the next section).

It follows from (3.1.27) that if the ground state is a singlet ($M_i(H=0)=0$) the phase shift achieves the unitary limit.

Using (3.1.27) one can derive the Fermi-liquid relation between the phase shift $\eta_\sigma$ and the magnetic and charge susceptibilities:

$$\chi^{\mathrm{i}}_{\mathrm{sp}}=\frac{1}{\pi}\frac{\partial}{\partial H}(\eta_\uparrow-\eta_\downarrow), \tag{3.1.28}$$

$$\chi^{\mathrm{i}}_{\mathrm{ch}}=\frac{1}{\pi}\frac{\partial}{\partial \mu}(\eta_\uparrow+\eta_\downarrow), \tag{3.1.29}$$

where $\mu$ is a chemical potential. Comparing formulae (3.1.26–3.1.29) we obtain

$$\chi^{\mathrm{i}}_{\mathrm{sp}}=\frac{1}{\pi}(\alpha+\rho\Phi), \tag{3.1.30}$$

$$\chi^{\mathrm{i}}_{\mathrm{ch}}=\frac{1}{\pi}(\alpha-\rho\Phi), \tag{3.1.31}$$

where $\rho$ is the density of state.

When $T_{\mathrm{K}}\ll\epsilon_{\mathrm{F}}$ the Kondo resonance is attached to the Fermi level $\mu$ and must move rigidly with $\mu$. Put another way, if one moves $\mu$ and the energy $z$ by the same amount the phase shift must be invariant and therefore we obtain

$$\chi^{\mathrm{i}}_{\mathrm{ch}}=0.$$

That gives

$$\alpha=\rho\Phi. \tag{3.1.32}$$

Substituting (3.1.32) into the expression for magnetic susceptibility we obtain

$$\chi^{\mathrm{i}}_{\mathrm{sp}}/\chi^{\mathrm{h}}_{\mathrm{sp}}=2\alpha/\pi\rho. \tag{3.1.33}$$

For the specific heat $C$, the change of occupation $\delta n_\sigma$ due to a temperature increase is zero: the increment due to the impurity is given by

$$C^{\mathrm{i}}/C^{\mathrm{h}}=\alpha/\pi\rho. \tag{3.1.34}$$

On combining (3.1.33) and (3.1.34) we finally obtain Wilson's result (3.1.25).

Except for this simple result the phenomenological theory predicts the low-temperature behaviour of resistivity (Nozières 1974):

$$R(T)=R_0(1-(\alpha\pi T)^2+O(T^4)), \tag{3.1.35}$$

where $R_0=3/\pi\rho^2v_{\mathrm{F}}^2e^2$ is the unitary limit. We do not consider this remarkable derivation as it does not yet have an analogy in the exact solution framework.

The Fermi-liquid theory has been successfully applied to systems described by hamiltonians (2.2.7) and (2.2.8). We first consider hamiltonian (2.2.8) in the absence

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

of crystal field effects. The phase shift must be invariant under rotations of the total angular momentum (3.1.21) and is thus replaced by

$$\eta_j(z)=\eta_0-\alpha z+\Phi\sum_{j'\neq j}\delta n_{j'}. \tag{3.1.36}$$

In order to dispose of the parameters $\alpha$ and $\Phi$, we make use of our universality requirement. Universality requires that $\eta$ be invariant if the energy $z$ and all chemical potentials move by the same amount. That condition yields

$$\alpha-(n-1)\rho\Phi=0, \tag{3.1.37}$$

where $\rho$ is the density of states per channel. The impurity part of the heat capacity is

$$C^{\mathrm{i}}/C^{\mathrm{h}}=\alpha/\pi\rho. \tag{3.1.38}$$

In order to calculate the magnetic susceptibility we again use the Friedel sum rule

$$\eta_j(z=jH)=\pi n_j, \tag{3.1.39}$$

where $n_j$ is the number of particles with $j$th projection of the total angular momentum.

If the impurity magnetism vanishes eqn. (3.1.39) yields

$$n_j=1/n; \qquad \eta_0=\pi/n \tag{3.1.40}$$

and

$$\chi^{\mathrm{i}}/\chi^{\mathrm{h}}=\frac{\alpha}{\pi}\frac{n}{n-1}. \tag{3.1.41}$$

Now the Wilson ratio is

$$\frac{(C^{\mathrm{i}}/C^{\mathrm{h}})}{(\chi^{\mathrm{i}}/\chi^{\mathrm{h}})}=\frac{n-1}{n} \tag{3.1.42}$$

(Nozières and Blandin 1980). We obtain this relation using the exact solution (see § 7).

Hamiltonian (2.2.7) is a more complex case. It is invariant under spin and orbital rotation. If the spin distribution is polarized in the $\hat{z}$ direction the most general form of the scattering phase is

$$\eta_{m\sigma}(z)=\eta_0-\alpha z+\sum_{m'\neq m}\{(\varphi+\psi)\delta n_{m'\sigma}+(\varphi-\psi)\delta n_{m',-\sigma}\}+(\varphi-3\psi)\delta n_{m,-\sigma}. \tag{3.1.43}$$

The terms containing $\delta n_{m'\sigma}$ are absent as before.

*Weak* universality requires that $\eta$ be invariant if the energy $z$ and all chemical potentials move by the same amount. That condition yields

$$\alpha+\rho(4l\varphi+\varphi-3\psi)=0. \tag{3.1.44}$$

Since scattering never changes $m$, *strong* universality also holds: $\eta_{m\sigma}$ must be unchanged if the Fermi level of another channel is moved. Thus

$$\varphi=0$$

and therefore

$$\alpha=3\psi\rho. \tag{3.1.45}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The Friedel sum rule defines the value of the phase shift on the Fermi level:

$$\eta_{m\sigma}(z=\sigma H)=\frac{\pi}{2(2l+1)}-\alpha H+(4l+3)H\rho\psi \tag{3.1.46}$$

and the magnetic susceptibility

$$\frac{\chi^{\mathrm{i}}}{\chi^{\mathrm{h}}}=\frac{\alpha}{\pi\rho}\frac{2(2l+3)}{3}. \tag{3.1.47}$$

The heat capacity is still equal to

$$\frac{C^{\mathrm{i}}}{C^{\mathrm{h}}}=\frac{\alpha}{\pi\rho}.$$

The Wilson ratio is

$$\frac{(C^{\mathrm{i}}/C^{\mathrm{h}})}{(\chi^{\mathrm{i}}/\chi^{\mathrm{h}})}=\frac{3}{2(2l+3)} \tag{3.1.48}$$

(Yoshimori 1976, Mihaly and Zawadowski 1978, Nozières and Blandin 1980).

Unfortunately, the Fermi-liquid analogy is restricted by a low-temperature limit. For example, it is impossible to evaluate in such a way the $(T/T_{\mathrm{K}})^2$ or $(T/T_{\mathrm{K}})^3$ terms in the expansions of the magnetic susceptibility or specific heat.

## 3.2. *The Anderson model*

### 3.2.1. *Introduction*

In the next subsections we shall discuss recent developments in the Anderson model. There exists a vast literature on the model, which is the generally adopted model for description of different phenomena in dilute magnetic alloys. For the early literature on the model we refer the reader to available review articles (Grüner and Zawadowski 1974, 1978, Blandin 1973, Mills *et al.* 1973). In this section we first consider some approaches developed recently: the Fermi-liquid approach based on the perturbation theory with respect to $U$ (Yamada 1975, Yosida and Yamada 1970, 1975), and the numerical renormalization group approach (Krishna-Murthy *et al.* 1975, 1980 a) to the symmetric Anderson model.

In the past few years many efforts have been made to study rare-earth intermetallics. This interest has been caused by the intermediate valence phenomena (for a review, see Varma 1976, Khomski 1979). Famous examples of systems with intermediate valence are traditional concentrated Sm systems (SmS, SmSe and SmTe). Meanwhile, the valence instability phenomena may also be observed in dilute rare-earth alloys. The modern theory of valence instability in concentrated compounds cannot reveal the relative role of single-ion effects against the interaction between impurity centres.

In such a situation microscopic investigations of the single-ion behaviour of a mixed-valence impurity were highly desirable both theoretically and experimentally. The valence instability phenomena in dilute rare-earth systems is conventionally described by the asymmetric Anderson model. This model has been intensively studied from the middle of the 1970s. The distinctive features of the asymmetric limit of the Anderson model have been found (Varma and Yafet 1976, Barabanov

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

*et al.* 1974, Haldane 1978 a). We shall discuss the main properties of the asymmetric Anderson model below.

The non-degenerate Anderson hamiltonian has the form

$$\mathscr{H}_{\mathrm{A}}=\sum_{k,\sigma}\epsilon_k c_{k\sigma}^{+}c_{k\sigma}+V\sum_{k,\sigma}(c_{k\sigma}^{+}d_\sigma+d_\sigma^{+}c_{k\sigma})+\epsilon_d(n_\uparrow+n_\downarrow)+Un_\uparrow n_\downarrow, \tag{3.2.1}$$

where $n_\sigma=d_\sigma^{+}d_\sigma$ is the particle number operator.

We start with a brief summary of various results that have so far been obtained for the Anderson model. There are five different regimes for different relations between temperature, $\Gamma$ and the energies $E_+=\epsilon_d+U$ and $E_-=-\epsilon_d$:

(A) *Free-atom regime*

$$E_+, E_- \gg \Gamma \gg T.$$

All four states with $n_d=0, \uparrow, \downarrow, 2$ are almost independent and the dominant part of the impurity susceptibility is given by

$$\chi_{\mathrm{i}}=\frac{1}{2T}(2+\exp(\epsilon_d/T)+\exp(-(\epsilon_d+U)/T))^{-1}.$$

(B) *Local-moment regime*

$$E_+, E_- \gg \Gamma, \qquad (U\Gamma)^{1/2}\exp\left(\frac{\pi\epsilon_d(\epsilon_d+U)}{2U\Gamma}\right)\ll T\ll T_0\equiv\min\left(\sqrt{(2U\Gamma)},\frac{\epsilon_d U}{\epsilon_d+2U}\right).$$

In this regime only two states with $n_d=\uparrow,\downarrow$ are available and the Kondo screening phenomenon is depressed by a sufficiently high temperature. The magnetic susceptibility is $\chi_{\mathrm{i}}=1/4T$.

(C) *Strong-coupling regime*

$$E_+, E_- \gg \Gamma, \qquad T\ll(U\Gamma)^{1/2}\exp\left(\frac{\pi\epsilon_d(\epsilon_d+U)}{2U\Gamma}\right).$$

In this region the Kondo phenomenon takes place. The susceptibility is predominantly constant, which in this case has the value

$$\chi_{\mathrm{i}}=\frac{1}{2(2U\Gamma)^{1/2}}\exp\left[-\frac{\pi\epsilon_d(\epsilon_d+U)}{2U\Gamma}\right].$$

(D) *The non-magnetic regime*

$$T\ll T_0, \qquad \Gamma\gg U.$$

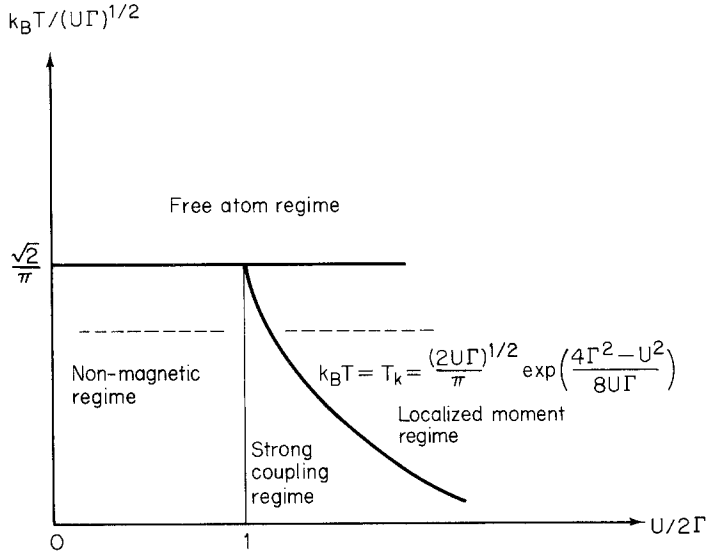
The interaction is small and the impurity behaves as the resonance level with width $\Gamma$. The magnetic susceptibility is

$$\chi_{\mathrm{i}}=\frac{2}{\pi}\frac{\Gamma}{\epsilon_d^2+\Gamma^2}.$$

The various regimes for the symmetric Anderson model are illustrated in fig. 3.5.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 3.5




Schematic sketch of the various regimes for the symmetric Anderson model. The separations between the various regimes, in contrast to the drawing, are actually quite fuzzy. The dashed line corresponds to the temperature at which the Anderson (1961) Hartree–Fock approach to the formation of a localized moment is qualitatively valid.

All these regimes are typical for the symmetric ($\epsilon_d \simeq -U/2$) as well as for the *asymmetric* models. In the latter case there is, additionally,

(E) *Valence-fluctuating regime*

$$\Gamma \gtrsim |\epsilon_d|, \qquad T \ll U.$$

In this case the states with different occupation $n_d = 0$ and $n_d = 1$ are strongly mixed, the state $n_d = 2$ being virtual. For $T \gg \Gamma$ we obtain $\chi_i = 1/6T$ and for $T \ll \Gamma$

$$\chi_i \sim \Gamma / \{\max(|\epsilon_d|, \Gamma)\}^2.$$

We discuss all enumerated regimes in detail below (§ 8).

### 3.2.2. *The Symmetric Anderson model*

We start with the magnetic regime $U \gg \Gamma$, when there are no real transitions into states with $n_d = 0$; 2 and a magnetic moment arises. This magnetic moment interacts with conduction electrons through the virtual transitions into excited states with $n_d = 0$; 2. The interaction is described by exchange hamiltonian (I) with the coupling constant

$$\rho(\epsilon_F) I = -8\Gamma/\pi U$$

(Anderson and Clogston 1962, Schrieffer and Wolf 1966) and leads to the Kondo effect. Consequently the impurity magnetism and $T\chi$, where $\chi$, the magnetic susceptibility, decrease and vanish as $T \to 0$. If $U \ll \epsilon_F$ the states $n_d = 0$ and $n_d = 2$ decouple from the local-moment for energies larger than $U$ and, therefore, one

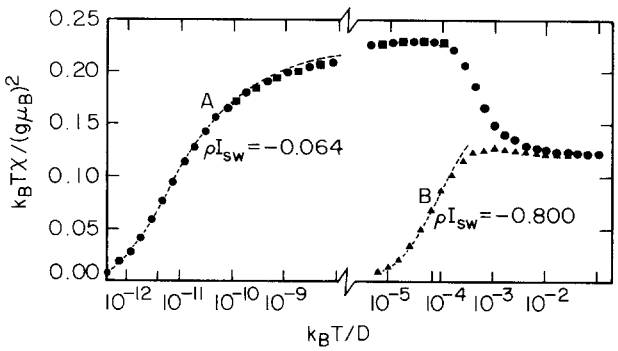
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

should consider the amplitude $U$ as a cut off for the low-energy processes. According to (2.4.19) and (2.4.22) one has the expression for the Kondo temperature

$$T_K \sim U(\rho I)^{1/2} \exp(-1/\rho I) \sim (\Gamma U)^{1/2} \exp(-\pi U/8\Gamma).$$

The mapping between the symmetric Anderson model and the Kondo model has been illustrated by means of Wilson's numerical renormalization group approach to the impurity susceptibility. It was applied by Krishna-Murthy *et al.* (1980 a) to the calculation of the magnetic susceptibility in various regimes in the Anderson model. Their numerical results are depicted in fig. 3.6.

Fig. 3.6




Plots $T\chi_i$ versus $\ln T/D$ on the symmetric Anderson model with parameters $\rho I = 0{\cdot}064$ (A), $0{\cdot}800$ (B), $U/\epsilon_F \simeq 10^{-3}$, $U/\pi\Gamma = 12{\cdot}66$ (A), $1{\cdot}013$ (B). The dashed curves are the universal Kondo susceptibility curves. The Kondo temperature is marked by an arrow on the abscissa. For $U \gg \Gamma$ (A) there is a well-developed local-moment regime ($T\chi \simeq 1/4$) between the free-orbital regime ($T\chi \simeq 1/8$) and the strong-coupling regime ($\chi = \text{const.}$), whereas for $U \sim \Gamma$ (B) there is a direct transition from the free-orbital to strong-coupling regime (after Krishna-Murthy *et al.* 1980 a).

The numerical correspondence between the Anderson and Kondo models gives the Kondo temperatures $T_K(U, \Gamma)$ for the relevant $U$ and $\Gamma$. These temperatures are indicated by the arrows in fig. 3.6. Having compared them the pre-exponential factor in the expression for Kondo temperature was obtained (Haldane 1978 b)†:

$$T_W = 0{\cdot}182 U(\rho I)^{1/2} \exp(-1/\rho I), \tag{3.2.2}$$

(remember that the definition of $T_W$ differs from that taken in the present review: $T_W = 0{\cdot}1032 \times 2\pi T_K$). As the temperature increases above $T_0$ the states with $n_d = 0{\cdot}2$ decouple. In a symmetric case this occurs at $T_0 \sim (U\Gamma)^{1/2}$ (Wiegmann *et al.* 1982); above this temperature the impurity is in the free-atom regime.

At $U \gg \Gamma$ and $T \gg T_K$ there is a wide region where a local-moment regime takes place: $T\chi_i \simeq 1/4$ at $T_K \ll T \ll (U\Gamma)^{1/2}$. At $T \gg U$ the impurity passes into the free-orbital regime where all impurity configurations are equally populated and the couplings between them are irrelevant. The transition from local-moment regime into a free-orbital one in which $T\chi_i \simeq 1/8$ is illustrated by fig. 3.6.

† The amplitude $U$ is customarily believed to be an energy cut-off.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

At $U \sim \Gamma$ the local-moment region vanishes (see fig. 3.5) and on being heated the system passes continuously from the strong-coupling regime to the free-orbital one. Finally, at $U < \Gamma$ the non-magnetic regime with $\chi_i \sim 1/\Gamma$ takes place.

The transition from the non-magnetic to the local-moment regime was first predicted by Anderson in his classical work in 1961 on the basis of the Hartree–Fock approximation. This theory qualitatively describes the situation only at high temperatures $T_K < T \lesssim (U\Gamma)^{1/2}$.

We shall come back to this discussion in § 8 where the dependence of magnetic susceptibility on $U/\Gamma$ and magnetic field derived from the exact solution will be discussed.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

### 3.2.3. *The Fermi-liquid approach, based on the perturbation theory in the Anderson model*

Besides the Nozières theory, another powerful approach based on the Fermi-liquid theory has been developed by Yosida and Yamada (Yosida and Yamada 1970, 1975) and Yamada (1975). It is based upon using the Fermi-liquid identities for analysis of perturbation series with respect to $U$ in the Anderson model and is a remarkable illustration of Nozières' phenomenological picture. The Anderson model has proved to be convenient due to the fact that the behaviour of all quantities is Fermi-liquid-like to all orders of the perturbation theory with respect to $U$. The first papers by Yamada and Yosida were devoted to the symmetric non-degenerate Anderson model. Subsequently their method has been extended to treatment of the impurity orbital shell by Yoshimori (1976) and Yoshimori and Zawadowski (1982). At low temperatures and frequencies the basic physical quantities may, in the spirit of the Fermi-liquid theory, be expressed through the self-energy part of $d$ electrons. The Fourier-transform of the $d$-electron Green function is defined in a standard way:

$$G_\sigma(\omega_n) = -\int_0^{1/T} d\tau \langle \hat{T} d_\sigma(\tau) d_\sigma^+(0) \rangle \exp(i\omega_n \tau)$$

and may be written as follows

$$G_\sigma(\omega_n) = (i\omega_n - \epsilon_d + \sigma H + i\Gamma \operatorname{sign} \omega_n - \Sigma_\sigma(\omega_n))^{-1},$$

where $\Gamma = \pi\rho(\epsilon_F)V^2$ is the width of the virtual impurity level, $\omega_n = (2n+1)\pi T$.

Using $G(\omega_n)$ one can express the impurity part of free energy as

$$F_i = T\sum_n \exp(i\omega_n \varepsilon) \ln G_\sigma(\omega_n) \qquad \varepsilon \to +0. \tag{3.2.3}$$

Expanding the function $\ln G_\sigma(\omega_n)$ near the singular point $\omega_n = 0$ one obtains the formula for the impurity heat capacity at $T \to 0$:

$$\frac{C_i}{T} = \frac{2\pi}{3} \sum_\sigma \operatorname{Im} G_\sigma(+i0) \left( 1 - \left. \frac{\partial \Sigma_\sigma(i\omega)}{\partial i\omega} \right|_{\omega = +0} \right), \tag{3.2.4}$$

where $\Sigma(i\omega)$ is an analytical continuation of the function $\Sigma(\omega_n)$.

Another relation which relates the magnetic susceptibility to the self-energy $\Sigma$ is based on the Friedel sum-rule

$$n_\sigma = \frac{1}{\pi} \operatorname{Im} \ln G_\sigma(+i0). \tag{3.2.5}$$

Thus, the impurity magnetic and charge susceptibilities have the form:

$$\chi_{\mathrm{sp}} = -\frac{1}{2\pi}\sum_{\sigma}\sigma\,\mathrm{Im}\,G_{\sigma}(+i0)\frac{\partial\Sigma_{\sigma}(+i0)}{\partial H} \tag{3.2.6}$$

$$\chi_{\mathrm{ch}} = -\frac{1}{\pi}\sum_{\sigma}\mathrm{Im}\,G_{\sigma}(+i0)\frac{\partial\Sigma_{\sigma}(+i0)}{\partial\epsilon_d}. \tag{3.2.7}$$

Relations analogous to (3.2.4) and (3.2.6) takes place in the ordinary Fermi-liquid theory (see, for example, Abrikosov *et al.* 1965). They follow from only the energy conservation law and, therefore, are still valid for nonhomogeneous systems.

The scattering $T$ matrix and, therefore, the electrical resistivity can easily be connected with the same function $G(i\omega)$. Indeed, the conduction electron Green function has the form

$$G_{kk'}(i\omega) = \delta_{kk'}G_k^{(0)}(i\omega) + V^2 G_k^{(0)}(i\omega)G(i\omega)G_{k'}^{(0)}(i\omega).$$

Therefore, $T_{\sigma}(\omega) = V^2 G_{\sigma}(i\omega)$ and using (3.2.5) one obtains

$$1 - 2\pi i T_{\sigma}(\omega) = (1 + 4\,\mathrm{Im}\,\Sigma_{\sigma}(\mathrm{i}\omega)/\Gamma)^{1/2}\exp(-2\pi i\eta_{\sigma}(\omega)), \tag{3.2.8}$$

where $\eta_{\sigma}(\omega)$ is a phase shift introduced in the usual way

$$\eta_{\sigma}(\omega) = \pi/2 - \tan^{-1}(\Sigma_{\sigma}(i\omega)/\Gamma)$$

(see, for example, Langreth 1966). Using eqn. (3.2.5) one gets the Friedel sum rule:

$$n_{d_{\sigma}} = \langle d_{\sigma}^{+} d_{\sigma}\rangle = \frac{1}{\pi}\eta_{\sigma}(0). \tag{3.2.9}$$

The conductivity $\sigma(T)$ of the system is given by the following well-known expression

$$\sigma(T) = \sigma_0 \int_{-\infty}^{+\infty} d\omega\, \tau(\omega)/2\cosh\omega/T. \tag{3.2.10}$$

$\tau^{-1}(\omega) = -2\,\mathrm{Im}\,T(\omega)$ ($\sigma_0$ is the value of $\sigma(T)$). In the saturated unitarity limit the formula for the magneto-resistance at $T=0$ according to (3.2.8)–(3.2.10) has the form (Sakurai and Yosida 1979):

$$R(H) = \frac{R_0}{2}\frac{(\cos\pi n_d - \cos 2\pi M_i)^2}{1 - \cos\pi n_d \cos 2\pi M_{\mathrm{i}}}, \tag{3.2.11}$$

where $n_d = \Sigma_{\sigma} n_{d_{\sigma}}$ is the average number of localized electrons. This formula generalizes the well-known formula (Ishii 1970):

$$R(H) = R_0 \cos^2 \pi M_{\mathrm{i}}, \tag{3.2.12}$$

which we have in the symmetric Anderson model ($n_d = 1$).

Using the general properties of perturbation series it is easy to prove that $\mathrm{Re}\,\Sigma(i\omega)$ is an odd function of $\omega$, $T$ and $\mathrm{Im}\,\Sigma(i\omega)$ is an even function, $\mathrm{Im}\,\Sigma(0)$ being equal to zero.

To find the term of order of $T^2$ in the expansion of conductivity it is sufficient to keep the terms of order of $\omega^2$ and $T^2$ in the expression for $\mathrm{Im}\,T(\omega, T)$. Since $\mathrm{Re}\,\Sigma(i\omega) \sim \omega$, $\mathrm{Im}\,\Sigma(i\omega) \sim \omega^2$, $T^2$ eqn. (3.2.8) is written down for low frequencies and low temperatures as

$$1 - 2\pi i T(\omega) = -(1 + 2\,\mathrm{Im}\,\Sigma(i\omega)/\Gamma)\exp(2i(\omega - \mathrm{Re}\,\Sigma(i\omega)).$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The imaginary part of the phase shift $\operatorname{Im}\Sigma/\Gamma$ represents contributions from inelastic channels.

The electrical resistivity has the following form:

$$R(T)=\frac{1}{\operatorname{Im}G(0)}-\frac{\pi^2T^2}{3}\operatorname{Im}G(0)\left[\left(1-\frac{\partial\Sigma}{\partial i\omega}\right)^2+\frac{\partial^2\Sigma}{\partial(i\omega)^2}+\pi^2\frac{\partial^2\Sigma}{\partial T^2}\right]\Bigg|_{\omega=0} \tag{3.2.13}$$

The formulae (3.2.4)–(3.2.6) and (3.2.13) are valid for the symmetric Anderson model in the presence of the magnetic field. Yamada calculated many quantities up to the fourth order of perturbation theory expansion in powers of $U/\Gamma$ in the symmetric Anderson model (see Yamada 1975). We list here several terms of the perturbation expansion for magnetic susceptibility:

$$\chi_{\mathrm{sp}}=\frac{1}{2\pi\Gamma}\left[1+\frac{U}{\pi\Gamma}+\left(3-\frac{\pi^2}{4}\right)\left(\frac{U}{\pi\Gamma}\right)^2+0{\cdot}0553\left(\frac{U}{\pi\Gamma}\right)^4+\ldots+3\left(5-\frac{\pi^2}{2}\right)\left(\frac{U}{\pi\Gamma}\right)^3+\ldots\right]. \tag{3.2.14}$$

By investigating the general terms in the perturbation expansions of thermodynamical quantities, some important relations among the magnetic and charge susceptibilities and self-energy part $\Sigma(i\omega)$ of the thermal Green function have been found by Yosida and Yamada (1970, 1975) and by Yamada (1975). These relations are simple consequences of the Ward indentities for the expansion of the self-energy and can be written in the following compact form:

$$\Sigma(i\omega)=-\omega\left(\tilde{\chi}_{\mathrm{even}}\left(\frac{U}{\Gamma}\right)-1\right)-\frac{i\Gamma}{2}\tilde{\chi}^2_{\mathrm{odd}}\left(\frac{U}{\Gamma}\right)\left(\frac{\omega^2}{\Gamma^2}+\frac{\pi^2T^2}{\Gamma^2}\right), \tag{3.2.15}$$

where $\tilde{\chi}_{\mathrm{even}}(U/\Gamma)$ and $\tilde{\chi}_{\mathrm{odd}}(U/\Gamma)$ are the even and odd parts of the normalized susceptibility at $T=0$, respectively. They are related to the magnetic and charge susceptibilities:

$$\chi_{\mathrm{sp}}=\frac{1}{2\pi\Gamma}(\tilde{\chi}_{\mathrm{even}}+\tilde{\chi}_{\mathrm{odd}}),$$

$$\chi_{\mathrm{ch}}=\frac{1}{2\pi\Gamma}(\tilde{\chi}_{\mathrm{even}}-\tilde{\chi}_{\mathrm{odd}}).$$

In other words, the quantities $\tilde{\chi}_{\mathrm{even}}$ and $\tilde{\chi}_{\mathrm{odd}}$ are the sums of diagrams of either even or odd order with respect to $U$. Thus the self-energy shows features characteristic of the Fermi-liquid theory. Using the eqns. (3.2.4), (3.2.6), (3.2.7) and (3.2.15) we obtain the well-known Fermi-liquid-like relationship between the low-temperature specific heat and magnetic and charge susceptibilities

$$\lim_{T\to 0}\frac{C_{\mathrm{i}}}{T}=\frac{2\pi^2}{3}(\chi_{\mathrm{sp}}+\chi_{\mathrm{ch}}).$$

Or, constructing the ratio:

$$\frac{3}{4\pi^2}\lim_{T\to 0}\frac{C_{\mathrm{i}}}{T\chi_{\mathrm{sp}}}=\frac{1}{2}\left(1+\frac{\chi_{\mathrm{ch}}}{\chi_{\mathrm{sp}}}\right). \tag{3.2.16}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Comparing eqns. (3.2.13) and (3.2.15) one obtains the expression for resistivity (Yamada 1975, Yosida and Yamada 1975):

$$R=R_0\left[1-\frac{\pi^2}{3}\left(\frac{T}{\Gamma}\right)^2(2\tilde{\chi}^2_{\text{odd}}+\tilde{\chi}^2_{\text{even}})+O(T^4)\right], \tag{3.2.17}$$

where $R_0$ is the unitary limit.

These relationships should be complemented by the Korringa relation for the impurity–nuclear spin-lattice relaxation at low temperature and magnetic field which is equivalent to

$$\lim_{\omega\to 0}\left[\frac{1}{\omega}\operatorname{Im}\chi_{\text{sp}}(\omega+i0)\right]=\frac{\chi^2_{\text{sp}}(0)}{\pi}, \tag{3.2.18}$$

where $\chi_{\text{sp}}(\omega)$ is the frequency-dependent impurity magnetic susceptibility (Shiba 1975). When $U\to 0$ $\tilde{\chi}_{\text{odd}}$ vanishes ($\chi_{\text{ch}}=\chi_{\text{sp}}$) and the ratio (3.2.16) coincides with the Fermi-liquid value. The following simple and elegant speculation (Yamada (1975)) enables us to derive the ratio $C_{\text{i}}/T\chi_{\text{sp}}$ for $U/\Gamma$, $(\epsilon_d+U)/\Gamma\to\infty$. In this region there is a localized moment and therefore the charge fluctuations vanish:

$$\lim_{U,\epsilon_d+U\to\infty}\chi_{\text{ch}}(U,\epsilon_d)=0.$$

Thus the ratio $C_{\text{i}}/T\chi_{\text{sp}}$ differs from that of the Fermi-liquid theory by a factor of 2 (Wilson 1975, Nozières 1975). In a quite analogous way we obtain the result for the electrical resistivity which coincides with that of Nozières' theory (Yosida and Yamada 1975, Yamada 1975):

$$R=R_0(1-(\pi T\chi_{\text{sp}})^2). \tag{3.2.19}$$

To illustrate this phenomenon as well as the transition from the non-magnetic to the strong-coupling regime we exhibit the exact expressions for the charge and magnetic susceptibilities and impurity part of the ground-state energy:

$$\chi_{\text{ch}}=\frac{1}{2(2U\Gamma)^{1/2}}\int_{-\infty}^{+\infty}\exp(-\pi k^2/2U\Gamma)\Delta(k)\,dk, \tag{3.2.20}$$

(Kawakami and Okiji 1982 c);

$$\chi_{\text{sp}}=\frac{1}{2(2U\Gamma)^{1/2}}\left[\exp\left(\frac{\pi(U^2-4\Gamma^2)}{8U\Gamma}\right)+\int_{-\infty}^{+\infty}\exp(-\pi k^2/2U\Gamma)\Delta(ik)\,dk\right],$$

(Wiegmann *et al.* 1982, Kawakami and Okiji 1982 c);

$$E_{\text{i}}^{(0)}=-\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{i\omega+0}\,\frac{1}{1+\exp(|\omega|)}\int_{-\infty}^{+\infty}\exp(i\omega k^2/2U\Gamma)\,\Delta(k)\,dk,$$

(Kawakami and Okiji 1982 a).

$$\Delta(k)=\frac{1}{\pi}\,\frac{\Gamma}{(k+U/2)^2+\Gamma^2}.$$

The integrals in (3.2.20) are bounded functions of $U/\pi\Gamma$ and determine the terms of perturbation expansion with respect to $U$. It is easy to check that they coincide

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

with four first terms (3.2.13) calculated by Yamada (1975). At $U \to \infty$ both integrals vanish and we have

$$\chi_{ch} = 0, \qquad \chi_{sp} = 1/2\pi T_K, \tag{3.2.21}$$

where in the symmetrical case the Kondo temperature is

$$T_K = \frac{(2U\Gamma)^{1/2}}{\pi} \exp(-\pi U/8\Gamma) \tag{3.2.22}$$

and coincides with the numerical expression (3.2.2).

The magnetic and charge susceptibilities, heat capacity, the ratio $T\chi_{sp}/C_i$ and the ground-state energy as function of $U/\Gamma$ are represented in figs. 3.7 and 3.8.

The Yamada–Yosida theory has been generalized for the orbital degenerate case. In the limit of the half-filled shell for the exchange hamiltonian (2.4.7) the relation (3.1.48) and the coefficient of $T^2$ terms in the electrical resistivity has first been obtained in (Yoshimori 1976)

$$R = R_0 \left( 1 - (\pi T \chi_{sp})^2 \left( \frac{8n+1}{n^2(n+2)^2} \right) \right); \qquad n = 2l+1$$

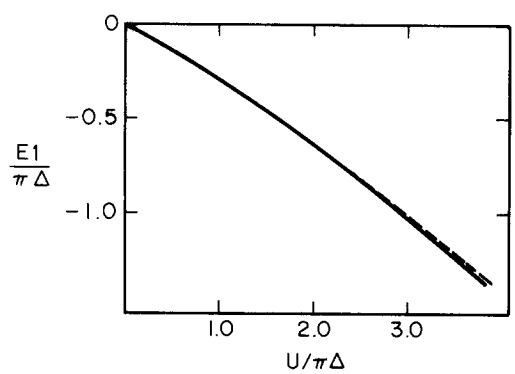
(see also the proof of the Korringa relation (Yoshimori and Zawadowski 1982)).

Unfortunately, one cannot go further either in this elegant framework or in that of Nozières' theory. For instance, the coefficient of the $T^2$ term in the magnetic susceptibility expansion is apparently not obtainable using this method. This is obvious as the Fermi-liquid analogy holds only at $T \to 0$.

### 3.2.4. *Properties of the asymmetric Anderson model*

In the asymmetric limit $\Gamma, |\epsilon_d| \ll U$ all transitions into the state with $n_d = 2$ are suppressed. Therefore, only states with $n_d = 0$ and $n_d = 1$ are mixed. In this limit

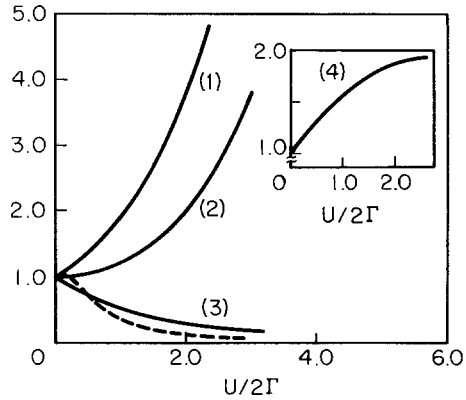
Fig. 3.7




Plots of the ground-state energy $(E^{(0)}(U) - E^{(0)}(0))/\Gamma$ versus $U/\Gamma$ for the symmetric Anderson model. The dashed line represents the perturbation-theory result up to the fourth order in $U/\Gamma$ (after Kawakami and Okiji 1982 a).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 3.8




Plots of the magnetic $\Gamma\pi\chi_s/(g\mu_B)^2$ and charge $\pi\Gamma\chi_c$ (3) susceptibilities, the specific heat $\pi\Gamma C_i/k_BT$ (2), and the ratio $\chi_s k_B T/C_i(g\mu_B)^2$ (4) for the symmetric Anderson model (expressions (3.2.20)). The dotted line represents the second-term of expression (3.2.20 *b*) (after Kawakami and Okiji 1982 c).

Anderson's hamiltonian can be studied using the perturbation theory with respect to $\Gamma$. It is convenient to choose another basis of states in which the hamiltonian

$$\mathscr{H}_{\text{atom}} = \sum_{\sigma=\uparrow,\downarrow} \epsilon_d n_{d_\sigma} + U n_\uparrow n_\downarrow + \frac{H}{2}(n_{d_\uparrow} - n_{d_\downarrow}) \tag{3.2.23}$$

is diagonal.

Stasük and Slobodyan (1974), Zaitsev (1976, 1977) and Haldane (1978 b) constructed the special diagram techniques which use the Green functions of the atomic hamiltonian (3.2.23). This technique greatly simplifies when $U \to \infty$. The following results have been obtained using the perturbation procedure mentioned.

Straightforward calculations yield the following expression for the magnetic susceptibility:

$$\chi = \chi_0\left(1 + \frac{\Gamma}{\pi\epsilon_d} + 2\left(\frac{\Gamma}{\pi\epsilon_d}\right)^2 \ln\frac{\max(|\epsilon_d|; T)}{T} + \dots\right)$$
$$+ \frac{d\chi_0}{d\epsilon_d}\frac{\Gamma}{\pi}\ln\frac{U}{\max(T, |\epsilon_d|)} + \frac{1}{2}\frac{d^2\chi}{d\epsilon_d^2}\frac{\Gamma}{\pi}\left(\ln\frac{U}{\max(T, |\epsilon_d|)}\right)^2 + \frac{2\Gamma}{\pi\epsilon_d^2}K + \dots,$$

where

$$\chi_0 = (2T(\exp(\epsilon_d/T) + 2))^{-1}; \quad K = (1 + \exp(-\epsilon_d/T)/(1 + 2\exp(-\epsilon_d/T);$$

Therefore at sufficiently small $\Gamma \ll \max(T, |\epsilon_d|)$ the corrections of the order of $(\Gamma/\max(T, |\epsilon_d|)\ln(\max(T, |\epsilon_d|))/U$ may be large and one should sum the leading logarithmic terms as well as the Kondo effect. Hence, a new feature characteristic of the asymmetric case: the position $\epsilon_d$ of the level is replaced by an effective temperature-dependent impurity orbital energy

$$E_d(T) = \epsilon_d + \frac{\Gamma}{\pi}\ln\frac{U}{\max(\epsilon_d, T)} \tag{3.2.24}$$

(Barabanov *et al.* 1974, Haldane 1978 a, Tsvelick and Barabanov 1978).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The simplest way to be convinced of this is to consider corrections to the impurity ground-state energy. The first-order perturbation theory diagrams of fig. (3.9 a, b) give

$$E_d(T)=\epsilon_d-V^2\left(\sum_{k>0}\frac{n(\epsilon_k)}{\epsilon_k-\epsilon_d}-2\sum_{k<0}\frac{1-n(\epsilon_k)}{\epsilon_k-\epsilon_d}\right)$$
$$\simeq\epsilon_d+\frac{\Gamma}{\pi}\ln\frac{U}{\max(T,\epsilon_d)}. \tag{3.2.25}$$

The summation through $k$ should be performed in the region of energies smaller than $U$ if $U\ll D$ ($D$ is the bandwidth). At such energies the state with $n_d=2$ decouples. Further, we shall assume $U\ll D$. However, if $D\ll U$ a cut-off should be chosen equal to the bandwidth.

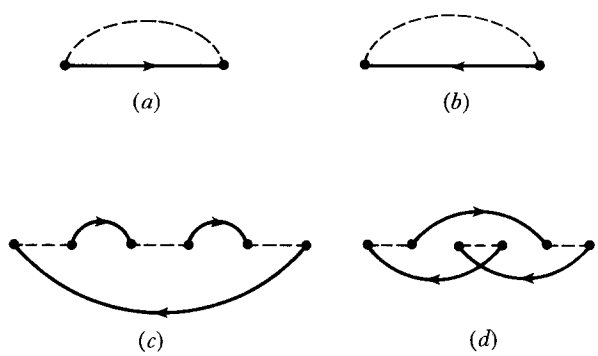
The cause of the above strong renormalization is that the state $n_d=0$ can mix with two states $n_d=\uparrow,\downarrow$, while the state $n_d=1$ only hybridizes with $n_d=0$ (because it decouples). That is the source of the factor '2' in eqn. (3.2.25).

At $U\to\infty$ in the asymmetric Anderson model there is one dimensionless parameter $\Gamma/\epsilon_d$, $U$ being a high-energy cut-off. The symmetric Anderson model is logarithmically renormalized.

The summation of leading logarithms in the ground-state energy expansion corresponds to taking into account the diagram depicted in fig. 3.9 (*c*). The diagram fig. 3.9. (*d*) is less dominant†.

The most economical way to study the universal properties of the model is a scaling approach. This approach was employed in an elegant form by Haldane (1978 a).

Fig. 3.9




Diagrams for the perturbation series, in $\Gamma$, of the ground-state energy for the asymmetric Anderson model. The time direction is fixed, and the dashed line represents the $\sigma$-electron line. The solid lines represent a conduction electron line to the right and a hole line to the left, and the dots represent the mixing $V$. The Pauli principle and the fact that $U\to\infty$ prevent two dotted lines from running at the same time. (*a* and *b*) The second-order diagrams in $V$. (*c*) The leading log's contribution (eqn. (3.2.26)) comes only from the diagrams without any crossings of electron and/or hole lines. (*d*) The simplet diagram with a crossing of the electron lines.

† Another approach to the calculation of $E_d(T)$ can be found in Tsvelick and Barabanov (1978), and Barabanov and Tsvelick (1979).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

In the leading-logarithmic approximation the scaling transformation leads to the renormalization group equation for an effective energy $E_d$ as a function of cut-off $w$:

$$\frac{dE_d}{d\ln w} = -\frac{\Gamma}{\pi}. \tag{3.2.26}$$

The boundary condition in eqn. (3.2.26) is $E_d(U) = \epsilon_d$ at $w = U$. At smaller $w$ the scaling trajectory is

$$E_d(w) = \epsilon_d - \frac{\Gamma}{\pi}\ln\frac{w}{U}. \tag{3.2.27}$$

One should rewrite eqn. (3.2.27) in terms of scale-independent quantities. Such a quantity is $E_d(\Gamma) \equiv \epsilon_d^*$

$$E_d(w) = \epsilon_d^* - \frac{\Gamma}{\pi}\ln\frac{w}{\Gamma}. \tag{3.2.28}$$

Now the scaling trajectory does not depend on the 'bare' initial values of $\epsilon_d$ and $U$.

The scaling law (3.2.28) holds at $\max(E_d, T) \leqslant w \leqslant U$. If either $w \leqslant T$ or $w \leqslant |E_d(w)|$ scaling stops and there is no renormalization of $E_d$.

First let us discuss the local-moment regime, where $-\epsilon_d^* \gg \Gamma$. Then scaling stops at an energy where the state $n_d = 0$ becomes decoupled. It occurs at $w \sim -E_d(w)$. Denoting this energy $-\epsilon_d^{**}$ we have

$$\epsilon_d^{**} = \epsilon_d^* + \frac{\Gamma}{\pi}\ln\frac{\alpha|\epsilon_d^{**}|}{\Gamma}, \tag{3.2.29}$$

where $\alpha$ is a constant.

The constant $\alpha$ should be fixed in such a way that all physical quantities do expand in power series in $\Gamma/\epsilon_d^{**}(\Gamma \ll -\epsilon_d^*)$. For example, the first terms of the expansion of the occupation number $n_d$ are (Tsvelick and Barabanov 1978, Haldane 1978 b)

$$n_d = 1 + \Gamma/\pi\epsilon_d^{**} + O(\Gamma^2/\epsilon_d^{**2}). \tag{3.2.30}$$

In the § 8.2.2 we derive the *exact value of* $\alpha$:

$$\alpha = \pi e. \tag{3.2.31}$$

For $T < -\epsilon_d^{**}$ charge fluctuations are frozen and the Schrieffer–Wolf transformation is valid. The Kondo hamiltonian describes a scattering of conduction electrons on the localized moment with 1/2 spin. The effective coupling constant is

$$I^{**} = -2\Gamma/\pi\epsilon_d^{**} \tag{3.2.32}$$

and the cut-off is $-\epsilon_d^{**}$. According to eqns. (2.4.19) and (2.4.22) the interaction (3.2.32) defines the Kondo temperature

$$T_K = \text{const}\,|\epsilon_d^{**}|(I^{**})^{1/2}\exp(-1/I^{**}) \tag{3.2.33}$$

Being rewritten in terms of the 'bare' quantities the Kondo temperature (3.2.33) gives the same pre-exponential factor as in the symmetric case (Haldane 1978 a, b,

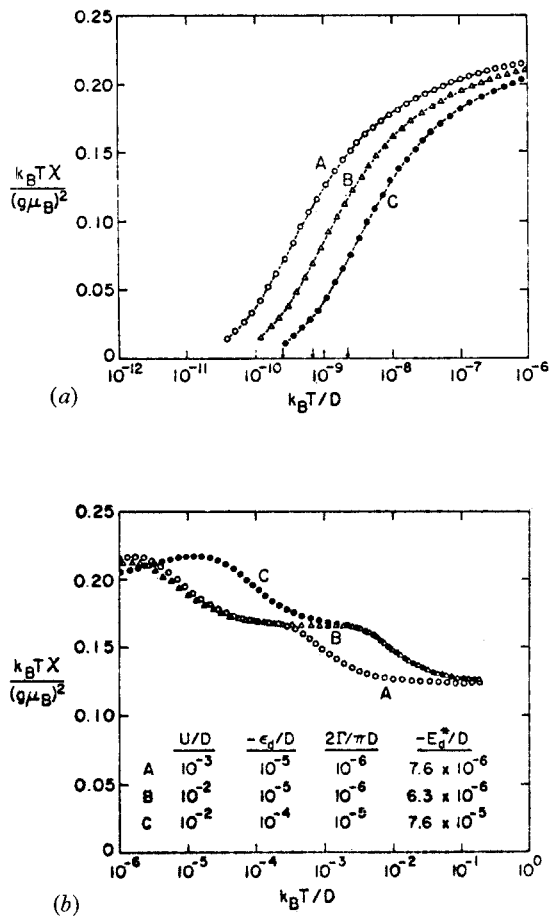
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Krishna-Murthy *et al.* 1980 b (eqn. (3.2.21)). We shall show below (§ 8) that these pre-exponential factors coincide modulo the numerical factor:

$$T_K = \frac{(2U\Gamma)^{1/2}}{\pi} \exp\left(\frac{\pi\epsilon_d(\epsilon_d + U)}{2U\Gamma}\right) \tag{3.2.34}$$

Figure 3.10 represents the results of the numerical renormalization group approach by Krishna-Murthy *et al.* (1980 b) for the magnetic susceptibility of the symmetric Anderson model. In the strong-coupling and local-moment regimes the curves for various $\epsilon_d$ and $\Gamma$ coincide with the universal curve calculated by Wilson

Fig. 3.10




Plots of $k_B T\chi_i(T)(g\mu_B)^2$ versus $\ln k_B T/D$ which illustrate the parameter dependence of transitions between the various regimes. (*a*) Transition from the strong-coupling regime to the local-moment one ($T\chi_i = 1/4$) occurs at a temperature of order $T_K$ which is indicated by arrows. All three curves lie along the universal Kondo-susceptibility curve indicated by the dashed curves. (*b*) Transition from the local-moment regime to the mixed-values one ($T\chi_i = 1/6$) occurs at $T \simeq -\epsilon_d^*$. As the temperature increases further transition to the free-orbital regime ($T\chi_i = 1/8$ occurs at $T \simeq U$. (after Krishna-Murthy *et al.* 1980 b).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

(1975) for the s–d exchange model fig. 3.10 (*a*). The local-moment regime holds up to $T \simeq -\epsilon_d^*$. At $T \gg -\epsilon_d^*$ the mixed-valence regime appears which extends up to $T \sim U$ ($T\chi_i = 1/6$ for $|\epsilon_d^*| \ll T \ll U$) see fig. 3.10 (*b*)).

Now let us consider the *mixed-valence* region where $|\epsilon_d^*| \sim \Gamma$. In this region there is no perturbation theory, so that Wilson's numerical technique (1974) and the exact solution come into their own. Somewhat forestalling events, we quote below an exact result (Wiegmann and Tsvelick 1982) for the magnetic susceptibility and occupation number (figs. 3.11 and 3.12)

$$n_d = 1 - \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{d\omega}{\omega + i0} \frac{\exp(-|\omega| - i\omega\epsilon_d^*/2\Gamma)}{G^{(-)}(\omega)}, \tag{3.2.35}$$

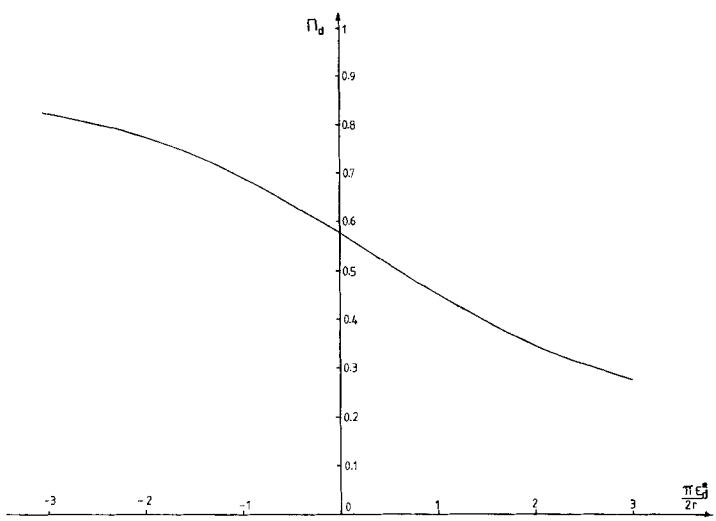
$$\left.\begin{aligned} \chi_i &= \frac{(2\pi e)^{1/2}}{8\Gamma}\left[\exp(-\pi\epsilon_d^*/2\Gamma) \right. \\ &\quad \left. + \frac{i}{2\sqrt{(\pi e)}} \int_{-\infty}^{+\infty} \frac{d\omega}{i\pi + \omega} \frac{\exp(-|\omega| - i\omega\epsilon_d^*/2\Gamma)}{G^{(-)}(\omega)}\right], \\ \epsilon_d^* &= \epsilon_d + \frac{\Gamma}{\pi} \ln \frac{\pi e U}{4\Gamma}, \end{aligned}\right\} \tag{3.2.36}$$

where

$$G^{(-)}(\omega) = \sqrt{(2\pi)} \left(\frac{i\omega + 0}{2\pi e}\right)^{i\omega/2\pi} \Big/ \Gamma\left(\frac{1}{2} + \frac{i\omega}{2\pi}\right),$$

postponing their derivation for § 8. The analytic properties of these integrands change when $\epsilon_d^*$ changes sign†. The perturbation-theory expansions in $\Gamma/\epsilon_d^{**}$ come

Fig. 3.11

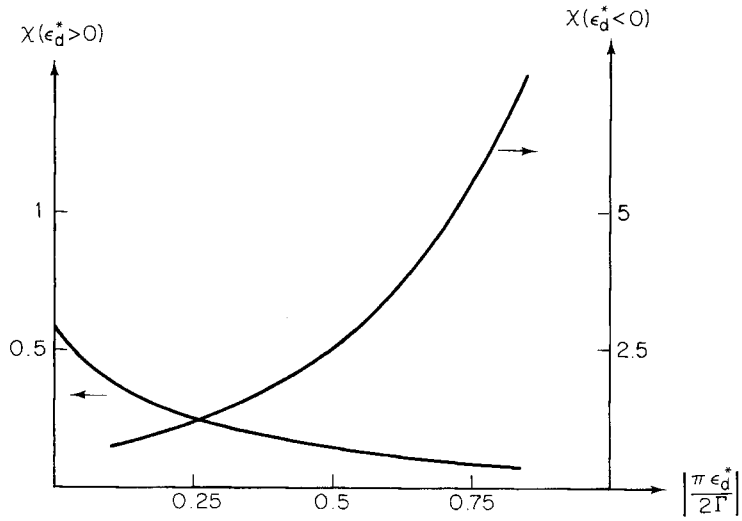



Universal plot of the occupation number $n_d$ versus $(\epsilon_d^* \pi)/2\Gamma$ for the asymmetric Anderson model (eqn. (3.2.25)) (after Melnicov 1982 b).

† Haldane (1978) noted that the criterion for the mixed valence is $|\epsilon_d^*| \lesssim \Gamma$ rather than $|\epsilon_d| \lesssim \Gamma$. Actually, $\epsilon_d^*$ may be arbitrarily large compared to $\epsilon_d$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 3.12




Universal plot of the magnetic susceptibility $\chi/(g\mu_B)^2$ versus $\pi\epsilon_d^*/2\Gamma$ for the asymmetric Anderson model (eqn. (3.2.36)) (after Melnicov 1982 b).

out of (3.2.35) and (3.2.36) as follows. In the integrands of (3.2.35) and (3.2.36) introduce a new integration variable $t=\omega\epsilon_d^{**}/2\Gamma$ ($\epsilon_d^{**}$ is defined by (3.2.29)). When $\epsilon_d^*<0$ we bend the integration contour in (3.2.35) into the upper half-plane and get

$$n_d=1+\frac{1}{\sqrt{\pi}}\int_0^\infty \frac{\tan(t(\Gamma/\epsilon_d^{**}))}{t}\,\frac{t^{-\Gamma t/\pi\epsilon_d^{**}}}{\Gamma(1/2-\Gamma t/\pi\epsilon_d^{**})} \times\exp(-t)\,dt+O(\exp(\pi\epsilon_d^*/2\Gamma)). \tag{3.2.37}$$

When $\Gamma/|\epsilon_d^*|\ll 1$ integral (3.2.37) can be expanded in powers of $\Gamma/\epsilon_d^{**}$. So we obtain (3.2.30). If $\epsilon_d^*>0$, one can bend the contour into the lower half-plane and get:

$$n_d(\epsilon_d^*/\Gamma)=2\Gamma/\pi\epsilon_d^{**}+O((\Gamma/\epsilon_d^{**})^2) \tag{3.2.38}$$

(Tsvelick and Barabanov 1978, Haldane 1978 b).

At $\epsilon_d^*<0$ corrections of the order of $\Gamma/\epsilon_d^{**2}$ to the magnetic susceptibility are much smaller than $T_K^{-1}$. When $\epsilon_d^*>0$ the situation is quite opposite: one can neglect exponential terms and expand (3.2.36) as follows (Haldane 1978 b):

$$\chi_i(\epsilon_d^*/\Gamma)=\Gamma/\pi\epsilon_d^{**2}+\dots. \tag{3.2.39}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

It is interesting to note that for $\epsilon_d^* \to 0$ the integrals ((3.2.35), (3.2.36)) can be calculated explicitly:

$$n_d(0) = 2 - \sqrt{2}; \qquad \chi_i(0) = \pi/4\sqrt{2}\Gamma. \tag{3.2.40}$$

The equality $\chi_i(0)\Gamma \sim 1$ was predicted by Varma and Yafet (1976). The case $-\epsilon_d^* \sim \Gamma$ is of most interest. The states $n_d = \uparrow, \downarrow$ get strongly mixed with the states $n_d = 0$. The local-moment regime and valence-fluctuation regime are no longer separated by a finite range of temperatures ($T_K \sim \Gamma$). As a result $T\chi_i$ makes a direct transition from the strong-coupling regime to the valence-fluctuation regime at a transition temperature of the order of $\Gamma$. Note that this is a case even for $-\epsilon_d \gg \Gamma$ as far as $-\epsilon_d \lesssim \Gamma \ln U/\Gamma$. The numerical renormalization group results for this case are presented in fig. 3.13. At a low temperature the system is in the strong-coupling regime and there are no deviations from the universal Kondo susceptibility (dashed curve (fig. 3.14). The magnetic susceptibility has a broad maximum at $T \sim \Gamma$ (fig. 3.14) after which it tends to the limiting curve $T\chi_i = 1/6$.

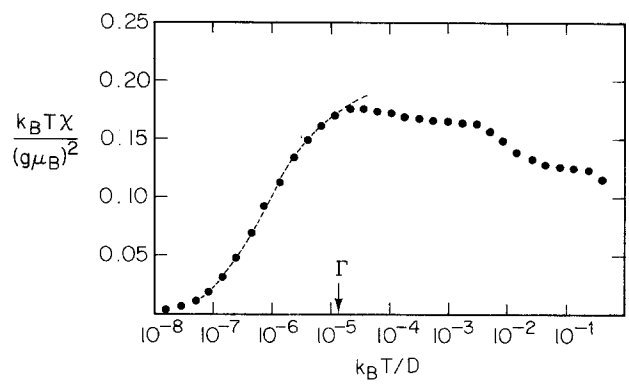
At $\epsilon_d^* \lesssim \Gamma$ as $\epsilon_d$ increases further even at a low temperature $T \sim \Gamma$ the magnetic susceptibility curves cannot be mapped on to the universal Kondo susceptibility curve (fig. 3.14). The magnetic susceptibility has a broad maximum at $T \sim \Gamma$ (fig. 3.14) after which it tends to the limiting curve $T\chi_i = 1/6$.

We next discuss what happens if $\epsilon_d^* \gg \Gamma$. The scaling formula (3.2.28) holds at energies up to $w \sim \epsilon_d(w)$ at which the states $n_d = \uparrow, \downarrow$ become decoupled from low-energy processes. This decoupling energy is still given by (3.2.29), where now $\epsilon_d^{**} > 0$. At $T \ll \epsilon_d^{**}$ charge fluctuations are frozen out, and physical quantities are given by perturbation theory. Apart from corrections to (3.2.38) and (3.2.39) of the order of $\Gamma/\epsilon_d^{**}$ there are also corrections of the order of $\exp(-\epsilon_d^{**}/T)$. If we substitute $E_d(T)$ instead of $\epsilon_d$ into the formula for the thermodynamic potential at $\Gamma = 0$

$$\mathscr{F}_i = -T \ln(1 + 2\cosh H/2T \exp(-E_d(T)/T)) \tag{3.2.41}$$

this formula will be valid even at $T < \epsilon_d^{**}$.

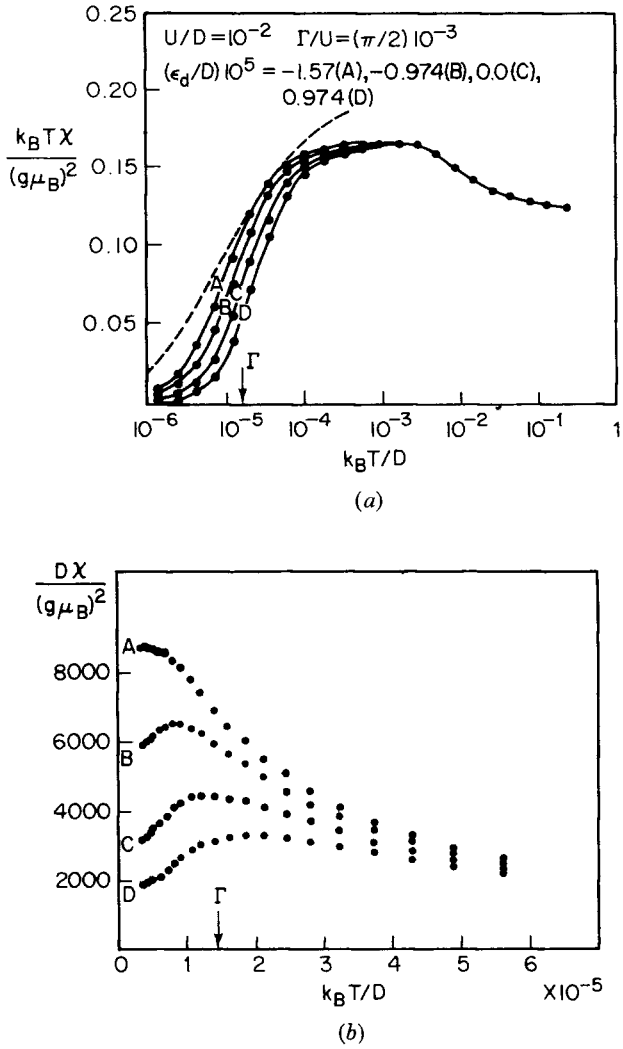
Fig. 3.13




Plot of $k_B T\chi_i/(g\mu_B)^2$ versus $\ln k_B T/D$ with parameters $\epsilon_d$, $\Gamma$, $U = 10^{-2}D$ such that $-\epsilon_d^* \gtrsim \Gamma$. The dashed curve is the universal Kondo susceptibility. Here $2\Gamma/\pi D = 10^{-5}$; $\epsilon_d/D = -0{\cdot}5 \times 10^{-4}$; $\epsilon_d^*/D = -1{\cdot}855 \times 10^{-5}$; $T_K/D = 4{\cdot}2 \times 10^{-7}$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 3.14




(*a*) Plots of $k_B T\chi/(g\mu_B)^2$ versus $\ln(k_B T/D)$ for $|\epsilon_d| \lesssim \Gamma$ and $\epsilon_d^* \gtrsim \Gamma$. Deviation from the universal shape, indicated by the dashed line, reveals the non-magnetic character of the impurity. (*b*) Plots of $D\chi/(g\mu_B)^2$ versus $\ln k_B T/D$ for the same parameters as (*a*). Deviations from universality correspond to the broad maxima in the magnetic susceptibilities curves (after Krishna-Murthy *et al.* 1980).

## §4. Bethe method

In this section we apply the Bethe-Ansatz approach to the solution of:

(i) The s–d exchange model §4.2.
(ii) The anisotropic s–d exchange model (§4.3).
(iii) The degenerate exchange model (§4.4).
(iv) The Anderson model (§4.5).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

A solution of the resonance-level model is given in the Supplement section.

Presentation is organized as follows. The fundamentals of the Bethe-Ansatz approach are presented in § 4.1. All other sections are intended for readers who are already acquainted either with Bethe's method or with § 4.2.

### 4.1. *General*

In 1931 only 5 years after Schrödinger's work, Hans Bethe constructed the exact wave function of a chain of 1/2-spins with a nearest-neighbour interaction. Thirty years passed and his work has initiated the development of a new interesting domain of mathematical physics, namely, the theory of quantum integrable systems.

The subject of the present review is the application of this theory to dilute magnetic alloys. However, the mathematical apparatus which we shall use for diagonalization and study of the integrable hamiltonians is to a certain extent common for different models of one-dimensional quantum-field theory and two-dimensional lattice statistics. The Bethe-Ansatz technique to be discussed below may equally well be applied to all integrable models. Therefore it is worth mentioning some general ideas related to the Bethe Ansatz.

Bethe studied a one-dimensional version of the model which had been suggested by Haisenberg (1926) for the description of ferromagnetism:

$$\mathscr{H} = I \sum_{n=1}^{N} \boldsymbol{\sigma}_n \cdot \boldsymbol{\sigma}_{n+1} \tag{4.1.1}$$

($\boldsymbol{\sigma}_n = (\sigma_n^x, \sigma_n^y, \sigma_n^z)$ are Pauli matrices). He proved that the eigenstates of this hamiltonian

$$|\Psi\rangle = \sum_{x_i} \Psi(x_1, \ldots, x_M) \sigma_{x_1}^+, \ldots, \sigma_{x_M}^+ |0\rangle; \qquad (x_i = 1, \ldots, N)$$

are given by a function of a special form, which has been christened the *Bethe Ansatz*:

$$\Psi(x_1, \ldots, x_M) = \sum_P \exp\left\{ i \sum_{j=1}^{M} k_{p_j} x_j + i \sum_{i>j=1}^{M} \operatorname{sign}(x_i - x_j) \Phi(k_{p_i}, k_{p_j}) \right\}, \tag{4.1.2}$$

where $P = \{p_1, \ldots, p_M\}$ is a permutation of the integers $\{1, \ldots, M\}$, $|0\rangle$ is the state with all spins down, $x_j$ are coordinates on the lattice, $k_j$ are quasimomenta of magnons, and

$$\Phi(k, p) = 2 \cot^{-1} \left[ \frac{\sin\left(\dfrac{k-p}{2}\right)}{\cos\left(\dfrac{k+p}{2}\right) - \cos\left(\dfrac{k-p}{2}\right)} \right], \tag{4.1.3}$$

is a two-particle scattering phase. The spin and energy of this state are equal to:

$$S^z = N/2 - M, \qquad E = I \sum_{j=1}^{M} \cos k_j.$$

It is convenient to use such parametrization for $k(\lambda)$, $p(\lambda')$ in which the scattering phase (4.1.3) depends on only the difference between the corresponding arguments $\lambda$ and $\lambda'$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The possibility of this parametrization is due to the presence of a special group of mutual rotations of a one-dimensional lattice and time. For the Haisenberg model this parametrization has the following form (Hulten 1938):

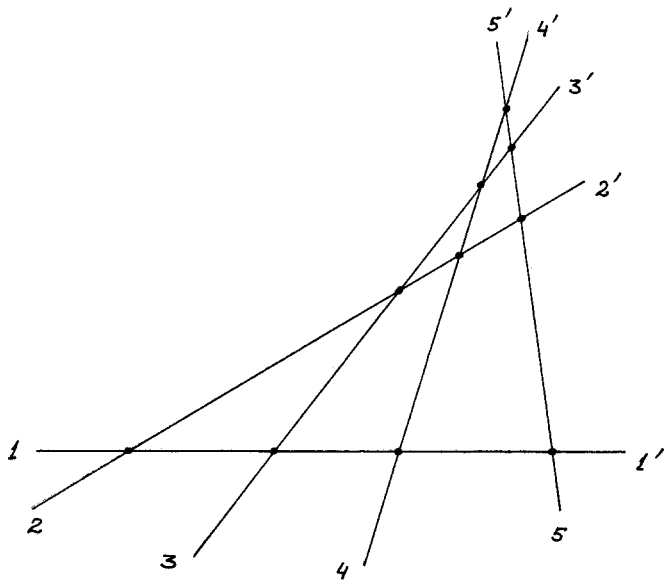
$$\left.\begin{aligned} k(\lambda) &= 2\tan^{-1}\lambda, \\ \Phi(k(\lambda), p(\lambda')) &= 2\tan^{-1}\left(\frac{\lambda-\lambda'}{2}\right). \end{aligned}\right\} \tag{4.1.4}$$

The analytical properties of the scattering phase as a function of $\lambda$ have a fairly simple form. By analogy with relativistic kinematics a quantity $\lambda$ will be called 'rapidity'.

The wavefunction (4.1.3) describes the so-called factorized scattering. We see from (4.1.3) that when a particle passes from one region $X_Q = \{x_{q_1} < \ldots < x_{q_M}\}$ to another region $X_{Q'}$, which differs from the first one by a permutation of some pair $(x_p, x_q)$, only two-particle processes occur. Furthermore, any $N$-particle scattering processes is expressed standardly in terms of the product of $N(N-1)/2$ two-particles processes (fig. 4.1). The absence of multipartiele processes is the Bethe hypothesis.

The two-particle processes in $1+1$ space-time conserve a set $\{k_1, k_2\}$ of momenta. Therefore, a set of momenta $\{k_1, \ldots, k_M\}$ in (4.1.3) is the same in all regions $X_Q$. In other words, there are no multiple production processes. Such dynamic systems are characterized by the existence of an infinite series of independent integrals of motion, which may be considered as a necessary condition of factorizability†.

Fig. 4.1




The graphical representation of the particle factorized $S$ matrix.

† Apparently, this relation was first pointed out by Polyakov (unpublished).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

As we mentioned above, the factorizability enables one to express the amplitude of any multiparticle process in terms of two-particle amplitudes. Obviously, one may bring particles from a region $X_Q$ to another region $X_{Q'}$ in several ways, i.e. decompose the permutation connecting $X_Q$ with $X_{Q'}$ into the product of two-particle permutations also in several ways. For the self-consistency of the Bethe hypothesis it is necessary that these ways lead to the same result.

The excitations in the Haisenberg model (4.1.1) have no internal degrees of freedom and a scattering process reduces only to a phase shift. Therefore, all possible transitions from the $|\text{in}\rangle$ to $|\text{out}\rangle$ states through the two-particle permutations automatically lead to the same result and the Bethe hypothesis is valid provided that the $N$-particle scattering phase has the following form:

$$\Phi(k_1, \ldots, k_N) = \sum_{i>j=1}^{N} \Phi(k_j, k_i). \tag{4.1.5}$$

The situation is more complicated in theories with certain internal symmetry (spectrum degeneracy). If a state of the particle is characterized by not only its mome tum but also by some index (colour) the colliding particles may exchange their colours. Factorized $S$ matrices still contain only purely elastic scatterings. Nevertheless, they are now far from trivial and are not, in general, diagonal. Non-diagonal processes are permissible in theories with spectrum degeneracy; they are responsible for the redistribution of momenta among particles of different types. The $S$-matrices form a finite-dimensional non-commutative space. The requirement of *independence of the final result of pair collisions of their ordering* imposes certain constraints on the two-particle $S$-marrix (in addition to the usual requirements of analyticity and unitarity), namely, the *factorization equations*.

However, before considering the integrable models with the internal symmetry we enumerate the main known models with diagonal $S$ matrices.

All these models are described by the Bethe-Ansatz wave function (4.1.2) with a special two-particle scattering phase.

(i) The *spin 1/2 anisotropic Haisenberg ring* (so-called *XXZ-chain*) (Orbach 1958)

$$\mathscr{H} = I \sum_{n=1}^{N} [(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y) + \cos \mu \sigma_n^z \sigma_{n+1}^z]. \tag{4.1.6}$$

$$\left.\begin{aligned} k(\lambda) &= 2 \tan^{-1} (\cot \mu/2 \tanh \mu\lambda), \\ \Phi(\lambda) &= 2 \tan^{-1} (\cot \mu \tanh \mu\lambda), \\ E &= I \sum_{\alpha=1}^{M} \cos k(\lambda_\alpha). \end{aligned}\right\} \tag{4.1.7}$$

(ii) The interacting Bose-gas (Lieb and Liniger 1963, Lieb 1963)

$$\mathscr{H} = \int \left[ -\varphi^* \frac{\partial^2}{\partial x^2} \varphi + g(\varphi\varphi^*)^2 \right] dx; \tag{4.1.8}$$

$\varphi$ is a Bose field

$$\left.\begin{aligned} \Phi(k) &= 2 \tan^{-1} (k/g), \\ E &= \sum_{\alpha=1}^{N} k_j^2. \end{aligned}\right\} \tag{4.1.9}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

(iii) *The massive Thirring model* (Berezin and Suschko 1965, Bergnoff and Thacker 1979)

$$\mathscr{L} = \int (\bar{\psi}_i \partial_\mu \gamma^\mu \psi - m\bar{\psi}\psi + g j_\mu j^\mu)\, dx; \tag{4.1.10}$$

here $j_\mu = \bar{\psi}\gamma_\mu\psi$, $\psi = (\psi_1, \psi_2)$ is a spinor, $\bar{\Psi} = \Psi^+\gamma_0$ and $\gamma_\mu$ are two-dimensional Dirac matrices

$$\{\gamma_\mu, \gamma_\nu\} = \delta_{\mu\nu}.$$

This model is equivalent to the *Sine–Gordon model* which was directly solved by Sklyanin *et al.* (1979).

$$\mathscr{L} = \int \left[ \frac{1}{2}(\partial_\mu \varphi)^2 - M_0(1 - \cos\beta\varphi) \right] dx, \tag{4.1.11}$$

$$\left.\begin{aligned} k(\lambda) &= m \sinh\lambda, \\ \Phi(\lambda) &= 2\tan^{-1}(\tan g \tanh\lambda/2), \\ E &= m \sum_{\alpha=1}^{M} \cosh\lambda_\alpha, \end{aligned}\right\} \tag{4.1.12}$$

where $m = M_0/2\Lambda$ ($\Lambda$ is an ultraviolet cutoff), and

$$\beta^2 = 4\pi + 8g \qquad \text{at } |g| \ll 1.$$

(iv) The *resonance-level model* (Filyov and Wiegmann 1980)

$$\mathscr{H} = \int \left\{ -ic^+(x)\frac{\partial}{\partial x}c(x) + V\delta(x)(c^+(x)d + d^+c(x)) + U\delta(x)c^+(x)c(x)d^+d \right\} dx, \tag{4.1.13}$$

$$\left.\begin{aligned} k(\lambda) &= V\exp(\lambda), \\ \Phi(\lambda) &= 2\tan^{-1}(\tan U \tanh\lambda/2), \\ E &= \sum_{\alpha=1}^{N} \tan^{-1}(V^2/k(\lambda_\alpha)). \end{aligned}\right\} \tag{4.1.14}$$

(v) The generalization of *the Haisenberg model for an arbitrary spin S* (Zamolodchicov and Fateev 1980, Tahktadjan 1982, Babujan 1982, Kulish and Sklyanin 1981)

$$\mathscr{H} = \sum_{n=1}^{N} \mathscr{P}(\mathbf{S}_n \cdot \mathbf{S}_{n+1}); \tag{4.1.15}$$

here $\mathscr{P}(x)$ is a polynomial of the order $2S$ of a special form,

$$\left.\begin{aligned} k(\lambda) &= 2\tan^{-1}\lambda/S, \\ \Phi(\lambda) &= 2\tan^{-1}\lambda, \\ E &= \sum_{\alpha=1}^{M} \cos k(\lambda_\alpha). \end{aligned}\right\} \tag{4.1.16}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

All the above models are interrelated. For example, it is known that magnetics (v) for large $S \to \infty$ are equivalent to the interacting bosons (ii). This follows from (4.1.16).

Until the early 1960s, as one may judge by the literature, Bethe's work had no considerable impact on either physicists or mathematicians. But there was a particular exception: work by Hulten (1938), in which the ground-state energy of the antiferromagnetic spin chain was calculated, stood by itself.

In 1963 Lieb and Liniger breathed a new life into the Bethe method, by solving the problem of the interacting Bose gas. The complete symmetrical many-body wavefunction for a problem with the $\delta$-function interaction was independently derived by McGuire (1964) and Berezin *et al.* (1964). A major breakthrough in the technology of the Bethe Ansatz has been a generalization of the Lieb–Liniger solution for a many-body problem without constraining the symmetry of the wavefunction. The solution of this problem required great effort (Flicker and Lieb 1967, McGuire 1966) and was carried out almost simultaneously by Gaudin (1967)† and Yang (1967). In the course of this solution the general special function relations between two-particle scattering amplitudes were derived. These relations are necessary and sufficient conditions for the validity of the Bethe Ansatz. These relations constitute the foundations of the theory of integrable two-dimensional statistical models (Baxter 1972) and of the theory of factorized scattering (Zamolodchicov and Zamolodchicov 1979, Zamolodchicov 1980, Karowski *et al.* 1977). They are well known as *triangle* (*or factorization*) equations (Zamolodchikov and Zamolodchicov 1979))‡. Often they are called the Yang–Baxter equations. In the general case of the one-dimensional quantum theory of particles with $n$ different colours these equations have the following form:

$$S^{a_1 a_1'}_{a_2 a_2'}(k_1, k_2) S^{a_1' a_1''}_{a_3 a_3'}(k_1, k_3) S^{a_2' a_2''}_{a_3' a_3''}(k_2, k_3) = S^{a_2 a_2'}_{a_3 a_3'}(k_2, k_3) S^{a_1 a_1'}_{a_3' a_3''}(k_1, k_3) S^{a_1' a_1''}_{a_2' a_2''}(k_1, k_2); \qquad (4.1.17)$$

here $S^{a_1 a_1'}_{a_2 a_2'}(k_1, k_2)$ is the two-particle scattering matrix (fig. 4.2).

The subscripts $(a_1, a_2)$ and $(a_1', a_2')$ correspond to particle colours in the $|\text{in}\rangle$ and $|\text{out}\rangle$ states with momenta $k_1, k_2$. In (4.1.17) summation over repeated indices is meant. The factorization equations imply that all the possible decompositions of the $N$-particle $S$ matrix as a product of two-particles $S$ matrices give the same result.

Let us consider a three-particle scattering matrix. The corresponding two-particle collisions may be ordered in two different ways as presented in fig. 4.3.

Let the particles in the $|\text{in}\rangle$ state be ordered in such a way that $x_1 < x_2 < x_3$, whilst after the collision the ordering is $x_3 < x_2 < x_1$. The pair collisions may occur in two different ways:

$$x_1 < x_2 < x_3 \to x_1 < x_3 < x_2 \to x_3 < x_1 < x_2 \to x_3 < x_2 < x_1,$$

$$x_1 < x_2 < x_3 \to x_2 < x_1 < x_3 \to x_2 < x_3 < x_1 \to x_3 < x_2 < x_1.$$

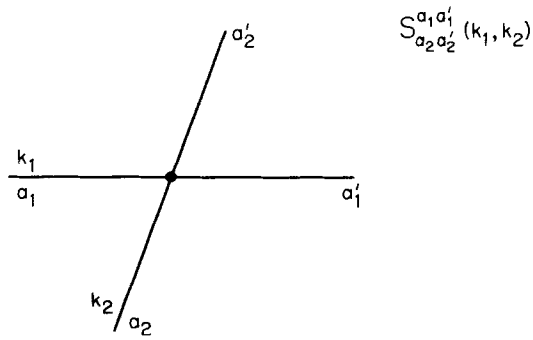
Their equivalence is an expression of the factorization condition (4.1.17). The validity of this condition for three particles leads to the validity of it for any $N$-

† Unfortunately, Gaudin has published only a brief list of his results. His work has not been published completely yet, not to mention his Thesis which is not available.

‡ Note that the factorization conditions sprang out earlier (McGuire 1966) in the connection with the many-body fermion problem.

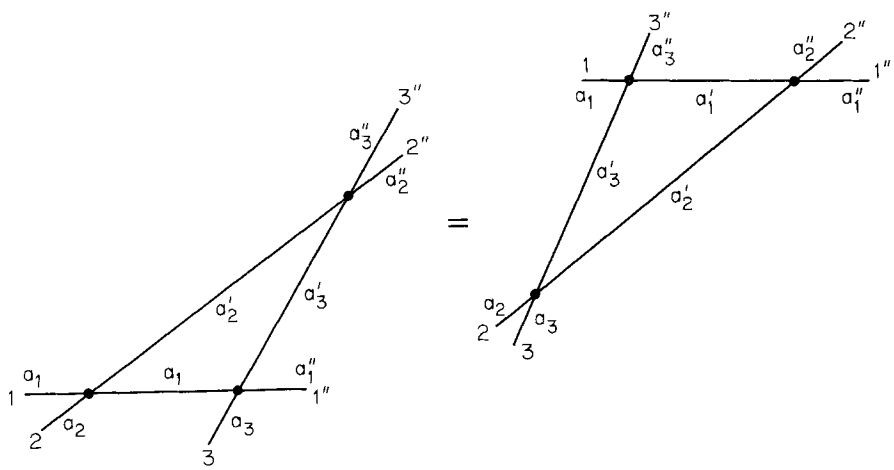
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 4.2




The graphical representation of a two-particle $S$ matrix.

Fig. 4.3




The equivalence of three-particle diagrams (the factorization equation).

particle process (fig. 4.1). As has been mentioned above for (i)–(v) without an internal symmetry the condition (4.1.17) is fulfilled trivially by virtue of the commutativity of $S$ matrices.

For systems possessing an internal symmetry the Bethe Ansatz has the following form. Let $Q=\{q_1,\ldots,q_N\}$ and $P=\{p_1,\ldots,p_N\}$ be permutations of the integers $\{1,\ldots,N\}$. Then in the region $X_Q=\{x_{q_1}<x_{q_2}<\ldots<x_{q_N}\}$ the wavefunction is

$$\Psi(X_Q)=\sum_P A_{a_1\ldots a_N}(P|Q)\exp\left\{i\sum_{j=1}^{N}k_{p_j}x_j\right\}. \tag{4.1.18}$$

The summation is carried out over all the permutations. $A(P|Q)$ in the given region does not depend on coordinates. $A(P|Q)$s from different regions are connected with

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

each other by $S$-matrix elements. For example, if the regions $X_Q$ and $X_{Q_{\langle ij\rangle}}$ differ from each other by the permutation of $i$ and $j$ particles then

$$A_{\ldots kl\ldots}(P|Q)=S_{lj}^{ki}A_{\ldots ij\ldots}(P|Q_{\langle ij\rangle}). \tag{4.1.19}$$

Qnce the two-particle $S$ matrix is shown all $A(P|Q)$s can be expressed in terms of $A(P|I)$ $(I=\{1,\ldots,N\})$ with $N$-particle $S$ matrices given by the product of two-particle matrices.

The factorizability conditions are very strict constraints on the scattering kinematics. Rewriting them in components it is easy to make sure that the number of equations considerably exceeds the number of unknown quantities. Nevertheless, today a considerable number of non-trivial solutions of the factorization equations is known. These solutions correspond to different models of the $1+1$-dimensional quantum-field theory. Among them we should point to the following:

(i) *Many-body problem with the $\delta$-function interaction*:

$$\mathscr{H}=\int\left[-\sum_{a=1}^{n}\psi_a^*\frac{\partial^2}{\partial x^2}\psi_a+g\sum_{a>b}\psi_a^*\psi_b^*\psi_b\psi_a\right]dx, \tag{4.1.20}$$

where $n$ is the number of colours.

This hamiltonian with $n=2$ was diagonalized by Yang (1967). Generalization to an arbitrary $n$ was done by Sutherland (1968).

The two-particle $S$ matrix of this model is

$$S_{a_2a_2'}^{a_1a_1'}(k,p)=\frac{k-p+igP_{a_2a_2'}^{a_1a_1'}}{k-p+ig}, \tag{4.1.21}$$

where $P_{a_2a_2'}^{a_1a_1'}=\delta_{a_1a_2'}\delta_{a_2a_1'}$ is a permutation operator.

The energy of the system is $E=\sum_{j=1}^{N}k_j^2$.

(ii) *Hubbard model* (Lieb and Wu 1968):

$$\mathscr{H}=t\sum_{n,\sigma}(c_{n\sigma}^+c_{n+1\sigma}+c_{n+1\sigma}^+c_{n\sigma})+U\sum_n c_{n\uparrow}^+c_{n\uparrow}c_{n\downarrow}^+c_{n\downarrow}; \tag{4.1.22}$$

$$S_{\sigma_2\sigma_2'}^{\sigma_1\sigma_1'}(k,p)=\frac{t(\sin k-\sin p)+iUP_{\sigma_2\sigma_2'}^{\sigma_1\sigma_1'}}{t(\sin k-\sin p)+iU}, \tag{4.1.23}$$

where $c_{n\sigma}^+$ is the creation operator of an electron with $\sigma$ spin at the $n$th site of a one-dimensional lattice.

The energy of the system is

$$E=t\sum_{j=1}^{N}\cos k_j. \tag{4.1.24}$$

(iii) *Generalization of the massive Thirring model* (Lipatov and Buhvostov 1980):

$$\mathscr{L}=\int\left[\sum_{a=1}^{2}\bar{\psi}_a(i\partial_\mu\gamma^\mu-m)\psi_a-g(\bar{\psi}_1\gamma_\mu\psi_1)(\bar{\psi}_2\gamma^\mu\psi_2)\right]dx. \tag{4.1.25}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$S^{a_2a_2'}_{a_1a_1'}(\lambda)=\delta_{a_1a_1'}\delta_{a_2a_2'}\delta_{a_1a_2}+\frac{1}{2}\epsilon_{a_1a_2}\epsilon_{a_1'a_2'}$$
$$\times\sinh\left(\frac{\lambda-ig}{2}\right)\Big/\sinh\left(\frac{\lambda+ig}{2}\right)+\frac{1}{2}(\sigma_x)_{a_1a_2}(\sigma_x)_{a_1'a_2'}$$
$$\times\cosh\left(\frac{\lambda-ig}{2}\right)\Big/\cosh\left(\frac{\lambda+ig}{2}\right);\qquad(4.1.26)$$

$$E=m\sum_{\alpha=1}^{N}\cosh\lambda_\alpha.\qquad(4.1.27)$$

(iv) *The s–d exchange model with an arbitrary impurity spin S*:

$$\mathscr{H}=\sum_\sigma\int dx\left\{-ic_\sigma^+(x)\frac{\partial}{\partial x}c_\sigma(x)+\frac{1}{2}Ic_\sigma^+(x)\boldsymbol{\sigma}_{\sigma\sigma'}c_{\sigma'}(x)\mathbf{S}\delta(x)\right\},\qquad(4.1.28)$$

where $\sigma=\pm1$, $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ are the conventional Pauli matrixes and $\mathbf{S}=(S_x,S_y,S_z)$ are the spin operators of the impurity.

$$S(\lambda)=(\lambda+iI\boldsymbol{\sigma}\cdot\mathbf{S})/(\lambda+iI);\qquad E=\sum_{j=1}^{N}k_j.\qquad(4.1.29)$$

The hamiltonian was diagonalized by Andrei (1980) and Wiegmann (1980 a, 1981) for $S=1/2$ and by Fateev and Wiegmann 1981 a) for arbitrary $S$.

(v) *The chiral invariant Gross–Neveu model* (*SU*(*n*) *isospin Thirring model*):

$$\mathscr{L}=\int dx\left\{\sum_{a=1}^{n}i\bar{\psi}_a\partial_\mu\gamma^\mu\psi_a-g\left[\left(\sum_{a=1}^{n}\bar{\psi}_a\psi_a\right)^2-\left(\sum_{a=1}^{n}\bar{\psi}_a\gamma_5\psi_a\right)^2\right]\right\}.\qquad(4.1.30)$$

This model was solved by Belavin (1979) and Andrei and Lowenstein (1979) for $n=2$. The solution describing $n$ arbitrarily was found by Andrei and Lowenstein (1980), Kulish and Reshetikhin (1981) and Arinstein (1980):

$$S^{a_1a_1'}_{a_2a_2'}(\tau,\tau')=\frac{\tau-\tau'+igP^{a_1a_1'}_{a_2a_2'}}{\tau-\tau'+ig},\qquad(4.1.31)$$

$\tau=\pm1$ is a particle chirality.

$$E=\sum_{\tau=\pm1}\tau\sum_{i=1}^{N_\tau}k_{\tau_i},$$

where $N_\tau$ and $k_{\tau_i}$ are the number and momenta of particles with the given chirality $\tau$.

(vi) *The Anderson model* (Wiegmann 1980 c):

$$\mathscr{H}=\int dx\sum_{\sigma=\uparrow,\downarrow}\left[-iC_\sigma^+(x)\frac{d}{dx}C_\sigma(x)+V\delta(x)(C_\sigma^+(x)d_\sigma\right.$$
$$\left.+d_\sigma^+C_\sigma(x))\right]+\epsilon_d(d_\uparrow^+d_\uparrow+d_\downarrow^+d_\downarrow)+Ud_\uparrow^+d_\uparrow d_\downarrow^+d_\downarrow\qquad(4.1.32)$$

where $C_\sigma^+(x)$ is a creation operator of a conduction electron with the spin $\sigma$ and $d_\sigma^+$ is a creation operator of an electron from the impurity orbital.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\left.\begin{aligned} S^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}(k,p) &= \frac{g(k)-g(p)+iP^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}}{g(k)-g(p)+i}, \\ g(k) &= (k-\epsilon_d-U/2)^2/2U\Gamma, \qquad \Gamma=V^2/2, \\ E &= \sum_{j=1}^{N} k_j. \end{aligned}\right\} \tag{4.1.33}$$

(vii) *The generalized Haisenberg chain* (Sutherland 1975, Kulish and Reshetikhin 1981):

$$\mathscr{H} = I\sum_{n=1}^{N} \mathbf{P}_{n,n+1}, \tag{4.1.34}$$

$$\left.\begin{aligned} S^{a_1a_1'}_{a_2a_2'}(\lambda) &= (\lambda+iP^{a_1a_1'}_{a_2a_2'})/(\lambda+i), \\ E &= I\sum_{\alpha=1}^{M} \cos k(\lambda_\alpha); \qquad k(\lambda)=2\tan^{-1}2\lambda. \end{aligned}\right\} \tag{4.1.35}$$

(viii) *The $O(n)$-invariant magnetic chain* (Reshetikhin 1983):

$$\mathscr{H} = I\sum_{m=1}^{N} [(n-2)\mathbf{P}_{m,m+1}-2\mathbf{K}_{m,m+1}]. \tag{4.1.36}$$

There $\mathbf{P}_{m,m+1}$ is a permutation operator, $K^{a_1a_1'}_{a_2a_2'}=\delta_{a_1a_2}\delta_{a_1'a_2'}$

$$\left.\begin{aligned} \mathbf{S} &= \left(\lambda\mathbf{I}+i\mathbf{P}-i\frac{\lambda}{\lambda+i(n-2)/2}\mathbf{K}\right)\Big/(\lambda+i), \\ E &= I\sum_{\alpha=1}^{M} \cos k(\lambda_\alpha), \qquad k(\lambda)=2\tan^{-1}2\lambda. \end{aligned}\right\} \tag{4.1.37}$$

Let us come back to the general properties of the Bethe Ansatz. The parameters $\{k_j\}$ of the wavefunction (4.1.18) are so far arbitrary quantities. In order to find the spectrum of the system we impose some boundary conditions. The limit of a large number of particles does not depend on the form of the boundary conditions. It is most convenient to choose them as periodic conditions (PBC)†. Let us put the system into a box with length $L$ and demand that

$$\psi(x_1,\ldots,x_j,\ldots,x_N)=\psi(x_1,\ldots,x_j+L,\ldots,x_N) \tag{4.1.38}$$

for any $j=1,\ldots,N$.

The resulting equations for the coefficients $A(P|Q)$ lead to the following eigenvalue problem (Yang 1967, Gaudin 1967):

$$\exp(ik_jL)\xi=\mathbf{T}_j\xi, \tag{4.1.39}$$

where $\xi=A(\mathbf{I}/\mathbf{I})$,

$$\mathbf{T}_j=\mathbf{S}_{jj+1}\ldots S_{jN}S_{j1}\ldots S_{jj-1}, \tag{4.1.40}$$

and $\mathbf{S}_{jk}$ means the operator matrix $\mathbf{S}_{jk}(\lambda_j-\lambda_k)$.

† Other kinds of boundary conditions were considered by Gaudin (1967).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

For models without an internal symmetry the $S$ matrix is not an operator but a $C$ number and (eqn (4.1.39) leads straight to the algebraic equation for $k(\lambda_\alpha)$ (Bethe 1931):

$$\exp(ik(\lambda_\alpha)L) = \prod_{\substack{\beta \neq \alpha \\ \beta = 1}}^{M} \exp(i\Phi(\lambda_\alpha - \lambda_\beta)). \tag{4.1.41}$$

Equation (4.1.41) describes the whole spectrum of the system.

The most useful form of PBCs is found by taking the logarithm of (4.1.41), for which one must choose a branch of the function $\Phi(\lambda)$. The log of (4.1.41) is written as

$$k(\lambda_\alpha)L = 2\pi N_\alpha + \sum_{\beta=1}^{M} \Phi(\lambda_\alpha - \lambda_\beta), \tag{4.1.42}$$

where $N_\alpha$ = integer are the quantum numbers of the system. The transcendental equation (4.1.42) was first found by Bethe (1931) for a 1/2-spin chain. We shall call them the Bethe-Ansatz equations below. For systems possessing an internal symmetry PBCs lead to the problem of simultaneously diagonalizing $N$ operators. Using the triangle equations it is easy to show that all operators $\mathbf{T}_j$ commute with each other so that the problem of simultaneous diagonalization may indeed be solved. The most remarkable aspect of Yang's and Gaudin's approaches is the treatment of the matrices $\mathbf{T}_j$. They have shown that the eigenvalue problem for the system with two kinds of coloured particles can be solved by a twofold application of the Bethe Ansatz. Sutherland (1968) has extended their method to include a treatment of an arbitrary number of colours, using a *hierarchy of Ansatzes*. The problem of diagonalization of similar sets of operators has arisen in different aspects of the application of the Bethe Ansatz. We mean the classical two-dimensional statistical lattice models.

The ideas of Kramers and Wannier (1941) and Onsager (1944) concerning the transfer matrix were developed further by Lieb (1967 a, b, c, d) who used the Bethe Ansatz to diagonalize the transfer matrices of the 'ice' and 'ferroelectric' models which are special cases of the *six-vertex model*. The two-dimensional Ising model (more precisely, two decoupled Ising models) is also a special case of these models (for a review see Lieb and Wu 1972). The various developments in solvable lattice models were unified and extended in the remarkable works of Baxter (1972 a–e). Baxter constructed the solution of the *eight-vertex model* including all the previously solved models as special cases, and put forward the method which became the ground of the modern development of the Bethe Ansatz.

There is a close relationship between exactly solvable models of lattice statistics, 1 + 1 quantum-field theory and factorized scattering theory (Zamolodchikov 1980). We consider this relationship in the framework of Baxter's scheme.

In particular, Baxter (1972 b) and Sutherland (1970) showed that the hamiltonian of a general anisotropic $XYZ$ Haisenberg spin chain

$$\mathscr{H}_{xyz} = \sum_n [I_x \sigma_n^x \sigma_{n+1}^x + I_y \sigma_n^y \sigma_{n+1}^y + I_z \sigma_n^z \sigma_{n+1}^z] \tag{4.1.43}$$

could be obtained as a logarithmic derivative of the eight-vertex model *transfer-matrix*.

Let us give the general definition of a vertex model. Consider a square lattice. The fluctuating variables $a = 1, 2, \ldots, n$ ('spins' or 'colours') are attached to each

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

bond connecting the nearest-neighbour lattice site. The vertex Boltzmann weight $S^{a_2 a_2'}_{a_1 a_1'}$ (see fig. 4.4) corresponds to each colour configuration around any lattice site. By definition, the partition function is the sum over all colour configurations of all the lattice bonds, each configuration being taken with the statistical weight equal to the product of vertex weights over all lattice vertices. The transfer matrix of a vertex model is the operator connecting the configurations on the vertical bonds placed between the rows $n-1, n(\{i_1, \ldots, i_N\})$ and $n, n+1(\{j_1, \ldots, j_N\})$. The transfer matrix is of the form

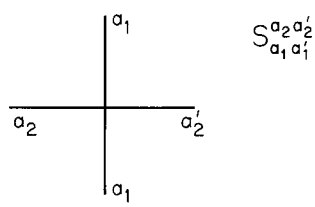
$$\mathbf{T} \equiv \mathbf{T}^{i_1 \ldots i_N}_{j_1 \ldots j_N} = \sum_{\substack{p_1 = p_{N+1} \\ \{p_k\}}} \prod_{k=1}^{N} S^{p_k p_{k+1}}_{i_k j_k}. \tag{4.1.44}$$

The partition function for a lattice with $N'$ rows is given by

$$Z = \mathrm{Tr}\,\{\mathbf{T}^{N'}\}.$$

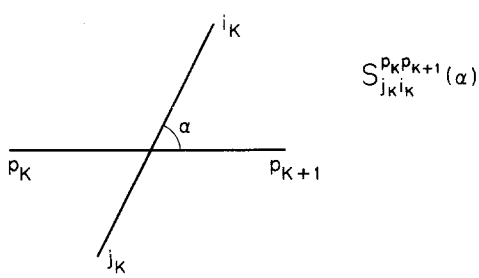
The problem is thus reduced to that of diagonalizing the transfer matrix (4.1.44). Baxter (1978) has shown that the remarkable properties of the solvable vertex model become more transparent if one puts it on a general non-regular lattice, consisting of a large number of arbitrarily directed straight lines (lattice axes). The model on the non-regular lattice remains exactly solvable, subject to the dependence of the vertex weight $\mathbf{S}(\alpha)$ on the intersection angle $\alpha$ of two straight lines in the given vertex of a special kind (fig. 4.5).

Fig. 4.4




The matrix of the Boltzmann weights (vertex) $S^{a_2 a_2'}_{a_1 a_1'}$ in the vertex models.

Fig. 4.5




The graphical representation of the vertex weights of the vertex model on a non-regular lattice.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

This angular dependence is a consequence of the remarkable symmetry of the Baxter models on the non-regular lattice (so-called $Z$ invariance). The partition function of the model is invariant under arbitrary parallel shifts of any lattice axes (note that such shifts can lead to a change in the coordinate structure of the lattice). It is easy to see that the $Z$ invariance is realized if the vertex weights $S^{a_2a_2'}_{a_1a_1'}(\alpha)$ do satisfy the triangle equations (4.1.17):

$$\mathbf{S}_{12}(\alpha_1-\alpha_2)\mathbf{S}_{13}(\alpha_1-\alpha_3)\mathbf{S}_{23}(\alpha_2-\alpha_3)=\mathbf{S}_{23}(\alpha_2-\alpha_3)\mathbf{S}_{13}(\alpha_1-\alpha_3)\mathbf{S}_{12}(\alpha_1-\alpha_2).$$

Let us consider the so-called monodromy matrix (fig. 4.6):

$$\begin{aligned}\mathbf{L}(\alpha)&\equiv L^{\{i_1\ldots i_N\},i}_{\{j_1\ldots j_N\},j}(\alpha;\alpha_1,\ldots,\alpha_N)\\&=S^{jp_1}_{i_1j_1}(\alpha_1-\alpha)S^{p_1p_2}_{i_2j_2}(\alpha_2-\alpha)\ldots S^{p_{N-1},i}_{i_Nj_N},\end{aligned}\tag{4.1.45}$$

an important object which we shall often use. The trace of the monodromy matrix on the non-regular lattice defines the transfer matrix of the vertex-lattice model:

$$\mathbf{T}(\alpha)=\operatorname{Tr}\mathbf{L}(\alpha)=\sum_i L^{\{i_1\ldots i_N\},i}_{\{j_1\ldots j_N\},i}(\alpha;\alpha_1,\ldots,\alpha_N).\tag{4.1.46}$$

Hereafter $\alpha$ is called a *spectral parameter*.

The most important property of the parametric set of transfer matrices (4.1.46) is their *commutativity at different values of the spectral parameter* (Baxter 1972 a)

$$[\mathbf{T}(\alpha),\mathbf{T}(\beta)]=0.\tag{4.1.47}$$

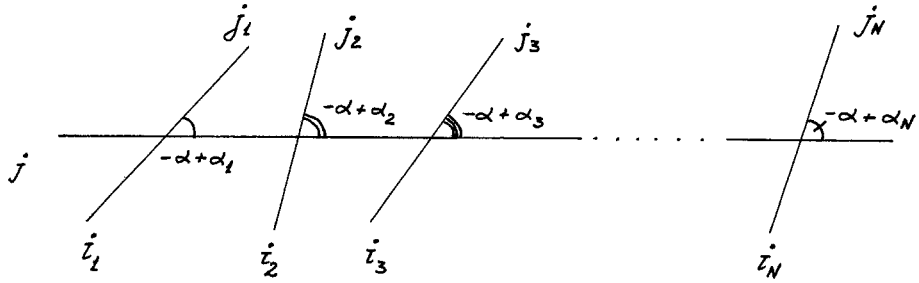
This is the consequence of the triangle equations and is the necessary condition for exact diagonalizability.

In the Baxter eight-vertex model the number of colours is equal to two and the colour of the bond is represented by the arrows. Each vertex has an even number of arrows entering and leaving it. The vertex in the eight-vertex model can be written as

$$S^{a_2a_2'}_{a_1a_1'}=\sum_{i=0}^{3} w_i\sigma^i_{a_1a_1'}\sigma^i_{a_2a_2'},\tag{4.1.48}$$

where $\boldsymbol{\sigma}^i$, $(i=1,2,3)$ are Pauli matrices and $\boldsymbol{\sigma}^0=1$. Baxter (1972 a) showed that the vertex weight (4.1.48) lies on the curve $S^{a_2a_2'}_{a_1a_1'}(\alpha)$ determined by the triangle equation.

Fig. 4.6




The graphical representation of the monodromy matrix.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The following parametrization for $w_i$ exists:

$$w_1 : w_2 : w_3 : w_0 = \frac{cn(\alpha, l)}{cn(\zeta, l)} : \frac{dn(\alpha, l)}{dn(\zeta, l)} : \frac{sn(\alpha, l)}{sn(\zeta, l)}, \tag{4.1.49}$$

where $l$ is the modulus of the elliptic functions and $\zeta$ is an arbitrary parameter. As has been mentioned above, the eight-vertex model is related to the spin-1/2 anisotropic Haisenberg ring (4.1.43). The following relation is valid for the hamiltonian of the spin ring:

$$\mathscr{H}_{xyz} = -\left(\mathbf{T}^{-1}(\alpha)\frac{d\mathbf{T}(\alpha)}{d\alpha}\right)_{\alpha=0} \tag{4.1.50}$$

(Sutherland 1970, Baxter 1972 b).

Due to the commutativity of the transfer matrices with different parameters, the model has a series of motion integrals

$$[\mathscr{H}_{xyz}, \mathbf{T}(\alpha)] = 0 \tag{4.1.51}$$

and is completely integrable on the quantum level. Using (4.1.51) one can construct the set of the local motion integrals $Q_n$:

$$Q_n = -\frac{d^n}{d\alpha^n} \ln \mathbf{T}(\alpha)|_{\alpha=0}. \tag{4.1.52}$$

The $Q_n$ operators are represented as the sum of terms containing only the products of spin-operators placed in the finite ($n$) number of the nearest sites of the chain.

The common lore is that the existence of a large class of exactly solvable two-dimensional system and/or one-dimensional quantum-field theories is due to the existence of the non-trivial solutions of the triangle equations (Zamolodchicov 1980).

These celebrated equations appeared later when the $1+1$-dimensional relativistic factorized $S$ matrices were studied (Zamolodchicov 1980). The factorization conditions impose non-trivial constraints on the two-particle amplitudes. Assuming certain symmetry properties of the $S$ matrix and using these relations as equations one can solve them together with the unitary and analyticity equations. The relativistic invariance, crossing symmetry and some quasiclassical results are often sufficient to derive the explicit formulae for the $S$ matrix elements. This is the way by which the $S$ matrices of many quantum-field theories have first been obtained (for a review see Zamolodchicov and Zamolodchicov 1979). We already know a considerable number of solutions of the triangle equations corresponding to different 'isotopic' symmetries. The general solution with the two-dimensional representation possessing $Z_2 \times Z_2$ symmetry was obtained by Baxter (1972) (4.1.48). For an arbitrary dimension of isotopic space the solutions with $O(n)$ symmetry, (Zamolodchicov and Zamolodchicov 1978) and $U(n/2)$ symmetry (for even $n$) (Berg *et al.* 1978) are known. Some of these solutions have been generalized to supersymmetric models (Schankar and Witten 1978). One can find other known solutions of the triangle equations in the review of Kulish and Sklyanin (1981).

A method also exists which allows us to construct the solution for arbitrary finite-dimensional irreducible representations of the given symmetry group starting from the solution for the fundamental representation of this group (Kulish and Sklyanin 1981, Kulish and Reshetikhin 1980, Kulish *et al.* 1981, Fateev 1980).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

One important property of the triangle equations was discovered by Belavin (1980): triangle equations possess symmetry under the action of the discrete subgroup of the Lorentz group, acting independently on particles with different momenta. It has been shown that this symmetry may be applied to the determination of all the elements of the $S$-matrix satisfying the triangle equations. In particular, Belavin constructed the solution with $Z_N \times Z_N$ symmetry generalizing Baxter's $Z_2 \times Z_2$ matrix.

The operators $\mathbf{T}_j$ born by the Bethe method appeared to be related with the trace of the monodromy matrix ((4.1.45), (4.1.46)). The latter is the central object of the modern theory of integrable systems. This relation was first noticed by Belavin (1979). Namely,

$$\mathbf{T}_j = \mathbf{T}(\alpha, \alpha_1, \ldots, \alpha_N)|_{\alpha=\alpha_j}. \tag{4.1.53}$$

In view of (4.1.47) it follows from (4.1.53) that the operators $\mathbf{T}_j$ are commutative. We prove that below.

A deep relation between the well-known 'inverse scattering method' applicable to the classical non-linear equations (for a review, see Zakharov *et al.* 1980), on the one hand, and the Bethe method in Baxter's version, on the other hand, has been elucidated recently. This relation has been realized by Faddeev, Sklyanin and Takhtajan and brought these authors to the remarkable method known as the *quantum inverse-scattering method.* It combines the main ideas and methods of both the quantum and classical theory of integrable systems (Faddeev and Sklyanin 1978, Sklyanin 1978, Faddeev 1980, Sklyanin *et al.* 1979, Kulish and Sklyanin 1979, Thacker and Wilkinson 1979, Honerkamp *et al.* 1979). Today, almost all the results obtained earlier by means of the Bethe Ansatz have been rederived in the framework of the quantum inverse-scattering method. This method enables one to derive the equations determining all eigenvalues of the trace of the monodromy matrix (4.1.45) within the framework of the general algebraic scheme, without writing down the eigenvectors in an explicit form. Thus, this procedure may be considered as the algebraization of the Bethe Ansatz (for a review see Sklyanin 1980, Takhtajan 1981). It is most convenient to use this method for diagonalization of the trace of the monodromy matrix $\mathbf{T}(\alpha)$ and we shall follow it below.

The triangle equations are an essential ingredient of the algebraic method. They must be satisfied by the matrix determining the commutation relations between the elements of the monodromy matrix. It is the quantum analogue of the $L$-operator of the classical inverse scattering method.

Namely,

$$S_{kk'}^{qq'}(\alpha-\alpha')\mathbf{L}_{q'}^{l}(\alpha')\mathbf{L}_{k}^{l'}(\alpha) = \mathbf{L}_{k}^{k'}(\alpha)\mathbf{L}_{q}^{q'}(\alpha')S_{q'l}^{k'l'}(\alpha-\alpha') \tag{4.1.54}$$

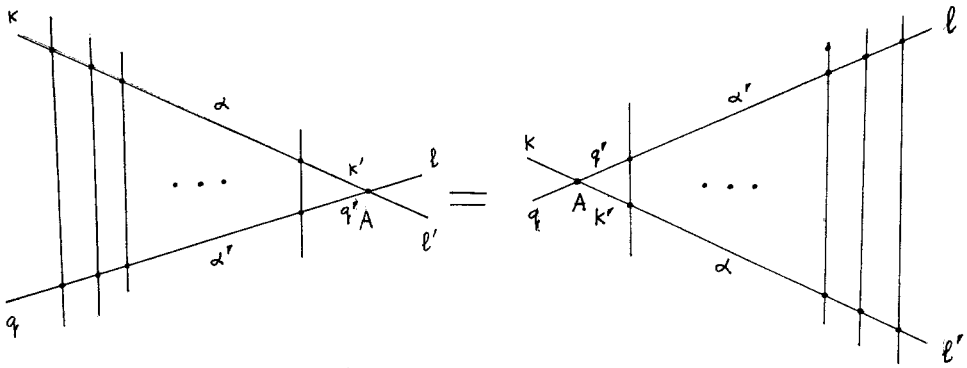
(for brevity we omit the operator indices) (Baxter 1972 a, Sklyanin *et al.* 1979). This relation is illustrated in fig. (4.7). By virtue of (4.1.54) it follows that the operators $\mathbf{T}(\alpha)$ are commutative (4.1.47). In the next section we prove this important relation.

The quantum inverse scattering method, first applied to the $S$ matrix with a dimension $n=2$ (Sklyanin 1978, Takhtajan and Faddeev 1979), was generalized to an arbitrary representation of $O(3)$ (Fateev (1980) and to the $SU(n)$ symmetric $S$ matrix (4.1.37) (Kulish and Reshetihin 1981, Arinstein 1980).

In conclusion let us mention another powerful approach to the eigenvalue problem for the $\mathbf{T}$-matrix. It may be shown that for $N \to \infty$ each member of the

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 4.7




The graphical representation of $L$-matrix commutation rules.

parametric set of $\mathbf{T}(\alpha)$ corresponds to another member of the same set $\mathbf{T}(\Phi(\alpha))$ satisfying the following relation

$$\lim_{N\to\infty} \mathbf{T}(\alpha)\mathbf{T}(\Phi(\alpha)) = \mathbf{I}\Psi^N(\alpha), \tag{4.1.55}$$

where $I$ is a unit matrix, and $\Phi(\alpha)$ and $\Psi(\alpha)$ are the known functions depending on the explicit form of the $\mathbf{T}$-matrix. From (4.1.55) it follows that in the thermodynamic limit $N\to\infty$ the eigenvalues of the $\mathbf{T}$ matrix satisfy the functional equation:

$$t(\alpha)t(\Phi(\alpha)) = \Psi(\alpha) \tag{4.1.56}$$

(Stroganov 1979, Zamolodchicov 1979, Baxter 1980).

It may easily be shown that the maximum eigenvalue of the transfer matrix $\mathbf{T}(\alpha)$, i.e. the partition function of a lattice model, is an analytical function of $\alpha$. The condition of analyticity enables us to solve eqn. (4.1.56) unambiguously. Other solutions of eqn. (4.1.56) correspond to the excited states of the $1+1$ dimensional quantum-field theory. In particular, this method permits us to reproduce the excitation spectrum of the $XYZ$ chain (Tetelman 1981).

Developing this approach, Reshetikhin (1983) and Baxter and Pearce (1982), obtained the functional equations for eigenvalues of $\mathbf{T}(\alpha)$ for a finite $N$. With the use of some additional symmetry and analyticity properties he derived the Bethe-Ansatz equations for some models for a case of finite $N$ (*the so-called analytical Bethe Ansatz*). The methods reviewed above reduce the problem of the spectrum of the many-body system to the solution of the transcendental Bethe-Ansatz equation. The simplest case corresponds to the system of eqns. (4.1.41); in more complicated cases one has a Bethe-Ansatz hierarchy.

Another branch of the theory of exactly integrable systems consists of the development of a mathematical technique for the investigation of equations of this kind in the continuous limit ($N\to\infty$) and obtaining physical results. This branch of theory is relatively independent of the methods discussed above and has its own history originating from the earlier Bethe work (1931). Let us consider the essential stages of its history.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Bethe constructed the wavefunction of the ground state of the antiferromagnetic spin ring, which contains $M=N/2$ parameters—rapidities of the up spin waves. So the ground state is described by the system of $N/2$ equations (4.1.41).

The precise form of these equations in the thermodynamic limit ($N\to\infty$) was adequately discussed by Hulten (1938). In the thermodynamic limit the state of the system can conveniently be described not by a discrete set of rapidities $\{\lambda_\alpha\}$ but by the rapidity distribution function:

$$\rho(\lambda)=\lim_{N\to\infty}\frac{1}{N(\lambda_{\alpha+1}-\lambda_\alpha)}. \tag{4.1.57}$$

The ground-state distribution is obtained from (4.1.42) and the integers $N_\alpha$ are chosen as closely spaced as possible: $N_{\alpha+1}=N_\alpha+1$ (the proof was given by Yang and Yang 1966 a). By subtracting Bethe-Ansatz equations (4.1.42) for adjacent $k_\alpha$'s and replacing the sum in (4.1.42) by an integral one, the Fredholm integral equation with the symmetrical kernel is obtained:

$$2\pi\rho(\lambda)=dk(\lambda)/d\lambda-\int_{-B}^{B}\Phi'(\lambda-\lambda')\rho(\lambda')d\lambda'. \tag{4.1.58}$$

The subsidiary condition determining the number of particles is

$$\frac{M}{N}=\int_{-B}^{B}\rho(\lambda)d\lambda. \tag{4.1.59}$$

While the ground-state energy is given by

$$\frac{E}{N}=\int_{-B}^{B}\cos k(\lambda)\rho(\lambda)d\lambda \tag{4.1.60}$$

(Hulten 1938, Lieb and Liniger 1963).

For the ground state of the Haisenberg chain one has $M=N/2$, $S^z=0$ and $B=\infty$ (for $|\cos\mu|<1$ or $B=\pi(\cos\mu<-1)$). The ground-state energy was found by Orbach (1958) and Walker (1959) and by Baxter (1972 b) for the $XYZ$ chain. Griffith (1964) suggested the method for obtaining the low field magnetic susceptibility of the Haisenberg chain (i.e. the method for the investigation of eqn. (4.1.58) in the limit of $B\gg1$). His method was developed by Yang and Yang (1966 b) and applied to the anisotropic Haisenberg chain.

The magnetic susceptibility and the ground-state energy as a function of the density of particles for the Hubbard model were investigated by Takahashi (1970 a, b) and Krivnov and Ovchinnicov (1974). Recently, the magnetic properties of interacting one-dimensional fermions were studied in an interesting paper of Japaridze and Nersisyan (1981). The isotopic Thirring model with the $U(1)$ isospin symmetry was considered in Japaridze *et al.* (1983).

The other line of investigation of Bethe-Ansatz equations is an analysis of the excitation spectrum. Bethe (1931) found that the solutions of (4.1.46) lie in the general case in the complex plane. In the thermodynamic limit, the roots of the Bethe-Ansatz equations are grouped in 'strings' characterized by a common real abscissa and an order $n$. A string of the order $n$ for the isotropic Haisenberg chain consists of the set

$$\lambda_\alpha^{(n,j)}=\lambda_\alpha^n+i(n+1-2j);\qquad j=1,\ldots,n. \tag{4.1.61}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

These states describe the excitations of the antiferromagnetic spin–1/2 chain (note that the ground state of the $S$-spin chain is formed by strings of the order $2S$) and play an important role for the elementary excitation classification and for the construction of equilibrium thermodynamics. A considerable part of the literature dealing with the Bethe method is devoted to the derivation of the excitation spectrum (see, for example, Des Cloizeaux and Pearson 1962, Des Cloiseaux and Gaudin 1966, Ovchinnicov 1969, Johnson *et al.* 1973). However, total clarity in this question has been attained only recently by Takhtajan and Faddeev (1981) and Faddeev and Takhtajan (1981).

The rich excitation spectrum of the Sine–Gordon model (or the equivalent massive Thirring model) was investigated by Bergnoff and Thacker (1979), Korepin (1979), and Japaridse *et al.* (1982) and by Andrei and Lowenstein (1980) for the chiral Gross–Neveu model. The spectrum of the one-dimensional Hubbard chain was studied in the original work of Lieb and Wu (1968) and also by Ovchinnicov (1969), Krivnov and Ovchinnikov (1974), Filyov (1977) and Woynarovich (1982). One can also easily calculate the elements of the scattering matrix. The method based on the Bethe-Ansatz equations was suggested by Korepin (1979).

An important step in the investigation of the integrable quantum model was made in the remarkable paper of Yang and Yang (1969). In this paper the method for evaluating the equilibrium thermodynamical properties of the system described the Bethe-Ansatz equation was suggested. Yang and Yang showed that in contrast to linear integral equations for $T=0$, the equilibrium thermodynamics at finite temperatures must be derived from the solution of the non-linear integral equations. A large system with all states being macroscopically populated is naturally described by density distributions of *particles* $\rho(\lambda)$ and *holes* $\tilde{\rho}(\lambda)$. These functions are related to each other by the Bethe-Ansatz equations and determine a contribution to the whole entropy of the state. At temperature $T$ we should maximize the contribution to the partition function from the states described by $\rho$ and $\tilde{\rho}$. Thus, we get the non-linear integral equation for the function $\varepsilon(\lambda)=T\ln\tilde{\rho}(\lambda)/\rho(\lambda)$. The determination of this basic function first introduced by Yang and Yang (1969) allows us to calculate all thermodynamic properties.

The method of Yang and Yang is the most natural and consistent approach to the investigation of Bethe-Ansatz equations with a large number of particles, even for the zero-temperature case. The main point is that the function $\varepsilon(\lambda)$ is the energy of elementary excitations (Yang and Yang 1969). For another derivation of this relation see Japaridse *et al.* (1982). Thus, the method of Yang and Yang allows us to evaluate low-lying excitations and equilibrium thermodynamics within a general framework. By means of this approach the spectrum of the elementary excitations of the anisotropic Haisenberg spin chain (Johnson 1974, Puga 1980, and the Sine–Gordon model (Japaridze *et al.* 1982) have been investigated. The original paper of Yang and Yang is devoted to a one-dimensional system of bosons with a repulsive delta-function interaction.

The reformulation of the Yang and Yang method for the thermodynamics of the one-dimensional Haisenberg chain was performed by Gaudin (1971 a) and Johnson and McCoy (1972) and in the interesting series of papers by Takahashi (1971 a, 1973) and Takahashi and Suzuki (1972).

Today, the thermodynamics for a number of one-dimensional many-body problems have been investigated on the basis of the exact solution. Namely, a one-dimensional system of fermions with repulsive delta-function interaction was

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

studied by Takahashi (1971 b), the Hubbard model by Takahashi (1972, 1974 a), the $SU(2)$ Thirring model by Japaridze and Nersisyan (1981), the Sine–Gordon model by Fowler and Zotos (1982) and the arbitrary spin Haisenberg chain by Babujan (1982).

The authors attach great importance to the Yang–Yang method. In the present review we consider this method in detail in the sections devoted to the exchange and Anderson models. We have enumerated the main applications of the quantum theory of integrable systems. Of course, our list (and references) does not pretend to be complete and is oriented primarily to the theory of magnetic alloys. So far there is only one review concerning exact integrability in one-dimensional quantum-field theory and two-dimensional lattice statistics (Thacker 1981).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

### 4.2. *The Bethe Ansatz for the s–d exchange model*

#### 4.2.1. *The effective hamiltonian*

As we saw in § 2.1, the problem of scattering by a single impurity is, in essence, one-dimensional. Here we shall show this once more by starting directly from the s–d exchange model (I)

$$\mathscr{H}_{s-d}=\sum_{\substack{k\\ \sigma=\uparrow,\downarrow}} \varepsilon_k c^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}+\frac{1}{2}I\sum_{\substack{k,k'\\ \sigma,\sigma'}} c^{+}_{\mathbf{k}\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}c_{\mathbf{k}'\sigma'}\mathbf{S}. \tag{4.2.1}$$

We expand the plane electronic wave in spherical waves about the impurity

$$c^{+}_{\mathbf{k}\sigma}=\sum_{l}\sum_{lm=-l}^{l} Y_{lm}\left(\frac{\mathbf{k}}{k}\right)c^{+}_{klm\sigma}. \tag{4.2.2}$$

Writing the hamiltonian (4.2.1) in terms of $c^{+}_{klm\sigma}$, we have

$$\mathscr{H}_{\text{s–d}}=\sum_{k,l,m,\sigma}\varepsilon_k c^{+}_{klm\sigma}c_{klm\sigma}+\frac{1}{2}I\sum_{\substack{k,k'\\ \sigma,\sigma'}} c^{+}_{k00\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}c_{k'00\sigma'}\mathbf{S}, \tag{4.2.3}$$

where only the $s$ wave interacts with the impurity.

Next, we assume that the interaction amplitude is small, so that $T_{\text{K}}\ll\epsilon_{\text{F}}$. Whence, at $H$, $T\ll\epsilon_{\text{F}}$ we can ignore the electronic states that lie far from the Fermi surface and consider a linear section of the spectrum near $k=k_{\text{F}}$

$$\varepsilon(k)=\epsilon_{\text{F}}+v_{\text{F}}(k-k_{\text{F}}). \tag{4.2.4}$$

In what follows we take $v_{\text{F}}$ equal to unity. Reckoning the momentum from $k_{\text{F}}$, we arrive at the effective hamiltonian for the s–d model†

$$\mathscr{H}_{\text{s–d}}=\sum_{p,\sigma=\uparrow,\downarrow} pc^{+}_{p\sigma}c_{p\sigma}+\frac{1}{2}I\sum_{\substack{p,p'\\ \sigma,\sigma'}} c^{+}_{p\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}c_{p'\sigma'}\mathbf{S}. \tag{4.2.5}$$

Here $c^{+}_{p\sigma}$ and $c_{p\sigma}$ are the creation and annihilation operators for an electron in an $s$ state with the momentum $p+k_{\text{F}}$.

The condition that (4.2.1) be integrable imposes stringent restrictions on the two-particle scattering amplitudes and, therefore, on the hamiltonian. For this

† The emerging problem could be called a one-half-dimensional, since the particles have only one Fermi point instead of two as is customary.

reason even small variations in the hamiltonian at small distances, which, practically, do not affect the properties of the system, almost always destroy the integrability. Below we shall show that the hamiltonian (4.2.5) is completely integrable.

4.2.2. *The coordinate Bethe Ansatz*

Here we formulate and prove Bethe's hypothesis for the exchange model. First, we shift the hamiltonian (4.2.5) to the coordinate representation. Suppose that $x$ is a coordinate on a straight line passing through the impurity and

$$c_\sigma(x) = \int \exp(ipx) c_\sigma(p) dp. \tag{4.2.6}$$

Then the hamiltonian (4.2.4) for the s–d model is

$$\mathscr{H}_{\text{s–d}} = \int dx \left[ -i \sum_\sigma c_\sigma^+(x) \frac{\partial}{\partial x} c_\sigma(x) + \frac{1}{2} I \delta(x) \sum_{\sigma,\sigma'} c_\sigma^+(x) \boldsymbol{\sigma}_{\sigma\sigma'} c_{\sigma'}(x) \mathbf{S} \right]. \tag{4.2.7}$$

We consider the eigenstate of (4.2.5) in which there are electrons with spin components $\sigma_1, \ldots, \sigma_N$ and a localized moment with the component $\mathscr{s} = -S, \ldots, S$:

$$|\Psi\rangle = \int \Psi_{\sigma_1 \ldots \sigma_N, \mathscr{s}}(x_1, \ldots, x_N) c_{\sigma_1}^+(x_1) \ldots c_{\sigma_N}^+(x_N) (S^+)^{\mathscr{s}+S_N} \prod_{j=1}^{\mathscr{s}+S_N} dx_j |0\rangle, \tag{4.2.8}$$

where $|0\rangle$ is the state without particles and with a component of the impurity moment equal to $-S$.

The wave function $\Psi_{\sigma_1 \ldots \sigma_N, \mathscr{s}}$ satisfies Schrödinger's equation

$$\left( -i \sum_{j=1}^N \frac{\partial}{\partial x_j} - E \right) \Psi_{\sigma_1 \ldots \sigma_N, \mathscr{s}} + \frac{1}{2} I \sum_{j=1}^N \delta(x_j) \boldsymbol{\sigma}_{\sigma_j \sigma_j'} \mathbf{S}_{\mathscr{s}\mathscr{s}'} \Psi_{\sigma_1 \ldots \sigma_j' \ldots \sigma_N, \mathscr{s}'} = 0. \tag{4.2.9}$$

Bethe's method provides the means for finding every solution of this equation for an arbitrary number of particles.

Suppose that $Q = \{q_0, \ldots, q_N\}$ is a permutation of the numbers $\{0, 1, \ldots, N\}$ while $Q' = \{q_1', \ldots, q_N'\}$ and $P = \{p_1, \ldots, p_N\}$ are permutations of the numbers $\{1, \ldots, N\}$. with $Q'$ coinciding with $Q$ from which $q_i = 0$ is excluded, then in the region $X_Q = \{x_{q_0} < x_{q_1} < \ldots < x_{q_N}\}$ the wavefunction is *Bethe Ansatz*:

$$\Psi_{\sigma_1 \ldots \sigma_N, \mathscr{s}}(x_1, \ldots, x_N) = \sum_P A_{\sigma_1 \ldots \sigma_N, \mathscr{s}}(Q; Q'|P) \exp\left( i \sum_{i=1}^N k_{p_i} x_i \right), \tag{4.2.10}$$

where the first sum is over all permutations $P$, $\{k_j\}$ is a sequence of different values of $k_j$ and $x_0 = 0$. The state (4.2.8) is the eigenstate of the hamiltonian (4.2.5) with the energy

$$E = \sum_{j=1}^N k_j. \tag{4.2.11}$$

The factors $A_{\sigma_1, \ldots, \sigma_N, \mathscr{s}}$ are, obviously, not independent. First we must require that $\Psi$ be antisymmetric under permutations in the pairs $(x_i, \sigma_i)$. As a result

$$A_{\sigma_1, \ldots, \sigma_N, \mathscr{s}}(Q; Q'|P) = A_{\sigma_{q'_1} \ldots \sigma_{q'_N}, \mathscr{s}}(Q; Q'P)(-1)^P, \tag{4.2.12}$$

where $Q'P$ is the product of the permutations and $(-1)^P$ is the parity of the permutation $P$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The factors $A$ for different regions are linked through the Schrödinger equation (4.2.9). As mentioned above, the hypothesis that the wavefunction consists of a finite number of waves implies that the $S$ matrix is two-particle factorized. In other words, the interrelation between the $A$'s in two neighbouring regions is determined by the characteristics of only two particles or a particle and an impurity on the boundary. Suppose that the boundary between the regions $X_Q$ and $X_{\tilde{Q}}$ is the plane $X_j=0$, i.e. $Q$ and $\tilde{Q}$ differ in the permutation of the $j$th particle and the impurity, then

$$A_{\ldots\sigma_j\ldots;\sigma}(\tilde{Q})=R^{\sigma_j\sigma_j'}_{\sigma\sigma'}A_{\ldots\sigma_j'\ldots;\sigma'}(Q), \tag{4.2.13}$$

where the matrix

$$R^{\sigma_j\sigma_j'}_{\sigma\sigma'}\equiv\mathbf{R}_{0j}=\exp(iI\boldsymbol{\sigma}_j\cdot\mathbf{S}/2). \tag{4.2.14}$$

Indeed, let us take the case of one particle scattered by an impurity. Then

$$-i\frac{d}{dx}\Psi_{\sigma,\sigma}(x)+\frac{1}{2}I\delta(x)\boldsymbol{\sigma}_{\sigma\sigma'}\cdot\mathbf{S}_{\sigma\sigma'}\Psi_{\sigma',\sigma'}(x)=E\Psi_{\sigma,\sigma}(x). \tag{4.2.15}$$

This equation is poorly defined. To redefine it, we substitute a smooth potential $V_\varepsilon(x)$ for the delta-function in (4.2.14) such that $\lim_{\varepsilon\to 0}V_\varepsilon(x)=1/2I\delta(x)$. Then the solution of eqn. (4.2.15) has the form

$$\Psi_{\sigma,\sigma}(x)=\exp(ikx)A_{\sigma,\sigma}(x), \tag{4.2.16}$$

where the dependence of the matrix $A$ on the coordinate $x$ is determined thus:

$$A_{\sigma,\sigma}(x)=\exp\left(i\boldsymbol{\sigma}_{\sigma\sigma'}\cdot\mathbf{S}_{\sigma\sigma'}\int_x^y V_\varepsilon(x')\,dx'\right)A_{\sigma',\sigma'}(y). \tag{4.2.17}$$

Tending $\varepsilon$ to zero, we find that

$$A_{\sigma,\sigma}(x<0)=R^{\sigma\sigma'}_{\sigma\sigma'}A_{\sigma',\sigma'}(x>0), \tag{4.2.18}$$

where the matrix $\mathbf{R}$ is given by (4.2.14).

Now let us assume that the plane $x_i=x_j$ is the boundary between $X_Q$ and $X_{\tilde{Q}}$. In this case the factors $A(Q)$ and $A(\tilde{Q})$ are connected via the permutation operator:

$$\begin{aligned}A_{\ldots\sigma_i\ldots\sigma_j\ldots}(\tilde{Q})&=P^{\sigma_i\sigma_i'}_{\sigma_j\sigma_j'}A_{\ldots\sigma_i'\ldots\sigma_j'\ldots}(Q)\\&=A_{\ldots\sigma_j\ldots\sigma_i\ldots}(Q),\end{aligned} \tag{4.2.19}$$

where

$$P^{\sigma_i\sigma_i'}_{\sigma_j\sigma_j'}=\frac{1}{2}(\mathbf{1}\cdot\mathbf{1}+\boldsymbol{\sigma}_{\sigma_i\sigma_i'}\cdot\boldsymbol{\sigma}_{\sigma_j\sigma_j'})=\delta_{\sigma_i\sigma_j'}\delta_{\sigma_j\sigma_i'}$$

is the permutation operator. This fact requires some explaining.

Let us take two particles far from the impurity, say $x_1$, $x_2<0$. The particles are free:

$$-i(\partial/\partial x_1+\partial/\partial x_2)\Psi(x_1,x_2)=E\Psi(x_1,x_2). \tag{4.2.20}$$

The usual solution of this equation providing the first perturbation-theory approximation is

$$\Psi_{\sigma_1,\sigma_2}(x_1,x_2)=\exp(ik_1x_1+ik_2x_2)A_{\sigma_1\sigma_2}-\exp(ik_2x_1+ik_1x_2)A_{\sigma_2\sigma_1}, \tag{4.2.21}$$

where the factors $A_{\sigma_1\sigma_2}$ do not depend on the position of the particles. What will

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

happen with the wave (4.2.21) after the particles scatter on the impurity? We can readily see that in the region $x_1, x_2 > 0$ the wavefunction is not given by (4.2.21). Indeed, in transferring from the region $x_1, x_2 < 0$ first to the region $x_1 < 0 < x_2$ and then to the region $0 < x_1 < x_2$ the factor $A_{\sigma_1\sigma_2;\sigma}$, according to (4.2.13), becomes $\mathbf{R}_{10}\mathbf{R}_{20}A$. Another sequence of events (say, the first particle is scattered by the impurity and then the second) leads to quite a different state. Suppose that the electrons, the first having spin 'up' and the second spin 'down', are scattered with a spin flip on the impurity having spin 'up'. The first electron cannot change the direction of the impurity spin, but the second flips this spin over. If the sequence is reversed, then the impurity spin flips twice and its direction as a result does not change. In other words, the matrices $\mathbf{R}_{10}$ and $\mathbf{R}_{20}$ do not commute:

$$\mathbf{R}_{10}\mathbf{R}_{20} \neq \mathbf{R}_{20}\mathbf{R}_{10}. \tag{4.2.22}$$

These arguments vividly demonstrate that particles cannot be considered individually in the presence of the impurity. The fact that the impurity has a degree of freedom is sufficient to make the problem a many-particle one.

To write the correct scattering wavefunction in the region $x_1, x_2 > 0$, we point once more to the peculiar feature of the hamiltonian (4.2.7). All particles move in one direction with the same velocity. Therefore, if $\Psi(x_1, x_2)$ is a solution of eqn. (4.2.20), then $f(x_1 - x_2)\Psi(x_1, x_2)$ is also a solution (here $f(x)$ is an arbitrary function that may have, for example, a discontinuity at $x = 0$). This property enables us easily to find the wavefunction in the region $x_1, x_2 > 0$. The wavefunction is again given by (4.2.21), but the factors have a discontinuity on the line $x_1 = x_2$:

$$\Psi(x_1, x_2) = [\mathbf{R}_{20}\mathbf{R}_{20}\theta(x_1 - x_2) + \mathbf{R}_{10}\mathbf{R}_{20}\theta(x_2 - x_1)] \times (\exp(ik_1x_1 + ik_2x_2) - \mathbf{P}_{12}\exp(ik_1x_2 + ik_2x_1))A. \tag{4.2.23}$$

Obviously, in this case the discontinuity in the wavefunction at $x_1 = x_2$ does not mean that there is an interaction far from the impurity. However, the scattering wavefunction does depend on the order of events in the scattering of particles, and the 'memory' of this is not lost, as the particles move away from the impurity.

The approach we have just studied is not very well suited for deriving a wavefunction of a system of $N$ particles that satisfies the given boundary conditions. The correct way to do this is to 'order' the spins of the incoming particles in the region $x_1, x_2 < 0$ so that the impurity 'knows' which particle it will encounter first. This is another solution of the Schrödinger equation (4.2.20):

$$\Psi(x_1, x_2) = (\exp(ik_1x_1 + ik_2x_2) - \exp(ik_1x_2 + ik_2x_1) \times [\theta(x_1 - x_2) + \mathbf{P}_{12}\theta(x_2 - x_1)]A. \tag{4.2.24}$$

Unlike solution (4.2.21), this function changes when both the spins of the particles and their momenta $k_1$ and $k_2$ are interchanged and corresponds to the particles being '*ordered*' on the straight line that passes through the impurity. Strictly speaking $k_1$ and $k_2$ are not the momenta of free particles. Indeed, $\Psi_{\sigma_1\sigma_2}(x_1, x_2)$ is not an eigenfunction of the operators $i\partial/\partial x_1$ and $i\partial/\partial x_2$ separately. Rather, $k_1$ and $k_2$ are the momenta of charge density waves, whose generation does not lead to a local change in a spin. They resemble momenta of spinless fermions: the wavefunction (4.2.24) vanishes at $k_1 = k_2$ irrespective of the total spin of the system. We see, therefore, that free particles with a linear spectrum are described equally well by

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

functions (4.2.21) and (4.2.24). The first function corresponds to a unit scattering matrix: $S^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'} = I^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'} \equiv \delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'}$, while the second corresponds to an $S$ matrix that is the permutation operator

$$S^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'} = P^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'} \equiv \delta_{\sigma_1\sigma_2'}\delta_{\sigma_2\sigma_1'}. \tag{4.2.25}$$

We return to the case of two particles scattered by an impurity. As usual, there are two ways in which we can go from the region $x_1 < x_2 < 0$ to, say, the region $x_1 > x_2 > 0$. The first path, i.e.

$$x_1 < x_2 < 0 \to x_1 < 0 < x_2 \to 0 < x_1 < x_2 \to 0 < x_2 < x_1$$

transforms $A$ into $\mathbf{P}_{12}\mathbf{R}_{10}\mathbf{R}_{20}A$. The other path, namely

$$x_1 < x_2 < 0 \to x_2 < x_1 < 0 \to x_2 < 0 < x_1 \to 0 < x_2 < x_1,$$

brings us to another transformation matrix:

$$A \to \mathbf{R}_{20}\mathbf{R}_{10}\mathbf{P}_{12}A.$$

But now the result in both cases must be the same, since

$$\mathbf{R}_{20}\mathbf{R}_{10}\mathbf{P}_{12} = \mathbf{P}_{12}\mathbf{R}_{10}\mathbf{R}_{20} \tag{4.2.26}$$

(see fig. 4.8).

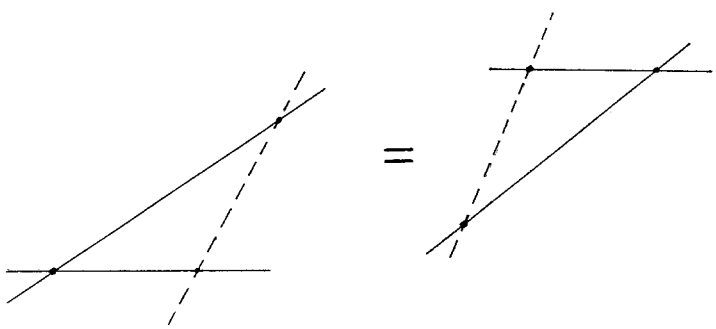
We have, therefore, proved the Bethe hypothesis: the general solution of the Schrödinger equation (4.2.9) is given by formula (4.2.10) together with conditions (4.2.12), (4.2.13) and (4.2.19) (Andrei 1980, Wiegmann 1980 a, 1981).

Applying these conditions, we can express $A(Q; Q'|P)$ in terms of $A(I; I'|P)$, with $I = \{1, \ldots, N\}$ being a unit permutation. To do it we must take $Q$ as one of the possible products of pair transpositions and to each cofactor assign either operator $\mathbf{P}_{ij}$ or operator $\mathbf{R}_{j0}$, depending on whether this transposition changes the position of particles $i$ and $j$ or of particle $j$ and the impurity. Condition (4.2.26), together with the unitary conditions

$$\mathbf{P}_{ji}\mathbf{P}_{ij} = \mathbf{I}, \qquad \mathbf{R}_{j0}\mathbf{R}_{0j} = \mathbf{I}, \tag{4.2.27}$$

guarantees that all ways of factorizing $Q$ into products of pair transpositions lead to the same results.

Fig. 4.8



The triangle equation for the s–d exchange model. The moving particle corresponds to the solid line and the impurity to the dashed line.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

In conclusion of this section we make the following remark. The factorization conditions, in which one $S$ matrix does not depend on a spectral parameter and is equal to the permutation operator, are satisfied for an arbitrary form of the $S$ matrix. It becomes obvious if one rewrites eqn. (4.2.26) as

$$\mathbf{P}_{12}\mathbf{R}_{10}\mathbf{R}_{20}\mathbf{P}_{21}=\mathbf{R}_{20}\mathbf{R}_{10}.$$

Thus the coordinate Bethe Ansatz (4.2.10) holds irrespective of the matrix structure of the interaction of Dirac's particles. We shall see it is not yet the integrability below.

Due to this fact Hewson (1982) gave an alternative approach which does not use the coordinate Bethe Ansatz and derived the coordinate wavefunction (4.2.10) as a general solution of the Schrödinger equation (4.2.15). Proof of the completeness of the states (4.2.10) was made by Schulz (1982).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

4.2.3. *Periodic boundary conditions*

Let us place our one-dimensional system on the ring with length $L$ and require that the $\Psi$ function satisfy the periodic boundary conditions (PBC):

$$\Psi(x_1,\ldots,x_j,\ldots,x_N)=\Psi(x_1,\ldots,x_j+L,\ldots,x_N). \tag{4.2.28}$$

The conditions (4.2.28) may be rewritten as the constraints on the coefficients $A(Q;Q'P)$ in formula (4.2.10). See, for example, the coefficient $A(I;I')=\xi$. To arrive from $x_j$ to $x_j+L$ one should successfully transpose $j$th particle with $j+1$, $j+2,\ldots$ particles, the impurity and $1,2,\ldots,j^{j-1}$ particles passing through a whole ring. On transposing with a particle the pre-exponent factor $A(I;I')$ transforms by the permutation operator $\mathbf{P}_{ji}$ (4.2.19) and on transposing with the impurity transforms by the operator $\mathbf{R}_{j0}$ (4.2.13). Between collisions the wavefunction acquires the phase shift $k_jL$. Thus PBCs lead us to the problem of simultaneous diagonalization of the operators

$$\mathbf{T}_j=\mathbf{P}_{jj+1}\ldots\mathbf{P}_{jN}\mathbf{R}_{j0}\mathbf{P}_{j1}\ldots\mathbf{P}_{jj-1}, \tag{4.2.29}$$

namely,

$$\exp(ik_jL)\xi=\mathbf{T}_j\xi. \tag{4.2.30}$$

Due to the factorization conditions (4.2.26) and (4.2.27) the operators $\mathbf{T}_j$ commute with each other. It guarantees the existence of a common set of the eigenvectors of operators $\mathbf{T}_j$. It is easy to make sure that here $\mathbf{T}_j$'s do not only commute but are simply equal to each other:

$$T^{\sigma_1'\ldots\sigma_N';\sigma'}_{j\sigma_1\ldots\sigma_N;\sigma}=\delta_{\sigma_1\sigma_2'}\delta_{\sigma_1'\sigma_2}\ldots\delta_{\sigma_{N-1}\sigma_N'}R^{\sigma\sigma'}_{\sigma_N\sigma_1'}. \tag{4.2.31}$$

This does not, however, make the problem of diagonalization simpler. For this reason we shall follow the general scheme. Namely, we start by building a parametric set of commuting operators $\mathbf{T}(\alpha)$, the $\mathbf{T}_j$ being members of this set. Next, we employ the method of the quantum inverse-scattering problem.

The analogous eigenproblem may be formulated for any coefficient $A(Q;Q'P)$. Then the other operators $\mathbf{T}_j$ appear but they have the same eigenvalues as operators (4.2.29). This statement will be proved in the process of diagonalization of the $\mathbf{T}(\alpha)$ matrix.

4.2.4. *The set of commuting operators*

We have already noticed in §4.2.3 that the validity of conditions (4.2.26) and, hence,, of the coordinate Bethe Ansatz (4.2.10), is not yet sufficient for the integrability. The integrability requires that the impurity-particle scattering matrix $\mathbf{R}_{j0}$ belongs to the parametric set of matrices satisfying the functional factorization equations (4.1.17).

For an arbitrary impurity spin the factorization equations include matrices of different rank. For this reason it is expedient to separate the matrices that refer only to the particles, $r^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}(\alpha)(\sigma=1,2)$ (the particle is depicted by the solid line in fig. 4.8), from those that refer to a particle and an impurity, $R^{\sigma\sigma'}_{\varsigma\varsigma'}(\alpha)$ $(\varsigma=-S,\ldots,+S)$ (the impurity corresponds to the dashed line in fig. 4.8). Equations (4.1.17) in these notations are

$$\mathbf{r}_{ij}(\alpha)\mathbf{R}_{i0}(\alpha+\alpha')\mathbf{R}_{j0}(\alpha')=\mathbf{R}_{j0}(\alpha')\mathbf{R}_{i0}(\alpha+\alpha')\mathbf{r}_{ij}(\alpha), \tag{4.2.32 a}$$

$$\mathbf{r}_{ij}(\alpha)\mathbf{r}_{ik}(\alpha+\alpha')\mathbf{r}_{jk}(\alpha')\mathbf{r}=\mathbf{r}_{jk}(\alpha')\mathbf{r}_{ik}(\alpha+\alpha')\mathbf{r}_{ij}(\alpha), \tag{4.2.32 b}$$

with the condition that at some $\alpha_0$:

$$\mathbf{R}_{j0}(\alpha_0)\exp(iI\boldsymbol{\sigma}\cdot\mathbf{S}/2). \tag{4.2.33}$$

Equation (4.2.32) is represented in fig. 4.8. The condition (4.2.33) is a sufficient one as the permutation operator belongs automatically to the set $\mathbf{r}_{ij}(\alpha)$. Indeed, putting $\alpha=0$ in eqn. (4.2.32) we obtain:

$$\mathbf{r}_{ij}(0)\mathbf{M}_{ij}(\alpha')=\mathbf{M}_{ji}(\alpha')\mathbf{r}_{ij}(0), \tag{4.2.34}$$

where $\mathbf{M}_{ij}(\alpha)=\mathbf{R}_{i0}(\alpha)\mathbf{R}_{j0}(\alpha)$ or $\mathbf{r}_{ij}(\alpha)\mathbf{r}_{jk}(\alpha)$. Therefore, we have that within an arbitrary factor

$$\mathbf{r}_{ij}(0)=\mathbf{P}_{ij}. \tag{4.2.35}$$

Then, let us subordinate matrices $\mathbf{r}$ and $\mathbf{R}$ to the functional unitarity conditions

$$\left.\begin{aligned}\mathbf{r}_{ij}(\alpha)\mathbf{r}_{ji}(-\alpha)&=\mathbf{I},\\ \mathbf{R}_{0j}(\alpha)\mathbf{R}_{j0}(-\alpha)&=\mathbf{I},\end{aligned}\right\} \tag{4.2.36}$$

which generalize the conditions (4.2.27).

In the next section we derive the solution of eqn. (4.2.32). Now let us assume that the conditions (4.2.32) and (4.2.33) are satisfied and construct the commutative set of operators $\mathbf{T}(\alpha)$. All following statements do not depend on an explicit form of $\mathbf{r},\mathbf{R}$ matrices and hold for all integrable models.

Let us consider the monodromy matrix

$$\begin{aligned}L^{\{j_1\ldots j_{N+1}\},k}_{\{i_1\ldots i_{N+1}\},l}(\alpha;\alpha_1,\ldots,\alpha_{N+1})&=r^{kk_1}_{i_1j_1}(\alpha_1-\alpha)\\ &\quad\times r^{k_1k_2}_{i_2j_2}(\alpha_2-\alpha)\ldots r^{k_{N-1}k_N}_{i_Nj_N}(\alpha_N-\alpha)R^{k_Nl}_{i_{N+1},j_{N+1}}(\alpha_{N+1}-\alpha),\end{aligned} \tag{4.2.37}$$

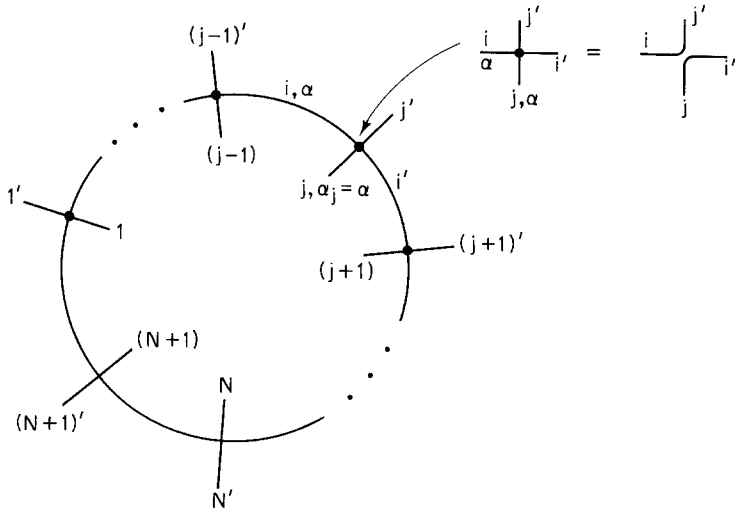
which is graphically represented in fig. 4.6. Omitting the operator and matrix indices rewrite (4.2.37) as

$$\mathbf{L}(\alpha;\alpha_1,\ldots,\alpha_{N+1})=\mathbf{r}_{*1}(\alpha_1-\alpha)\ldots\mathbf{r}_{*N}(\alpha_N-\alpha)\mathbf{R}_{*0}(\alpha_{N+1}-\alpha), \tag{4.2.38}$$

where * corresponds to indices of the particle depicted in fig. 4.9 as the horizontal line. The matrix indices $k$ and $l$ correspond to the ends of this line 'rail' and the

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 4.9




The graphical demonstration of the proof of eqn. (4.2.45).

operator indices $\{i\}=\{i_1,\ldots,i_{N+1}\}$ and $\{j\}=\{j_1,\ldots,j_{N+1}\}$ correspond to the ends of the crossing lines 'sleepers'. The dashed line corresponds to the impurity.

The trace of the monodromy matrix is the transfer matrix $\mathbf{T}(\alpha)$:

$$\mathbf{T}(\alpha)=T^{\{i\}}_{\{j\}}(\alpha)=\sum_{k=1}^{2} L^{\{i\},k}_{\{j\},k}(\alpha). \tag{4.2.39}$$

We shall show that a consequence of the factorized equation (4.2.32) is that the operators $\mathbf{T}(\alpha)$ are commutative at different values of $\alpha$. To do this, we use the graphic representation of the operator $\mathbf{r}(\alpha-\alpha')\mathbf{L}(\alpha')\mathbf{L}(\alpha)$ of fig. 4.7. Using the condition (4.2.32) let us translate the 'sleepers' over point $A$. Thus we obtain (see fig. 4.7) (Baxter1972 a, Sklyanin *et al.* 1979, Faddeev 1980):

$$r^{qq'}_{kk'}(\alpha-\alpha')\mathbf{L}^{q'}_{l}(\alpha')\mathbf{L}^{k'}_{l'}(\alpha)=\mathbf{L}^{k}_{k'}(\alpha)\mathbf{L}^{q}_{q'}(\alpha')r^{q'l}_{k'l'}(\alpha-\alpha'). \tag{4.2.40}$$

Multiplying both sides of eqn. (4.2.40) by $\mathbf{r}(\alpha'-\alpha)$ and taking eqn. (4.2.27) into account, we obtain the similarity relationship†:

$$\mathbf{L}^{n}_{l}(\alpha')\mathbf{L}^{m}_{l'}(\alpha)=r^{nq}_{mk}(\alpha'-\alpha)\mathbf{L}^{k}_{k'}(\alpha)\mathbf{L}^{q}_{q'}(\alpha')\times r^{q'l}_{k'l'}(\alpha-\alpha') \tag{4.2.41}$$

(we omit the operator indices of the matrix $\mathbf{L}^{n}_{l}$). Summing over the index pairs $n, l$ and $m, l'$ and once again using (4.2.36) we obtain:

$$\mathbf{T}(\alpha)\mathbf{T}(\alpha')=\mathbf{T}(\alpha')\mathbf{T}(\alpha). \tag{4.2.42}$$

† The proof was borrowed from Zamolodchicov (1980).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Now let us prove the relationship (4.1.43) connecting the operators $\mathbf{T}_j$ with $\mathbf{T}(\alpha)$ (Belavin 1979). Rewriting the operator (4.2.29) as

$$\mathbf{T}_j = \mathbf{r}_{jj+1}(0)\ldots\mathbf{r}_{jN}^{(0)}\mathbf{R}_{j0}(\alpha_0)\mathbf{r}_{j1}(0)\ldots\mathbf{r}_{jj-1}(0) \tag{4.2.43}$$

and setting in eqn. (4.2.38) $\alpha=\alpha_j (j=1,\ldots,N)$, $\alpha_{N+1}-\alpha=\alpha_0$ with help of eqns. (4.2.35) and (4.2.33) we obtain

$$\mathbf{T}_j = \mathrm{Tr}_{(*)}\{\mathbf{r}_{*1}(0)\ldots\mathbf{r}_{*j-1}(0)\mathbf{P}_{*j}\mathbf{r}_{*j+1}(0)\ldots\mathbf{r}_{*N}(0)\times\mathbf{R}_{*0}(\alpha_0)\}. \tag{4.2.44}$$

Thus

$$\mathbf{T}(\alpha,\alpha_1,\ldots,\alpha_{N+1})|_{\alpha=\alpha_1=\ldots=\alpha_N=0,\alpha_{N+1}=\alpha.} = \mathbf{T}_j \tag{4.2.45}$$

(the proof is demonstrated in fig. 4.9). Obviously, the operators $\mathbf{T}_j$ having arbitrary set of $\alpha_j$ commute also. But in our simple case they are equal.

4.2.5. *Factorization equations*

For the case of $S=1/2$, eqns. (4.2.32) were cited by Yang (1967). We shall show below that their solution does not depend on the magnitude of $S$ (Fateev and Wiegmann 1981 a). The most general case, including various representations of the $O(3)$ group, is studied by Kulish *et al.* (1981) and Zamolodchikov and Fateev (1980).

First, we write $\mathbf{R}(\alpha_0)$ in the form

$$\exp(iI\boldsymbol{\sigma}\cdot\mathbf{S}/2) = w_0' + 2w'\boldsymbol{\sigma}\cdot\mathbf{S}, \tag{4.2.46}$$

where $\omega_0'$ and $w'$ are functions of $I$ (we recall that $\boldsymbol{\sigma}^2=3$). The simplest way to find these functions is as follows. The total spin $\boldsymbol{\sigma}/2+\mathbf{S}$ can assume the values $S\pm 1/2$, and either $\boldsymbol{\sigma}\cdot\mathbf{S}=S$ or $\boldsymbol{\sigma}\cdot\mathbf{S}=-(S+1)$. Therefore

$$\exp(iIS/2) = w_0' + 2w'S, \qquad \exp(-iI(S+1)/2) = w_0' - 2w'\times(S+1). \tag{4.2.47}$$

Now we turn to eqns. (4.2.32). In view of the fact that conditions (4.2.33) are invariant under the transformations of the $O(3)$ group, the matrices $\mathbf{r}$ and $\mathbf{R}$ must be sought for in the form

$$R_{\sigma\sigma'}^{\sigma\sigma'}(\alpha) = w_0'(\alpha)\delta_{\sigma\sigma'}\delta_{\sigma\sigma'} + 2w'(\alpha)\boldsymbol{\sigma}_{\sigma\sigma'}\cdot\mathbf{S}_{\sigma\sigma'}, \tag{4.2.48}$$

$$r_{\mu\mu'}^{\sigma\sigma'}(\alpha) = w_0(\alpha)\delta_{\sigma\sigma'}\delta_{\mu\mu'} + w(\alpha)\boldsymbol{\sigma}_{\sigma\sigma'}\cdot\boldsymbol{\sigma}_{\mu\mu'}. \tag{4.2.49}$$

It is expedient to introduce the following notations:

$$\left.\begin{array}{lll} a=w_0+w\,, & b=w_0-w\,, & c=2w \\ a'=w_0'+w', & b'=w_0'-w', & c'=2w'. \end{array}\right\} \tag{4.2.50}$$

Substituting (4.2.49) into eqns. (4.2.32 a), we find that

$$h(\alpha) \equiv \frac{b(\alpha)}{c(\alpha)} = \frac{b'(\alpha)}{c'(\alpha)} \tag{4.2.51}$$

and

$$b'(\alpha)c'(\alpha+\alpha')c(\alpha') + c'(\alpha)c'(\alpha+\alpha')b(\alpha) = c'(\alpha)b'(\alpha+\alpha')c(\alpha'). \tag{4.2.52}$$

In terms of $h(\alpha)$ the above equation assumes the form

$$h(\alpha)+h(\alpha') = h(\alpha+\alpha'), \tag{4.2.53}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

whence, without loss of generality, we can assume that

$$h(\alpha)=\alpha/ig, \tag{4.2.54}$$

where $g$ is a parameter.

Equations (4.2.51) and (4.2.54) define $b(\alpha)$ and $c(\alpha)$ within an arbitrary factor. Conditions (4.2.47) determine the value of this factor at the points $\alpha=0$ and $\alpha=\alpha_0$. In all other respects the factor is arbitrary. It is convenient to select it in such a way that the unitarity condition (4.2.36) is valid for any $\alpha$:

$$\left.\begin{aligned} b(\alpha)&=\frac{\alpha}{\alpha+ig}a(\alpha), \qquad b'(\alpha)=\frac{\alpha}{\alpha+ig}a'(\alpha),\\ c(\alpha)&=\frac{ig}{\alpha+ig}a(\alpha), \qquad c'(\alpha)=\frac{ig}{\alpha+ig}a'(\alpha),\\ a(\alpha)a(-\alpha)&=1, \qquad a'(\alpha)a'(-\alpha)=\frac{-\alpha^2+g^2}{-\alpha^2+g^2(S+1/2)^2}. \end{aligned}\right\} \tag{4.2.55}$$

Using (4.2.33) and (4.2.35) and setting $\alpha_0=1$ we obtain

$$a(0)=1,$$

$$g=\frac{2}{2S+1}\tan(I2S+1/4),$$

and

$$a(1)=\frac{\exp(iIS/2)(2S+3)-(2S-1)\exp(-iI(S+1)/2)}{2(2S+1)}.$$

The characteristic feature of the factorized matrices (4.2.49) is that the function $h(\alpha)$ does not depend on the impurity spin $S$. This is because eqns. (4.2.32) are bilinear in the impurity spin operator $\hat{S}$ and contain only commutators of the type $[\hat{S}_a, \hat{S}_b]=i\varepsilon_{abc}\hat{S}_c$, whose form does not depend on group representation.

### 4.2.6. *Diagonalization of the trace of the monodromy matrix*

Let us denote the matrix elements of the operator matrix $L_l^k$ (4.2.37) as

$$\mathbf{L}_1^1=\mathbf{A}, \qquad \mathbf{L}_2^1=\mathbf{B}, \qquad \mathbf{L}_1^2=\mathbf{C}, \qquad \mathbf{L}_2^2=\mathbf{D}. \tag{4.2.56}$$

The matrix $\mathbf{r}(\alpha-\alpha')$ in (4.2.40) according to formulae (4.2.49) and (4.2.50) is

$$r_{kk'}^{qq'}(\alpha)=b(\alpha)\delta_{qq'}\delta_{kk'}+c(\alpha)\delta_{qk'}, \delta_{kq'}, \tag{4.2.57}$$

where $b(\alpha)$ and $c(\alpha)$ are given by (4.2.55). Rewriting (4.2.40) in components we have

$$\begin{aligned} &b(\alpha-\alpha')\mathbf{L}_l^q(\alpha')\mathbf{L}_{l'}^k(\alpha)+c(\alpha-\alpha')\mathbf{L}_l^k(\alpha')\mathbf{L}_{l'}^q(\alpha)\\ &\qquad=b(\alpha-\alpha')\mathbf{L}_{l'}^k(\alpha)\mathbf{L}_l^q(\alpha')+c(\alpha-\alpha')\mathbf{L}_l^k(\alpha)\mathbf{L}_{l'}^q(\alpha'). \end{aligned} \tag{4.2.58}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

We need only the following commutation relations from (4.2.58):

$$[\mathbf{A}(\alpha), \mathbf{A}(\beta)] = [\mathbf{D}(\alpha), \mathbf{D}(\beta)] = [\mathbf{A}(\alpha), \mathbf{D}(\beta)]$$
$$= [\mathbf{C}(\alpha), \mathbf{C}(\beta)] = [\mathbf{B}(\alpha), \mathbf{B}(\beta)] = 0, \tag{4.2.59 a}$$

$$b(\alpha-\beta)\mathbf{A}(\alpha)\mathbf{B}(\beta) = a(\alpha-\beta)\mathbf{B}(\beta)\mathbf{A}(\alpha) - c(\alpha-\beta)\mathbf{B}(\alpha)\mathbf{A}(\beta), \tag{4.2.59 b}$$

$$b(\beta-\alpha)\mathbf{D}(\alpha)\mathbf{B}(\beta) = a(\beta-\alpha)\mathbf{B}(\beta)\mathbf{D}(\alpha) - c(\beta-\alpha)\mathbf{B}(\alpha)\mathbf{D}(\beta). \tag{4.2.59 c}$$

The commutativity of traces of the $L$ matrices (4.2.42)

$$[\mathbf{A}(\alpha)+\mathbf{D}(\alpha), \mathbf{A}(\beta)+\mathbf{D}(\beta)] = 0$$

is the consequence of eqn. (4.2.59).

Let us consider the state $\Omega_0$ with all particle's spins up, the impurity spin projection being $+S$. The matrices $\mathbf{r}_{*j}(\alpha_j-\alpha)$, $\mathbf{R}_{*0}(\alpha_{N+1}-\alpha)$, when applied to the vacuum $\Omega_0$, become triangular matrices:

$$\mathbf{r}_{*j}(\alpha)\Omega_0 = \begin{pmatrix} a(\alpha) & c(\alpha)\boldsymbol{\sigma}_j^- \\ 0 & b(\alpha) \end{pmatrix}\Omega_0 \tag{4.2.60}$$

$$\mathbf{R}_{*0}(\alpha)\Omega_0 = \begin{pmatrix} (S+1/2)a'(\alpha)-(S-1/2)b'(\alpha) & 2c'(\alpha)S^- \\ 0 & -(S-1/2)a'(\alpha)+(S+1/2)b'(\alpha) \end{pmatrix}\Omega_0. \tag{4.2.61}$$

As the result, the action of the diagonal elements $A$ and $D$ of the matrices $\mathbf{r}_{*j}$ and $\mathbf{R}_{*0}$, to the vacuum

$$\left.\begin{aligned} &\mathbf{C}(\alpha)\Omega_0 = 0, \\ &\mathbf{A}(\alpha)\Omega_0 = \Lambda_A(\alpha)\Omega_0, \qquad \mathbf{D}(\alpha)\Omega_0 = \Lambda_D(\alpha)\Omega_0, \end{aligned}\right\} \tag{4.2.62}$$

where

$$\left.\begin{aligned} \Lambda_A(\alpha) &= \prod_{j=1}^{N} a(\alpha_j-\alpha)[(S+1/2)a'(\alpha_{N+1}-\alpha)-(S-1/2)b'(\alpha_{N+1}-\alpha)], \\ \Lambda_D(\alpha) &= \prod_{j=1}^{N} b(\alpha_j-\alpha)[-(S-1/2)a'(\alpha_{N+1}-\alpha)+(S+1/2)b'(\alpha_{N+1}-\alpha)]. \end{aligned}\right\} \tag{4.2.63}$$

Let us examine the vector

$$\Omega(\alpha'_1, \ldots, \alpha'_M) = \prod_{\beta=1}^{M} \mathbf{B}(\alpha'_\beta)\Omega_0 \tag{4.2.64}$$

and show that it is an eigenvector of the operator $\mathbf{A}(\alpha)+\mathbf{D}(\alpha)$, if $\{\alpha'_\beta\}$ satisfy a certain system of transcendental equations. Let us note that by virtue of (4.2.59) and (4.2.64) carrying $\mathbf{A}(\alpha)$, $\mathbf{D}(\alpha)$ through all the $\mathbf{B}(\alpha'_\beta)$ in (4.2.64), we have

$$(\mathbf{A}(\alpha)+\mathbf{D}(\alpha)) \prod_{\beta=1}^{M} \mathbf{B}(\alpha'_\beta)\Omega_0 = \Lambda(\alpha, \{\alpha'_\beta\}) \prod_{\beta=1}^{M} \mathbf{B}(\alpha'_\beta)\Omega_0$$
$$+ \sum_{\gamma=1}^{M} \Lambda_\gamma(\alpha, \{\alpha'_\beta\}) \prod_{\substack{\beta=1 \\ \beta\neq\gamma}}^{M} \mathbf{B}(\alpha'_\beta)\mathbf{B}(\alpha)\Omega_0, \tag{4.2.65}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where

$$\Lambda(\alpha, \{\alpha'_\beta\}) = \prod_{\beta=1}^{M} \frac{a(\alpha-\alpha'_\beta)}{b(\alpha-\alpha'_\beta)} \Lambda_A(\alpha) + \prod_{\beta=1}^{M} \frac{a(\alpha'_\beta-\alpha)}{b(\alpha'_\beta-\alpha)} \Lambda_D(\alpha); \tag{4.2.66}$$

and

$$\Lambda_\gamma(\alpha; \{\alpha'_\beta\}) = -\frac{c(\alpha-\alpha'_\gamma)}{b(\alpha-\alpha'_\gamma)} \prod_{\substack{\beta=1\\ \beta\neq\gamma}}^{M} \frac{a(\alpha'_\gamma-\alpha'_\beta)}{b(\alpha'_\gamma-\alpha'_\beta)} \Lambda_A(\alpha'_\gamma)$$
$$- \frac{c(\alpha'_\gamma-\alpha)}{b(\alpha'_\gamma-\alpha)} \prod_{\substack{\beta=1\\ \beta\neq\gamma}}^{M} \frac{a(\alpha'_\beta-\alpha'_\gamma)}{b(\alpha'_\beta-\alpha'_\gamma)} \Lambda_D(\alpha'_\gamma). \tag{4.2.67}$$

The first summand on the right-hand side of (4.2.65) is obtained when we carry $A(\alpha), D(\alpha)$ through $B(\alpha'_\beta)$, using only the first term on the right hand-side of (4.2.59 *b*, *c*). The second summand is obtained from the remaining commutations. The operator expression

$$\mathbf{B}(\alpha'_2) \ldots \mathbf{B}(\alpha'_M)\mathbf{B}(\alpha)\Omega_0$$

appears if we commute $A(\alpha), D(\alpha)$, with $B(\alpha'_1)$, using the second term in (4.2.59 *b*, *c*), while for further commutations we use the first term. This observation brings us to the expression (4.2.67) for $\Lambda_1(\alpha; \{\alpha'_\beta\})$. The validity of the remaining formulae follows from the symmetry of all expressions with respect to the permutation of $\alpha'_1, \ldots, \alpha'_M$.

As a result we see that $\Omega(\{\alpha'_\beta\})$ is an eigenvector of $\mathbf{A}(\alpha)+\mathbf{D}(\alpha)$—operator with a spin projection $S^z = N/2 - M + S$ and eigenvalue (4.2.66) if $\{\alpha'_\beta\}$ satisfy the system of equations

$$\prod_{j=1}^{N} \frac{a(\alpha_j-\alpha'_\gamma)}{b(\alpha_j-\alpha'_\gamma)} \frac{[(S+1/2)a'(\alpha_{N+1}-\alpha'_\gamma)-(S-1/2)b'(\alpha_{N+1}-\alpha'_\gamma)]}{[-(S-1/2)a'(\alpha_{N+1}-\alpha'_\gamma)+(S+1/2)b'(\alpha_{N+1}-\alpha'_\gamma)]}$$
$$= -\prod_{\beta=1}^{M} \frac{a(\alpha'_\beta-\alpha'_\gamma)}{a(\alpha'_\gamma-\alpha'_\beta)} \frac{b(\alpha'_\gamma-\alpha'_\beta)}{b(\alpha'_\beta-\alpha'_\gamma)}. \tag{4.2.68}$$

It is interesting to note that condition (4.2.68) removing the 'unwanted' terms in (4.2.65) also follows from the analyticity of $\Lambda(\alpha, \{\alpha'_\beta\})$ with respect to the spectral parameter $\alpha$ (Manackov, unpublished). Indeed, the operator $(\alpha+ig)r(\alpha)/a(\alpha)$ is analytical in the complex plane of $\alpha$. Therefore, the operator

$$\prod_{j=1}^{N+1} \frac{\alpha_j-\alpha+ig}{a(\alpha_j-\alpha)} \mathbf{T}(\alpha)$$

is analytical also and, moreover, it is a polynomial of the $N$th order. Due to commutativity of the set $\mathbf{T}(\alpha)$ the coefficients at various powers of $\alpha$ also commute. Hence, the eigenvalues of $\mathbf{T}(\alpha)$ are polynomials of $\alpha$. It is easy to see that requiring the poles at $\alpha=\alpha'_\beta$ to vanish in (4.2.66) one immediately gets eqn. (4.2.68).

Setting $\alpha'_\beta = g(-\lambda_\beta + i/2)$, $\alpha=0$, $\alpha_j = \delta_{N+1,j}$ and using eqns. (4.2.65) and (4.2.66) with $b(0)=0$ we obtain

$$\exp(ik_jL) = \exp\left(\frac{iIS}{2}\right) \prod_{\alpha=1}^{M} \left(\frac{\lambda_\alpha+i/2}{\lambda_\alpha-i/2}\right). \tag{4.2.A}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Equation (4.2.68) yields the following equations for $\lambda_\alpha$:

$$\left(\frac{\lambda_\alpha+i/2}{\lambda_\alpha-i/2}\right)^N\left(\frac{\lambda_\alpha+1/g+iS}{\lambda_\alpha+1/g-iS}\right)=-\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta+i}{\lambda_\alpha-\lambda_\beta-i}. \tag{4.2.B}$$

We shall call, below, eqns. (4.2.A) and (4.2.B) the Bethe-Ansatz equations. The Bethe-Ansatz equations solve the problems of diagonalization of the s–d exchange hamiltonian and completely describe its spectrum.

Note, that the eigenvalue of energy is determined by the momenta $\{k_j\}$ of the charge density waves and by the rapidities $\{\lambda_\alpha\}$ of the spin density waves:

$$E=\sum_{j=1}^{N}k_j \tag{4.2.C}$$

and the spin projection is given by $S^z=N/2-M+S$.

Equations (4.2.A)–(4.2.C) for $S=1/2$ were obtained by Andrei (1980) and Wiegmann (1980 a, 1981) and by Fateev and Wiegmann (1981 a) and Furuya and Lowenstein (1982) for arbitrary $S$.

### 4.3. *Bethe Ansatz for the anisotropic exchange model*

The modern theory of exactly integrable quantum models provides the means for diagonalization of the s–d exchange model with an arbitrary impurity spin and anisotropy of a general type. However, for the sake of simplicity we restrict ourselves to the most interesting case of 1/2-spin impurity with $U(1)$ symmetry

$$\mathscr{H}=\mathscr{H}_0+\frac{1}{2}\sum_{\substack{k,k'\\ \sigma,\sigma'}}c^+_{k\sigma}[I_\parallel\boldsymbol{\sigma}^z_{\sigma\sigma'}\mathbf{S}^z+I_\perp(\boldsymbol{\sigma}^x_{\sigma\sigma'},\mathbf{S}^x+\boldsymbol{\sigma}^y_{\sigma\sigma'},\mathbf{S}^y)]c_{k'\sigma'}. \tag{4.3.1}$$

Investigation of the thermodynamic properties of even this simple model with arbitrary $I_\parallel$ and $I_\perp$ is a difficult task and may be performed only for the exchange term of easy-plane type:

$$I_\parallel>I_\perp>0. \tag{4.3.2}$$

Our consideration is restricted to this simplest case.

We must admit that we do not know of any physical realization of the anisotropic exchange (4.3.1). Nevertheless, from the point of view of a 'theorist' the properties of the anisotropic model are richer than those of the isotropic model and open up some new possibilities for understanding the nature of the Kondo effect.

An excellent example is the paper by Anderson *et al.* (1970) in which much information about the isotropic s–d model was derived from consideration of the anisotropic model. The RL model is related closely to the anisotropic s–d model. We describe its solution in the Supplement section.

#### 4.3.1. *Two-particle scattering matrix and the Bethe-Ansatz equations*

This section is written for the reader who has studied the Bethe Ansatz for the isotropic s–d model (see § 4.2).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The coordinate Bethe wavefunction ((4.2.10)–(4.2.13), (4.2.19)) as well as all speculations, expounded in § 4.2.2 for the isotropic s–d model, are valid for the anisotropic case, but the particle-impurity scattering matrix has now another form:

$$\mathbf{R}_{0j}=\exp\left[i\frac{I_{\parallel}}{2}\boldsymbol{\sigma}^z\mathbf{S}^z+i\frac{I_{\perp}}{4}(\boldsymbol{\sigma}^+\mathbf{S}^-+\boldsymbol{\sigma}^-\mathbf{S}^+)\right]. \tag{4.3.3}$$

We have already noted in § 4.2.2 that the factorization conditions (4.2.26) are fulfilled for an arbitrary matrix $\mathbf{R}$. A non-trivial question is whether the matrix (4.3.3) lies on the algebraic curve $\mathbf{R}(\alpha)$ defined by the triangle equations (4.2.32). It has been explained in § 4.2.4 that this condition is necessary and sufficient for the factorization of the spin scattering and makes it possible to diagonalize the $T$ operators (4.2.29). The answer to this question is positive because the solution of the triangle equations possessing $U(1)$ symmetry contains the additional parameter (Baxter 1972 a), Zamolodchicov and Zamolodchicov 1979):

$$\mathbf{R}(\alpha)=w_0(\alpha)+w_{\parallel}(\alpha)\boldsymbol{\sigma}^z\otimes\boldsymbol{\sigma}^z+w_{\perp}(\alpha)(\boldsymbol{\sigma}^x\otimes\boldsymbol{\sigma}^x+\boldsymbol{\sigma}^y\otimes\boldsymbol{\sigma}^y) \tag{4.3.4}$$

$$\left.\begin{aligned}
b(\alpha)&\equiv w_0(\alpha)-w_{\parallel}(\alpha)=\frac{\sinh\alpha f}{\sinh(\alpha f+i\mu)}a(\alpha)\\
c(\alpha)&\equiv 2w_{\perp}(\alpha)=\frac{i\sin\mu}{\sinh(\alpha f+i\mu)}a(\alpha)\\
a(\alpha)&\equiv w_0(\alpha)+w_{\parallel}(\alpha),
\end{aligned}\right\} \tag{4.3.5}$$

where $a(\alpha)a(-\alpha)=1$. The eigenvalues of the $T_j$ operators (4.2.29) do not depend on the function $a(\alpha)$. Therefore, we put $a(\alpha)=1$. The solutions of the triangle equations and relations (4.3.5) are proved in the Appendix to § 4.3.1.

To find the relation between $(\mu,f)$ and $(I_{\parallel},I_{\perp})$, we rewrite the scattering matrix (4.3.3)

$$\mathbf{R}\equiv\mathbf{R}(1)=\frac{a(1)}{2}(\mathbf{1}\otimes\mathbf{1}+\boldsymbol{\sigma}_1^z\otimes\boldsymbol{\sigma}_2^z)+\frac{b(1)}{2}(\mathbf{1}\otimes\mathbf{1}-\boldsymbol{\sigma}_1^z\otimes\boldsymbol{\sigma}_2^z)$$
$$+\frac{1}{2}c(1)(\boldsymbol{\sigma}_1^+\otimes\boldsymbol{\sigma}_2^-+\boldsymbol{\sigma}_1^-\otimes\boldsymbol{\sigma}_2^+), \tag{4.3.6}$$

$$\left.\begin{aligned}
&a(1)=\exp(iI_{\parallel}/2-iI_{\perp}/4), \qquad b(1)=\cos I_{\perp}/2\exp(-iI_{\parallel}/4)\\
&c(1)=\frac{i}{4}\sin\frac{I_{\perp}}{2}\exp(-iI_{\parallel}/4)
\end{aligned}\right\} \tag{4.3.7}$$

and put $w_i(1)=w_i$. This equation yields

$$\cos\mu=\frac{\cos I_{\parallel}/2}{\cos I_{\perp}/2}; \qquad (\coth f)^2=\frac{\sin^2 I_{\parallel}/2}{\sin\left(\dfrac{I_{\parallel}+I_{\perp}}{2}\right)\sin\left(\dfrac{I_{\parallel}-I_{\perp}}{2}\right)}. \tag{4.3.8}$$

Taking the limit $g^{-1}\equiv\lim_{\mu\to 0}f/\mu=\cot I/2$ we obtain the $SU(2)$ invariant solution ((4.2.49), (4.2.55)).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The method of diagonalization of the

$$\mathbf{T}_j = \mathbf{T}(\alpha; \alpha_1, \ldots, \alpha_{N+1})|_{\alpha=0;\alpha_j=\delta_{j,N+1}}$$

matrices considered in (4.2.6) is valid for the anisotropic case. The state $\Omega_0$ with all spins up is still the eigenstate of the $T(\alpha)$ operator. Other eigenstates are constructed by a successive action of $\mathbf{B}(\alpha'_\beta)$ (4.2.66). The corresponding eigenvalues of the $T(\alpha)$ matrix are calculated using commutation rules between the $T$ matrix elements. These elements have the same form as those obtained for the isotropic case (4.2.60), but $a(\alpha)$, $b(\alpha)$, $c(\alpha)$ being determined by (4.3.5). Therefore, the eigenvalues of the $T(\alpha)$ operator have the same form as in § 4.2.6:

$$\Lambda(\alpha; \{\alpha'_\beta\}) = \prod_{\beta=1}^{M} \frac{a(\alpha-\alpha'_\beta)}{b(\alpha-\alpha'_\beta)} \prod_{j=1}^{N+1} a(\alpha_j-\alpha) + \prod_{\beta=1}^{M} \frac{a(\alpha'_\beta-\alpha)}{b(\alpha'_\beta-\alpha)} \prod_{j=1}^{N+1} b(\alpha_j-\alpha). \quad (4.3.9)$$

The quantities $\alpha'_\beta$ satisfy the following equations

$$\prod_{j=1}^{N+1} \frac{a(\alpha_j-\alpha'_\beta)}{b(\alpha_j-\alpha'_\beta)} = -\prod_{\gamma-1}^{M} \frac{a(\alpha'_\gamma-\alpha'_\beta)}{a(\alpha'_\beta-\alpha'_\gamma)} \frac{b(\alpha'_\beta-\alpha'_\gamma)}{b(\alpha'_\gamma-\alpha'_\beta)}. \quad (4.3.10)$$

Setting $\alpha=0$ and $\alpha'_\beta = -\mu/f(\lambda_\beta - i/2)$; $\alpha_j = \delta_{j,N+1}$ one obtains

$$\exp(ik_jL) = \exp(i(I_\parallel/2 - I_\perp/4)) \sum_{\alpha=1}^{M} \frac{\sinh[\mu(\lambda_\alpha+i/2)]}{\sinh[\mu(\lambda_\alpha-i/2)]} \quad (4.3.\mathrm{A})$$

$$\left[\frac{\sinh\mu(\lambda_\alpha+i/2)}{\sinh\mu(\lambda_\alpha-i/2)}\right]^N \frac{\sinh\mu(\lambda_\alpha+f/\mu+i/2)}{\sinh\mu(\lambda_\alpha+f/\mu-i/2)} = -\prod_{\beta=1}^{M} \frac{\sinh\mu(\lambda_\alpha-\lambda_\beta+i)}{\sinh\mu(\lambda_\alpha-\lambda_\beta-i)}, \quad (4.3.\mathrm{B})$$

$$E = \sum_{j=1}^{N} k_j, \qquad S^z = N/2 - M + 1/2. \quad (4.3.\mathrm{C})$$

Equations (4.3.A)–(4.3.C) were obtained by Wiegmann (1981).

### 4.4. *The Bethe Ansatz for the degenerate exchange model*

In this section the Bethe-Ansatz technique is applied to the degenerate exchange model which has been discussed in § 2.4.1.

$$\mathscr{H} = \sum_{k,j} k c^+_{kj} c_{kj} + \frac{I}{2} \sum_{\substack{k,k'\\ j,j'}} c^+_{kj} \mathbf{P}_{j'j} c_{k'j'} + \sum_j E_j \mathbf{P}_{jj} \qquad (j=1,\ldots,n), \quad (4.4.1)$$

where $I = -2V^2/\epsilon_f$, and $\mathbf{P}_{j'j}$ is a permutation operator.

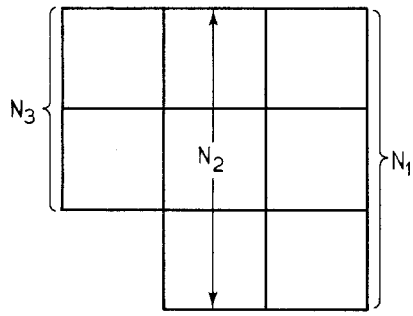
The hamiltonian (4.4.1) describes dilute rare-earth alloys. The energy of the $f$-electron level is assumed to be much larger than crystal field splittings ($-\epsilon_f \gg E_j$). Therefore effects related to the unspherical environment are taken into account only in the last term of (4.4.1).

#### 4.4.1. *The coordinate Bethe Ansatz*

The hamiltonian (4.4.1) commutes with a permutation operator. Therefore, we may construct the eigenstates of (4.4.1) for an arbitrary irreducible representation of the permutation group. This representation is characterized by the Young tableau $[1^{N_1-N_2}, 2^{N_2-N_3}, \ldots, n^{N_n}]$ (see fig. 4.10). The number $N_j (j=1,\ldots,n)$ is the number of particles with the $(j-(n+1)/2)$ the projection of the angular momentum. It is

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 4.10




The Young tableau corresponding to the representation of the permutation group $[2^2, 3^3, 3^3]$

convenient to characterize an eigenstate by a set of numbers $m_1, \ldots, m_n$ related with $N_j$ as

$$m_j = \sum_{k=1}^{j} N_k. \tag{4.4.2}$$

It is easy to generalize the coordinate Bethe wavefunction, constructed in § 4.2.1 for the case $n=2$, to the case of arbitrary $n$.

As has been shown for the s–d exchange model, linearity of the conduction electron spectrum enables one to choose a permutation operator $\mathbf{P}$ as the $S$ matrix of the non-interacting particles. Hence, the factorization condition (4.2.26) is satisfied irrespective of the form of the $R$ matrix:

$$\mathbf{R}_{0j} = \exp(iI\mathbf{P}_{0j}) = \cos I\mathbf{I}_{0j} + i \sin I\mathbf{P}_{0j} \tag{4.4.3}$$

and the Bethe hypothesis is valid. Now one should treat the indices in (4.2.26) taking the values from 1 up to $n$. The periodic boundary conditions lead to the problem of diagonalization of the matrix

$$\mathbf{T}_j = \mathbf{P}_{jj+1}\mathbf{P}_{jj+2} \ldots \mathbf{R}_{j0}\mathbf{P}_{j1} \ldots \mathbf{P}_{jj-1}. \tag{4.4.4}$$

The method for solving this problem was suggested by Sutherland (1968). His method enables one to generalize the solution with $n=2$ to the case of arbitrary $n$. Other versions of this method were discussed by Kulish and Reshetikhin (1981) and Arinstein (1980).

Let us define the following set of the $R$ matrices:

$$\mathbf{R}(\alpha) = b(\alpha) + c(\alpha)\mathbf{P}, \tag{4.4.5}$$

where

$$b(\alpha)/c(\alpha) = \alpha/gi; \qquad c(\alpha) = \frac{ig}{\alpha + ig}; \qquad g = \tan I/2.$$

These matrices satisfy the factorization conditions (4.2.32). The following relations are valid:

$$\mathbf{R}(0) = \mathbf{P}$$

$$\mathbf{R}(1) = \mathbf{R}\exp(-iI/2), \tag{4.4.6}$$

where $\mathbf{R}$ is given by (4.4.3).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

4.4.2. *Bethe-Ansatz hierarchy*

We construct the monodromy matrix according to the general scheme considered in § 4.3.6:

$$\mathbf{L}(\alpha)=\prod_{j=1}^{N}\mathbf{R}_{*j}(\alpha_j-\alpha)\mathbf{R}_{*0}(\alpha_{N+1}-\alpha). \tag{4.4.7}$$

Transfer matrices $\mathbf{T}(\alpha)=\mathrm{Tr}_*\mathbf{L}(\alpha)$ form a commuting set of operators.

Let us diagonalize the operator $\mathbf{T}(\alpha)$. It is convenient to express the permutation operator in terms of elementary matrices $\mathbf{X}_{pq}$:

$$P^{\beta\beta'}_{\gamma\gamma'}=\sum_{p,q=1}^{n}(X_{pq})^{\beta\beta'}(X_{qp})^{\gamma\gamma'} \tag{4.4.8}$$

$$(X_{pq})^{\alpha\beta}=\delta_{\alpha p}\delta_{q\beta}. \tag{4.4.9}$$

The matrix $\mathbf{R}(\alpha)$ is

$$\mathbf{R}(\alpha)=\begin{bmatrix} b(\alpha)+c(\alpha)\mathbf{X}_{11} & c(\alpha)\mathbf{X}_{21} & \dots & c(\alpha)\mathbf{X}_{n1} \\ c(\alpha)\mathbf{X}_{12} & b(\alpha)+c(\alpha)\mathbf{X}_{22} & \dots & c(\alpha)\mathbf{X}_{n2} \\ \vdots & \vdots & \dots & \vdots \\ c(\alpha)\mathbf{X}_{1n} & c(\alpha)\mathbf{X}_{2n} & \dots & b(\alpha)+c(\alpha)\mathbf{X}_{nn} \end{bmatrix}. \tag{4.4.10}$$

There exists an $\alpha$-independent vector $\Omega^j_\sigma$ which reduces $\mathbf{R}_{*j}(\alpha)$ to a triangular form. It is the state with the maximum value of colour:

$$\mathbf{X}^j_{ik}\Omega^j_0=\delta_{k1}\mathbf{X}^j_{i1}\Omega^j_0 \qquad (\Omega^j_{0\beta}=\delta_{\beta 1}). \tag{4.4.11}$$

Acting on it, $R_{*j}(\alpha)$ gives

$$\mathbf{R}_{*j}(\alpha)\Omega^j_0=\left[\begin{array}{c|ccc} 1 & b(\alpha)\mathbf{X}_{21} & \dots & b(\alpha)\mathbf{X}_{n1} \\ \hline & b(\alpha) & & \\ & & \ddots & \\ 0 & & & 0 \\ & 0 & & \ddots \\ & & & b(\alpha) \end{array}\right]\Omega^j_0 \tag{4.4.12}$$

(we bear in mind that $b(\alpha)+c(\alpha)=1$.

Now we construct a vector $\Omega_0$ putting

$$\Omega_0=\prod_{j=1}^{N+1}\otimes\Omega^j_0, \qquad \Omega_{0,\beta_1,\dots,\beta_{N+1}}=\prod_{j=1}^{N+1}\delta_{\beta_j,1}. \tag{4.4.13}$$

Computed on this vector, called 'bare' vacuum, all $R_{*j}, R_{0*}$ and the monodromy matrix (4.4.6) become triangular:

$$\mathbf{L}(\alpha;\alpha_1,\dots,\alpha_{N+1})\Omega_0$$

$$=\left[\begin{array}{c|ccc} 1 & \mathbf{B}_1(\alpha) & \mathbf{B}_2(\alpha) & \dots & \mathbf{B}_{n-1}(\alpha) \\ \hline & b^N(-\alpha)b(-\alpha+1) & & \dots & 0 \\ & & \ddots & & \\ 0 & & & \ddots & \\ & 0 & & & \\ & & & & b^N(-\alpha)b(-\alpha+1) \end{array}\right]\Omega_0. \tag{4.4.14}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

In view of these results is is natural to split $L(\alpha)$ into blocks

$$\mathbf{L}(\alpha)=\begin{pmatrix} \mathbf{A}(\alpha) & \mathbf{B}_a(\alpha) \\ \mathbf{C}_b(\alpha) & \mathbf{D}_{ab}(\alpha) \end{pmatrix} \tag{4.4.15}$$

(compare with (4.2.56)).

The blocks $\mathbf{A}$, $\mathbf{D}_{ab}$ act on the 'bare' vacuum as follows

$$\mathbf{A}(\alpha)\Omega_0=\Omega_0, \qquad \mathbf{D}_{ab}(\alpha)\Omega_0=\delta_{ab}b^N(-\alpha)b(-\alpha+1). \tag{4.4.16}$$

One may consider the blocks $\mathbf{C}_b$ and $\mathbf{B}_a$ as annihilation and creation operators respectively:

$$\left.\begin{aligned} \mathbf{C}_b(\alpha)\Omega_0&=0 \\ \mathbf{B}_a(\alpha)\Omega_0&=\Omega(\alpha, a). \end{aligned}\right\} \tag{4.4.17}$$

As above (4.2.6) the triangle equation gives the necessary commutation relations between the elements of $\mathbf{L}(\alpha)$:

$$\mathbf{R}^{qq'}_{kk'}(\alpha-\beta)\mathbf{L}^{q'}_{l}(\beta)\mathbf{L}^{k'}_{l'}(\alpha)=\mathbf{L}^{k}_{k'}(\alpha)\mathbf{L}^{q}_{q'}(\beta)\mathbf{R}^{q'l}_{k'l'}(\alpha-\beta). \tag{4.4.18}$$

Using (4.2.4), and (4.2.14) and rewriting (4.4.18) in components we obtain:

$$\mathbf{A}(\alpha)\mathbf{B}_a(\beta)b(\alpha-\beta)=\mathbf{B}_a(\beta)\mathbf{A}(\alpha)-c(\alpha-\beta)\mathbf{B}_a(\alpha)\mathbf{A}(\beta), \tag{4.4.19 a}$$

$$\begin{aligned} \mathbf{D}_{ab}(\alpha)\mathbf{B}_c(\beta)b(\alpha-\beta)&=\mathbf{B}_p(\beta)\mathbf{D}_{am}(\alpha)r^{cp}_{bm}(\beta-\alpha) \\ &\quad -c(\beta-\alpha)\mathbf{B}_b(\alpha)\mathbf{D}_{ac}(\alpha), \end{aligned} \tag{4.4.19 b}$$

$$\mathbf{B}_a(\beta)\mathbf{B}_b(\alpha)=r^{bd}_{ac}(\alpha-\beta)\mathbf{B}_c(\alpha)\mathbf{B}_d(\beta), \tag{4.4.19 c}$$

$$r^{ap}_{bq}(\alpha-\beta)\mathbf{D}_{pc}(\beta)\mathbf{D}_{qd}(\alpha)=\mathbf{D}_{bm}(\alpha)\mathbf{D}_{an}(\beta)r^{mc}_{nd}(\alpha-\beta), \tag{4.4.19 d}$$

$$\begin{aligned} r^{cd}_{ab}(\alpha)&=b(\alpha)I^{cd}_{ab}+c(\alpha)\,{}_1P^{cd}_{ab}; \\ I^{cd}_{ab}&=\delta_{ab}\delta_{cd}; \qquad {}_1P^{cd}_{ab}=\delta_{ad}\delta_{cb}, \end{aligned} \tag{4.4.19 e}$$

where ${}_1P$ is a permutation operator in $(n-1)\times(n-1)$ dimensional space.

We have one eigenvector of the $\mathrm{Tr}_*\mathbf{L}(\alpha)$ matrix $\Omega_0$ and a set of the creation operators $\mathbf{B}_a(\alpha)$. The algebraic approach to the Bethe Ansatz enables one to construct the other eigenvectors of $\mathrm{Tr}_*\mathbf{L}(\alpha)$. One has to apply the creation operators $\mathbf{B}_a(\lambda^a_\alpha)$ to $\Omega_0$ and using commutation rules (4.4.19) and the properties of 'bare' state $\Omega_0$ (4.4.14) obtain transcendental equations for the rapidities $\lambda^a_\alpha$.

More explicitly, consider the vector

$$\Omega({}_1\{\lambda_i, a_i\}_{m_1})=F_1(a_1,\ldots,a_{m_1})\prod_{i=1}^{m_1}\mathbf{B}_{a_i}(\lambda_i)\Omega_0 \tag{4.4.20}$$

(we assume the summation over the repeated indices).

Let us act by $\mathrm{Tr}\,\mathbf{D}_{ab}(\alpha)$ and $\mathbf{A}(\alpha)$ on the state (4.4.18). Using the commutation relations (4.4.19) we obtain:

$$\begin{aligned} \mathbf{A}(\alpha)\Omega({}_1\{\lambda_i, a_i\}_{m_1})&=\prod_{i=1}^{m_1}\frac{1}{b(\alpha-\lambda_i)}\Omega({}_1\{\lambda_i, a_i\}_{m_1}) \\ &\quad -\frac{c(\alpha-\lambda_1)}{b(\alpha-\lambda_1)}\prod_{i=2}^{m_1}\frac{1}{b(\lambda_1-\lambda_i)}\mathbf{B}_{a_1}(\alpha)\Omega({}_2\{\lambda_i, a_i\}_{m_1})+\ldots \end{aligned} \tag{4.4.21}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\begin{aligned}\operatorname{Tr}\mathbf{D}_{ab}(\alpha)\Omega({}_1\{\lambda_i, a_i\}_{m_1}) &= b^N(-\alpha)b(-\alpha+1)\prod_{i=1}^{m_1}\frac{1}{b(\lambda_1-\alpha)}\\ &\quad\times r^{a_1p_1}_{aq_1}(\lambda_1-\alpha)r^{a_2p_2}_{q_1q_2}(\lambda_2-\alpha)\ldots r^{a_{m_1}p_{m_1}}_{q_{m_1}a}(\lambda_{m_1}-\alpha)\\ &\quad\times\Omega({}_1\{\lambda_i, p_i\}_{m_1})-\frac{c(\lambda_1-\alpha)}{b(\lambda_1-\alpha)}b^N(-\lambda_1)b(-\lambda_1+1)\\ &\quad\times\prod_{i=2}^{m_1}\frac{1}{b(\lambda_i-\lambda_1)}\delta_{ap_1}\delta_{a_1q_1}r^{a_2p_2}_{q_1q_2}(\lambda_2-\lambda_1)\\ &\quad\times r^{a_3p_3}_{q_2q_3}(\lambda_3-\lambda_1)\ldots r^{a_{m_1}p_{m_1}}_{q_{m_1}a}(\lambda_{m_1}-\lambda_1)\\ &\quad\times\mathbf{B}_a(\alpha)\Omega({}_2\{\lambda_i, p_i\}_{m_1}), \Omega({}_2\{\lambda_i, p_i\}_{m_1})\\ &= F_1(a_1,\ldots,a_{m_1})\mathbf{B}_{p_2}(\lambda_2)\ldots\mathbf{B}_{p_{m_1}}(\lambda_{m_1}).\end{aligned}\tag{4.4.22}$$

The first summands in the right-hand side of eqns. (4.4.21) and (4.4.22) are obtained when we carry $\mathbf{A}(\alpha)$ or $\operatorname{Tr}\mathbf{D}_{ab}(\alpha)$ through $\mathbf{B}_{ai}(\lambda_i)$, using only the first terms in the right-hand side of (4.4.19 *a*, *b*). The second summands are obtained if $\mathbf{A}(\alpha)$ or $\operatorname{Tr}\mathbf{D}_{ab}(\alpha)$ commute with $\mathbf{B}_{a_1}(\lambda_1)$, and the second terms in (4.4.19 *a*, *b*) are used while for further commutations are denoted by points.

As in (4.2.6) the summands of the first type give the eigenvalue of $\mathbf{T}(\alpha)$ and the summands of the second type give the transcendental equations for the rapidities $\lambda_i$. In the previous cases these equations contain $c$ numbers but now they contain the new operators acting on the isotopic structure of the function $F_1(\alpha_1,\ldots,a_{m_1})$:

$$\mathbf{A}(\alpha)\mathbf{F}_1=\prod_{i=1}^{m_1}\frac{1}{b(\alpha-\lambda_i)}\mathbf{F}_1,\tag{4.4.23 a}$$

$$[\operatorname{Tr}\mathbf{D}_{ab}(\alpha)]\mathbf{F}_1=b^N(-\alpha)b(-\alpha+1)\prod_{i=1}^{m_1}\frac{1}{b(\lambda_i-\alpha)}\mathbf{T}_1(\alpha)\mathbf{F}_1,\tag{4.4.23 b}$$

where

$$\mathbf{T}_1(\alpha)=\operatorname{Tr}\mathbf{L}_1(\alpha)\equiv\operatorname{Tr}{}_1\mathbf{r}_{*1}(\lambda_1-\alpha)\ldots{}_1\mathbf{r}_{*m_1}(\lambda_{m_1}-\alpha)\tag{4.4.24}$$

and

$${}_1\mathbf{r}_{*j}(\alpha)=b(\alpha)+c(\alpha){}_1\mathbf{P}_{*j}.\tag{4.4.25}$$

A necessary and sufficient condition for the vector $\Omega({}_1\{\lambda_i, a_i\}_{m_1})$ to be an eigenvector is that $\mathbf{F}_1$ be an eigenvector of $\mathbf{T}_1(\alpha)$ and the rapidities $\lambda_i$ satisfy the vector equation

$$\begin{aligned}\mathbf{T}^{a_1'\ldots a_{m_1}'}_{a_1\ldots a_{m_1}}(\lambda_i)F_1(a_1',\ldots,a_{m_1}') &= b^{-N}(-\lambda_i)b^{-1}(-\lambda_i+1)\\ &\quad\times\prod_{\substack{j=1\\ j\neq i}}^{m_1}\frac{b(\lambda_j-\lambda_i)}{b(\lambda_i-\lambda_j)}F_1(a_1,\ldots,a_{m_1})\end{aligned}\tag{4.4.26}$$

resulting from the vanishing of the 'unwanted' terms in (4.4.21) and (4.4.22).

The operators $\mathbf{T}_1(\lambda)$, $\mathbf{L}_1(\lambda)$ and ${}_1\mathbf{r}(\lambda)$ and the eigenproblem (4.4.22) and (4.4.26) reproduce our initial construction with the following modifications. There are now sites in the chain and the operators ${}_1\mathbf{r}_{*j}(\lambda_j-\lambda)$ in $C_*^{n-1}\otimes C_j^{n-1}$ depend through $\lambda_j$ on the label of the site. Thus *the Bethe-Ansatz hierarchy* appears.

Let us consider the simplest case $n=3$, when the *Bethe-Ansatz* chain contains only two links.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The $L_1(\alpha)$ operator for $n=3$ coincides with that of § 4.2.6. The number $m_1$ plays the role of the number of particles. The eigenvalues of $\mathbf{T}_1(\alpha)$ are calculated from (4.2.67) and (4.2.68):

$$\Lambda(\alpha;\{\Lambda_k\})=\prod_{i=1}^{m_1} b(\lambda_i-\alpha)\prod_{k=1}^{m_2}\frac{1}{b(\Lambda_k-\alpha)}+\prod_{k=1}^{m_2}\frac{1}{b(\alpha-\Lambda_k)}, \tag{4.4.27}$$

where $\Lambda_k$ satisfy the following equations

$$\prod_{i=1}^{m_1}\frac{\Lambda_k-\lambda_i}{\Lambda_k-\lambda_i+ig}=-\prod_{j=1}^{m_2}\frac{\Lambda_k-\lambda_j-ig}{\Lambda_k-\Lambda_j+ig}. \tag{4.4.28}$$

To solve the problem (4.4.26) we need the eigenvalues $\Lambda_1(\lambda_i,\{\Lambda_k\})$. As $b(0)=0$, the first term in (4.4.27) vanishes. One obtains

$$\Lambda_1(\lambda_i;\{\Lambda_k\})=\prod_{k=1}^{m_2}\frac{1}{b(\lambda_i-\Lambda_k)}. \tag{4.4.29}$$

Substituting (4.4.29) in (4.4.26) we obtain the equation

$$\left(\frac{\lambda_i}{\lambda_i-ig}\right)^N\left(\frac{\lambda_i-1}{\lambda_i-1-ig}\right)\prod_{k=1}^{m_2}\frac{\lambda_i-\Lambda_k}{\lambda_i-\Lambda_k-ig}=\prod_{\substack{j=1\\ j\neq i}}^{m_1}\frac{\lambda_i-\lambda_j+ig}{\lambda_i-\lambda_j-ig}. \tag{4.4.30}$$

Equations (4.4.28) and (4.4.30) determine rapidities $\{\lambda_i\}$, $\{\Lambda_k\}$.

As $b(0)=0$ the eigenvalues of the $\mathbf{T}$ operator are defined only from $\mathbf{A}(\alpha)$. Equation (4.4.23) gives

$$T(0)=\prod_{i=1}^{m_1}\left(\frac{\lambda_i-ig}{\lambda_i}\right) \tag{4.4.31}$$

What do the numbers $m_1$, $m_2$ mean? As follows from above, $m_1$ is the total number of the creation operators $\mathbf{B}_{a_i}$ acting on the 'bare' vacuum. It means that $m_1$ is the total number of 'coloured' particles (we consider the 'bare' vacuum as white). In the present case the coloured particles have two colours, the number of particles with the first colour being $m_2$. Thus, the Young tableau consists of three columns: $[3^{m_2}, 2^{m_1-2m_2}, 1^{N-2m_1+m_2}]$ (see fig. 4.10).

Induction arguments enable us to write the Bethe-Ansatz hierarchy. Substituting $g(-\lambda+i/2)$, $-\Lambda g$ instead of $\lambda$ and $\Lambda$ one obtains for arbitrary $n$:

$$\exp(ik_jL)=\prod_{\alpha=1}^{m_1}\left(\frac{\lambda_\alpha^{(1)}+i/2}{\lambda_\alpha^{(1)}-i/2}\right), \tag{4.4.A}$$

$$\prod_{\tau=\pm1}\prod_{\beta=1}^{m_{j+\tau}}\left(\frac{\lambda_\alpha^{(j)}-\lambda_\beta^{(j+\tau)}+i/2}{\lambda_\alpha^{(j)}-\lambda_\beta^{(j+\tau)}-i/2}\right)=-\prod_{\beta=1}^{m_j}\left(\frac{\lambda_\alpha^{(j)}-\lambda_\beta^{(j)}+i}{\lambda_\alpha^{(j)}-\lambda_\beta^{(j)}-i}\right), \tag{4.4.B}$$

where $\lambda_\alpha^{(0)}=-1/g\delta_{\alpha,N+1}, j=1,\ldots,n-1$, $m_0=N+1$, $m_n=0$. The eigenvalue of the energy is

$$E=\sum_{j=1}^{N}k_j. \tag{4.4.C}$$

The number of particles with momentum projection $j-(n+1/2)$ is equal to $m_j-m_{j-1}$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Consider some details omitted in the previous discussion. The elimination of 'unwanted' terms in (4.4.20) and (4.4.21) leads to the following relation:

$$\frac{c(\lambda_1-\alpha)}{b(\lambda_1-\alpha)}b^N(-\lambda_1)b(-\lambda_1+1)\prod_{i=2}^{m_1}\frac{1}{b(\lambda_i-\lambda_1)}\delta_{ap_1}\delta_{a_1q_1}r^{a_2p_2}_{q_1q_2}(\lambda_2-\lambda_1)$$
$$\ldots\times r^{a_{m_1}p_{m_1}}_{q_{m_1}a}(\lambda_{m_1}-\lambda_1)\mathbf{B}_a(\alpha)\mathbf{B}_{p_2}(\lambda_2)\ldots\mathbf{B}_{p_{m_1}}(\lambda_{m_1})F_1(a_1,\ldots,a_{m_1})$$
$$+\frac{c(\alpha-\lambda_1)}{b(\alpha-\lambda_1)}\prod_{i=2}^{m_1}\frac{1}{b(\lambda_1-\lambda_i)}\mathbf{B}_{a_1}(\alpha)(\lambda_2)\ldots\mathbf{B}_{a_{m_1}}(\lambda_{m_1})F_1(a_1,\ldots,a_{m_1})=0. \qquad (4.4.32)$$

Using the relation $c(-\alpha)/b(-\alpha)=-c(\alpha)/b(\alpha)$ one can rewrite (4.4.32) as

$$b^N(-\lambda_1)b(-\lambda_1+1)\prod_{i=2}^{m_1}\delta_{aa_1}\delta_{p_1q_1}r^{p_2a_2}_{q_1q_2}(\lambda_2-\lambda_1)\ldots$$
$$r^{p_{m_1}a_{m_1}}_{q_{m_1}a}(\lambda_{m_1}-\lambda_1)F_1(p_1,\ldots,p_{m_1})\mathbf{B}_{a_1}(\alpha)\mathbf{B}_{a_2}(\lambda_2)\ldots\mathbf{B}_{a_{m_1}}(\lambda_{m_1})$$
$$-\prod_{i=2}^{m_1}\frac{b(\lambda_i-\lambda_1)}{b(\lambda_1-\lambda_i)}F(a_1,\ldots,a_{m_1})\mathbf{B}_{a_1}(\alpha)\mathbf{B}_{a_2}(\lambda_2)\ldots\mathbf{B}_{a_{m_1}}(\lambda_{m_1})=0. \qquad (4.4.33)$$

The terms containing the identical products of the **B** operators should be equal. Therefore, we have

$$b^N(-\lambda_1)b(-\lambda_1+1)\sum_a r^{p_1a_1}_{aq_1}(0)r^{p_2a_2}_{q_1q_2}(\lambda_2-\lambda_1)\ldots r^{p_{m_1}a_{m_1}}_{q_{m_1}a}(\lambda_{m_1}-\lambda_1)$$
$$\times F_1(p_1,\ldots,p_{m_1})=\prod_{i=2}^{m_1}\frac{b(\lambda_i-\lambda_1)}{b(\lambda_1-\lambda_i)}F_1(a_1,\ldots,a_{m_1}). \qquad (4.4.34)$$

Note that

$$\mathbf{r}(\alpha)={}_1\mathbf{r}(\alpha)$$

and particularly

$$r^{p_1q_1}_{aq_1}(0)=\delta_{aa_1}\delta_{p_1q_1},$$

where ${}_1\mathbf{r}$ is the matrix from (4.4.3) acting in $C^{n-1}\otimes C^{n-1}$. Using these equations it is easy to obtain from eqn. (4.4.34) the condition (4.4.26).

The Bethe-Ansatz hierarchy for the degenerate exchange model (4.4.A)–(4.4.C) was constructed by Tsvelick and Wiegmann (1981, 1982 a).

### 4.5. *The Bethe Ansatz for the Anderson model*

In the idealized case with the orbital structure of an impurity ion neglected, the hamiltonian of the so-called non-degenerate Anderson model is

$$\mathscr{H}_A=\sum_{k,\sigma=\uparrow,\downarrow}\varepsilon_k c^+_{k\sigma}c_{k\sigma}+V\sum_{k,\sigma}(c^+_{k\sigma}d_\sigma+d^+_\sigma c_{k\sigma})+\mathscr{H}_{\text{atom}}, \qquad (4.5.1)$$

where $c^+_{k\sigma}$, $c_{k\sigma}$ are the creation and annihilation operators of the band electron with the wave-vector $k$ and the spin $\sigma=\uparrow,\downarrow$, and $d^+_\sigma$, $d_\sigma$ are the creation and annihilation operators of an electron localized on the impurity orbital. The operator $\mathscr{H}_{\text{atom}}$ describes the dependence of the impurity orbital energy on the occupation orbital number $\hat{n}_\sigma=d^+_\sigma d_\sigma$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The atomic part of the hamiltonian is conventionally written as

$$\mathscr{H}_{\text{atom}} = \sum_{\sigma} \epsilon_d \hat{n}_\sigma + U \hat{n}_\uparrow \hat{n}_\downarrow, \tag{4.5.2}$$

where $\varepsilon_d$ is the energy of the impurity orbital measured from the Fermi level, $U$ is the Coulomb repulsion on the impurity orbital ($U>0$). The energies $E_+ = \epsilon_d + U$ and $E_- = -\epsilon_d$ are related to the variation of a number of $d$ electrons by $\pm 1$. The interaction of band and localized electrons is phenomenologically described by the hybridization $V$ (see §§ 2.1, 3.4 and 3.5). Integrability and the Bethe hypothesis for the Anderson model were briefly studied by Wiegmann (1980 b). This solution will be given below.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

### 4.5.1. *The effective hamiltonian*

The simplifying assumptions adopted while solving the Anderson hamiltonian (4.5.1) are identical to those used previously to construct the exact solution of the Kondo hamiltonian (s–d exchange model) (see § 4.1.2). Namely, it is our assumption that

(i) the mixing amplitude $V$ does not depend on momenta $k$; and
(ii) the amplitudes $U$, $\epsilon_d$ and $\Gamma$ are small in comparison with the Fermi energy.

According to (i) the hamiltonian (4.5.1) describing only a unique impurity is spherically symmetric and consequently reduces to a one-dimensional problem. Further, according to (ii) one can neglect electron states lying far from the Fermi surface so in the vicinity of $k \simeq k_F$ the spectrum can be considered as linear $\varepsilon(k) = (k - k_F) v_F$. We shall set, below, that $v_F = 1$. Therefore, the density of states on the Fermi surface $\rho(\varepsilon_F)$ is $1/2\pi$. Thus, one can reformulate the problem in terms of the coordinate along an arbitrary line intersecting the impurity position

$$\mathscr{H}_A = \sum_{\sigma} \int dx \left\{ -i c_\sigma^+(x) \frac{\partial}{\partial x} c_\sigma(x) + V \delta(x) [c_\sigma^+(x) d_\sigma + d_\sigma^+ c_\sigma(x)] \right\} + \epsilon_d \sum_{\sigma} \hat{n}_\sigma + U \hat{n}_\uparrow n_\downarrow, \tag{4.5.3}$$

where $x$ is the corresponding one-dimensional coordinate.

### 4.5.2. *The two-particle scattering matrix*

As is known, to prove the integrability of the hamiltonian and the validity of the Bethe hypothesis, it suffices to find out whether the two-particle $S$ matrix satisfies the factorization conditions.

Obviously the total number of particles is conserved:

$$N = \sum_{\sigma} \left[ \hat{n}_\sigma + \int dx\, c_\sigma^+(x) c_\sigma(x) \right]. \tag{4.5.4}$$

Elements of the two-particle $S$ matrix are determined by the Schrödinger equation for $N=2$. For instance, in the case $S^z=0$ the eigenvector of the hamiltonian is of the form

$$|\Psi\rangle=\left\{\int dx_1dx_2g(x_1,x_2)c_\uparrow^+(x_1)c_\downarrow^+(x_2)+\int dxe(x)\right.$$
$$\left.\times\left[c_\uparrow^+(x)d_\downarrow^+-c_\downarrow^+(x)d_\uparrow^+\right]+fd_\uparrow^+d_\downarrow^+\right\}|0\rangle, \qquad (4.5.5)$$

where the vacuum $|0\rangle$ is a state without particles: $c_\sigma(x)|0\rangle=d_\sigma|0\rangle=0$. The wavefunctions $g(x_1,x_2)$, $e(x)$ and $f$ satisfy the Schrödinger equation $\mathscr{H}_A|\Psi\rangle=E|\Psi\rangle$, which in our case is of the form

$$[-i(\partial_{x_1}+\partial_{x_2})-E]g(x_1,x_2)+V[\delta(x_1)e(x_2)+\delta(x_2)e(x_1)]=0, \qquad (4.5.6)$$

$$\left.\begin{aligned}(-i\partial_{x_1}-E+\epsilon_d)e(x)+Vg(0,x)+V\delta(x)f=0,\\ (U+2\epsilon_d)f+2Ve(0)=Ef.\end{aligned}\right\} \qquad (4.5.7)$$

Above all, let us find a solution of eqn. (4.5.6) at $U=0$. In this case the problem is one-particle, therefore the two-particle eigenvector (4.5.5) must be a direct product of two one-particle eigenvectors

$$|\Psi_{k\sigma}\rangle=\left(\int dxg_k(x)c_\sigma^+(x)+e_kd_\sigma^+\right)|0\rangle. \qquad (4.5.8)$$

With energies $k$ and $p$ such that $k+p=E$

$$|\Psi\rangle=|\Psi_{k\uparrow}\rangle\otimes|\Psi_{p\downarrow}\rangle+|\Psi_{p\uparrow}\rangle\otimes|\Psi_{k\downarrow}\rangle. \qquad (4.5.9)$$

Therefore at $U=0$

$$\left.\begin{aligned}g(x_1,x_2)=g_k(x_1)g_p(x_2)+g_k(x_2)g_p(x_1),\\ e(x)=e_kg_p(x)+e_pg_k(x);\qquad f=2e_ke_p.\end{aligned}\right\} \qquad (4.5.10)$$

The one-particle wave functions $g_k(x)$ and $e_k$ satisfy the equations

$$\left.\begin{aligned}(-i\partial_x-k)g_k(x)+V\delta(x)e_k=0\\ \epsilon_de_k+Vg_k(0)=ke_k.\end{aligned}\right\} \qquad (4.5.11)$$

The solution of these equations is

$$g_k(x)=\exp(ikx+i/2\,\mathrm{sign}\,x\delta(k)),\qquad g_k(0)=\cos\delta(k), \qquad (4.5.12)$$

$$e_k=\frac{V}{k-\epsilon_d}g_k(0),$$

where

$$\delta(k)=-2\tan^{-1}\left(\frac{V^2}{k-\epsilon_d}\right) \qquad (4.5.13)$$

is the one-particle phase of the scattering of a particle on the resonance level.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

At $U \neq 0$ we derive the solution in the form

$$g(x_1, x_2) = Z_{kp}(x_1 - x_2) g_k(x_1) g_p(x_2) + Z_{kp}(x_2 - x_1) g_p(x_1) g_k(x_2), \tag{4.5.14}$$

where $Z_{kp}$ is a so far unknown function.

Inserting (4.5.14) into (4.5.6) we get

$$e(x) = g_p(x) e_k Z_{kp}(x) + g_k(x) e_p Z_{kp}(-x).$$

where

$$Z_{kp}(x) = 1 + i \operatorname{sign} x \frac{\Gamma U}{(k-p)(k+p-U-2\epsilon_d)}. \tag{4.5.15}$$

If the spin of the particles is parallel, the interaction is absent and $g(x_1, x_2)$ is determined by (4.5.10) and (4.5.12).

Here as in the solution of the s–d exchange model, we encounter the following interesting circumstances. Even far from the impurity, e.g. in the region $x_1, x_2 < 0$, the particles described by the wavefunctions (4.5.14) and (4.5.15) have a non-unitary scattering matrix. Actually according to (4.5.14) and (4.5.15) the particle with the momentum $k$, scattered by another particle with the opposite spin, acquires the phase

$$i \ln \left[ \frac{g(k) - g(p) + i/2}{g(k) - g(p) - i/2} \right],$$

where

$$g(k) = (k - \epsilon_d - U/2)^2 / 2U\Gamma. \tag{4.5.16}$$

This circumstance, discussed in detail in § 4.2.2., does not, of course, imply any interaction and is a consequence of the linear particle spectrum. It is easy to check that the wavefunction (4.5.14) at arbitrary $Z_{kp}(x)$ is a solution of the Schrödinger equation

$$-i \left( \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) g(x_1, x_2) = E g(x_1, x_2). \tag{4.5.17}$$

One-dimensional free particles with a linear spectrum allow representations with an arbitrary scattering phase (for instance, constructing the perturbation theory ($U \to 0$) one uses a representation of free particles with a unitary scattering matrix). The presence of an impurity unambiguously fixes the free particle representation.

The hamiltonian (4.5.1) has rotational invariance. Therefore, the general form of the $S$-scattering matrix far from the impurity with the momenta $k, p$ and spins $\sigma_1, \sigma_2$ is

$$S^{\sigma_2 \sigma_2'}_{\sigma_1 \sigma_1'}(k, p) = \omega_0(k, p) + w(k, p) \boldsymbol{\sigma}_{\sigma_1 \sigma_1'} \boldsymbol{\sigma}_{\sigma_2 \sigma_2'} = b + c \mathbf{P}_{12}, \tag{4.5.18}$$

where $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are Pauli matrices and $\mathbf{P}_{12} = 1/2(\mathbf{1} \times \mathbf{1} + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)$ is a permutation operator. Comparing (4.5.18) with (4.5.14) we get

$$b(k, p) - c(k, p) = \frac{Z_{kp}(x > 0)}{Z_{kp}(x < 0)} = \frac{g(k) - g(p) + i/2}{g(k) - g(p) - i/2}.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

If the spins of the particles are parallel, the interaction with the impurity is absent and the particles passing through each other do not change their phase

$$b(k,p)+c(k,p)=1.$$

Therefore,

$$\mathbf{S}(k,p)=\frac{g(k)-g(p)+(i/2)\mathbf{P}}{g(k)-g(p)+i/2}. \tag{4.5.19}$$

It is easy to check that the matrix (4.5.19) satisfies (4.1.17). Actually, in terms of the functions $b(k,\mathrm{p})$ and $c(k,p)$ the factorization equation is

$$h(k,p)+h(p,r)=h(k,r), \tag{4.5.20}$$

where

$$h(k,p)=b(k,p)/c(k,p).$$

The general solution of (4.5.20) is $h(k,p)=g(k)-g(p)$, where $g(k)$ is an arbitrary function. For the Anderson model the function $g(k)$ is determined by formula (4.5.16).

4.5.3. *The coordinate Bethe Ansatz*

Let us now formulate the Bethe Ansatz. Let $Q$ and $P$ be permutations of the integers $\{1,\ldots,N\}$. In each domain $X_Q=\{X_{q_1}<\ldots<X_{q_N}\}$ $\{q\}\epsilon Q$, the wavefunction $g_{\alpha_1\ldots\alpha_N}(x_1,\ldots,x_N)$, where $\alpha_j$ are spins of the particles, is of the form

$$g_{\alpha_1\ldots\alpha_N}(x_1,\ldots,x_N)=\sum_{P=\{p_1\ldots p_N\}} A_{\alpha_1\ldots\alpha_N}(Q|P)\prod_{j=1}^{N} g_{k_p}(x_j), \tag{4.5.21}$$

where $\{k_j\}$ is a set of unequal numbers and $g_k(x)$ is given by (4.5.12). It is possible to write down similar expressions for $e_{\alpha_1\ldots\alpha_N}(x_1,\ldots,x_{N-1})$ as well. The underlying hypothesis is that in each domain the wavefunction is described by a unique set of $Q$-independent parameters. The energy of the state with the wavefunction (4.5.21) is

$$E=\sum_{j=1}^{N} k_j.$$

There is a number of constraints imposed on the $N!\times N!$ matrix $A(Q|P)$ by the Schrödinger equation, continuity conditions at the boundaries of the domain $X_Q$ and antisymmetry. The number of these constraints exceeds the number of elements of the matrix $A(Q|P)$. The consistency of these constraints is guaranteed by the factorization condition which proves the Bethe hypothesis. Let $I=\{1,\ldots,N\}$, then $A(Q|P)$ is related to $A(I|P)$ by the matrix $\mathbf{S}(Q|P)$:

$$A_{\alpha_1\ldots\alpha_N}(Q|P)=S^{\alpha_1'\ldots\alpha_N'}_{\alpha_1\ldots\alpha_N}(Q|P)A_{\alpha_1'\ldots\alpha_N'}(I|P).$$

Then $\mathbf{S}(Q|P)$ is a multiparticle scattering matrix. Due to the validity of factorization conditions (4.1.17) it is the product of two-particle $S$ matrices (fig. 4.1). The antisymmetry requirement with the wavefunction (4.5.21) at the pair permutations $(x_j,\alpha_j)$ leads to the condition

$$A_{\alpha_1\ldots\alpha_N}(Q|P)=(-1)^P A_{\alpha_{q_1}\ldots\alpha_{q_N}}(QP).$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

To study the spectrum of the system, we must impose boundary conditions on the wavefunctions. As has been established in § 4.2.3 we arrive at the following eigenvalue problem:

$$\mathbf{T}_j\xi = \exp(ik_jL + i\delta(k_j))\xi, \tag{4.5.22}$$

where

$$\mathbf{T}_j = \mathbf{S}_{jj+1}(k_j, k_{j+1})\ldots\mathbf{S}_{jN}(k_j, k_N)\mathbf{S}_{j1}(k_j, k_1)\ldots\mathbf{S}_{jj-1}(k_j, k_{j-1}). \tag{4.5.23}$$

Since this eigenvalue problem is not specific for the Anderson model we do not give its solution here, referring the reader to § 4.2.6.

The eigenvalues of the operators $\mathbf{T}_j$ with the total spin projection $S^z = N/2 - M$ are given by the equations

$$\exp(ik_jL + i\delta(k_j)) = \prod_{\alpha=1}^{M} \frac{g(k_j) - \lambda_\alpha + i/2}{g(k_k) - \lambda_\alpha - i/2}, \tag{4.5.A}$$

where the quantities $\lambda_\alpha$ satisfy the conditions

$$\prod_{j=1}^{N} \frac{\lambda_\alpha - g(k_j) + i/2}{\lambda_\alpha - g(k_j) - i/2} = -\prod_{\beta=1}^{M} \frac{\lambda_\alpha - \lambda_\beta + i}{\lambda_\alpha - \lambda_\beta - i}. \tag{4.5.B}$$

Equations (4.5.A) and (4.5.B) with the condition

$$E = \sum_{j=1}^{N} k_j \tag{4.5.C}$$

completely determine the spectrum of the Anderson hamiltonian. They describe the quantization of the rapidities of the charge $\{k_j\}$ and spin $\{\lambda_\alpha\}$ excitations. Note that in the s–d exchange (Kondo) model these excitations are not coupled.

### 4.6. *The Bethe Ansatz for the degenerate Anderson model*

We present below the Bethe-Ansatz solution of the degenerate Anderson model. For the origin of this model see § 2.1.3. The degenerate Anderson hamiltonian (2.1.14) describes the cerium or ytterbium impurity in both the localized-moment and mixed-valence regimes.

The effective hamiltonian of the degenerate Anderson model has the form:

$$\mathscr{H}_{\mathrm{A}} = \sum_{j=1}^{n} \int dx \left\{ -ic_j^+(x)\frac{\partial}{\partial x}c_j(x) + V\delta(x)[c_j^+(x)\mathbf{X}_{0j} + \mathbf{X}_{j0}c_j(x)] \right\} + \sum_{j=1}^{n} (\epsilon_d + E_j)\mathbf{X}_{jj}, \tag{4.6.1}$$

where $E_j$ is a crystal field splitting and $\mathbf{X}_{ij}$ is a projection operator, defined in § 2. As in the previous subsections, we have assumed that $\Gamma$ and $\epsilon_d$ are small compared to the Fermi energy and considered only the linear part of the electron spectrum. However, in this section we assert that the intra-atomic energy $E_+$, related with adding one additional electron to the impurity shell, is infinite, i.e. much larger than the band width.

The methods described in §§ 4.4 and 4.5 are all that we need to solve the problem (4.6.1). Hence, the presentation will be brief with frequent references to §§ 4, 5 and 6. In the particular case $n = 2$ we arrive at the asymmetric non-degenerate Anderson

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

model $U \to \infty$. In this limit in eqns. (4.5.6) and (4.5.7) the amplitude $f \to 0$. The two-particle $S$ matrix has the form (4.5.19) with

$$g(k) = \frac{\epsilon_d - k}{2\Gamma}. \tag{4.6.2}$$

The Bethe-Ansatz equations (4.5.A)–(4.5.C) must be changed according to the above.

After this note we are ready to solve the problem. Consider the state

$$|\Psi\rangle = \left[ \int c^+_{j_1}(x_1) c^+_{j_2}(x_2) g_{j_1 j_2}(x_1, x_2) dx_1 dx_2 + \int dx\, e^{j_2}_{j_1}(x) c^+_{j_1}(x) \mathbf{X}_{j_2 0} \right] |0\rangle. \tag{4.6.3}$$

The amplitudes $g_{j_1 j_2}(x_1, x_2)$ and $e^{j_2}_{j_1}(x)$ satisfy the equations:

$$\left.\begin{aligned} [-i(\partial_{x_1} + \partial_{x_2}) - E] g_{j_1 j_2}(x_1, x_2) + V(\delta(x_1) e^{j_1}_{j_2}(x_2) - \delta(x_2) e^{j_2}_{j_1}(x)) = 0, \\ (-i\partial_x - E + \epsilon_d) e^{j_1}_{j_2}(x) + V g_{j_1 j_2}(0, x) = 0. \end{aligned}\right\} \tag{4.6.4}$$

The solution of these equations is given by the following expressions:

$$\begin{aligned} g_{j_1 j_2}(x_1, x_2) = (g_k(x_1) g_p(x_2) - g_k(x_2) g_p(x_1)) \\ \times (A_{j_1 j_2} \theta(x_1 - x_2) + S^{j_2 j_2'}_{j_1 j_1'}(k, p) A_{j_1' j_2'} \theta(x_2 - x_1)); \end{aligned} \tag{4.6.5}$$

$$e^{j_2}_{j_1}(x) = (g_k(x) e_p - g_p(x) e_k)(A_{j_1 j_2} \theta(x) + S^{j_2 j_2'}_{j_1 j_1'}(k, p) A_{j_1' j_2'} \theta(-x)), \tag{4.6.6}$$

where the functions $g_k(x)$ and $e_k$ are given by (4.5.12) and the two-particle $\mathbf{S}$ matrix has the form

$$S^{j_2 j_2'}_{j_1 j_1'}(k, p) = (p - k + 2i\Gamma P^{j_2 j_2'}_{j_1 j_1'})/(p - k + 2i\Gamma). \tag{4.6.7}$$

Here $\mathbf{P}$ is permutation operator of rank $n$:

$$P^{j_2 j_2'}_{j_1 j_1'} = \delta_{j_1 j_2'} \delta_{j_2 j_1'} \qquad (j = 1, \ldots, n).$$

Evidently the matrix (4.6.7) satisfies the factorization condition.

The coordinate Bethe Ansatz for our problem, formulated in the same manner as in § 4.5.3, leads us to the eigenvalue problem of the operator (4.5.23), where the $\mathbf{S}$ operator is given by (4.6.7). For the solution of this problem we refer the reader to § 4.4.2.

The eigenvalues of the operators $\mathbf{T}_j$ are given by the Bethe-Ansatz hierarchy

$$\exp(ik_j L) \left( \frac{k_j - \epsilon_d - i\Gamma}{k_j - \epsilon_d + i\Gamma} \right) = \prod_{\alpha=1}^{m_1} \frac{k_j/2\Gamma + \lambda^{(1)}_\alpha - i/2}{k_j/2\Gamma + \lambda^{(1)}_\alpha + i/2}, \tag{4.6.A}$$

$$\prod_{\tau = \pm 1} \prod_{\beta=1}^{m_{j+\tau}} \left( \frac{\lambda^{(j)}_\alpha - \lambda^{(j+\tau)}_\beta + i/2}{\lambda^{(j)}_\alpha - \lambda^{(j+\tau)}_\beta - i/2} \right) = - \prod_{\beta=1}^{m_j} \left( \frac{\lambda^{(j)}_\alpha - \lambda^{(j)}_\beta + i}{\lambda^{(j)}_\alpha - \lambda^{(j)}_\beta - i} \right), \tag{4.6.B}$$

where $\lambda^{(0)}_\alpha = -k_\alpha/2\Gamma$, $m_0 = N$, $m_n = 0$ and the numbers $m_j (j = 1, \ldots, n-1)$ are defined by the Young tableau (fig. 4.10)

$$m_j = \sum_{j=k}^{n-1} N_k, \tag{4.6.8}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where $m_k$ is the number of particles with $(k-(n-1)/2)$ projection of the angular momentum. The energy of this state is

$$E=\sum_{j=1}^{N} k_j+\sum_{j=1}^{n} E_j N_j. \tag{4.6.C}$$

The Bethe-Ansatz hierarchy for the degenerate Anderson model (4.6.A)–(4.6.C) was constructed by Schlottmann (1982).

### 4.7. *General remarks*

The physical properties of a system containing a large number of particles ($N\to\infty$, $N/L=$const.) will be studied in the next sections with the use of eqns. (A)–(C) of §§4.2–4.6. Before that we discuss some properties of the derived equations and their relation to other models.

First, note that eqns. (A)–(C) of §§4.2–4.6 in the absence of the impurity describe a non-interacting electron gas. The impurity terms are of the order of $1/N$ with respect to others and can easily be selected from all these equations. For the exchange hamiltonians the appropriate factors in eqns. (B) of §§4.2–4.6 are

$$\left(\frac{\lambda+1/g+iS}{\lambda+1/g-iS}\right) \quad \text{for the Kondo model (eqn. (4.2.B)),}$$

$$\left(\frac{\sinh\mu(\lambda+f/\mu+i/2)}{\sinh\mu(\lambda+f/\mu-i/2)}\right) \quad \text{for the anisotropic Kondo model (eqn. (4.3.B)),}$$

$$\left(\frac{\lambda^{(1)}+1/g+i/2}{\lambda^{(1)}+1/g-i/2}\right) \quad \text{for the degenerate exchange model (eqn. (4.4.B)).}$$

The presence of the impurity in the Anderson model is reflected by the factor

$$\frac{k-\epsilon_d+i\Gamma}{k-\epsilon_d-i\Gamma}$$

in eqns. (A) of §§4.5 and 4.6.

Obviously, for either $g=0$ or $S=0$ and either $f=0$ or $\Gamma=0$ the interaction with the impurity vanishes and all these factors are equal to unity. In these limits the corresponding Bethe-Ansatz equations must describe the non-interacting electron gas. The explicit proof of this statement is given in §6.1.4. Here we only show that the excitation spectrum coincides with that of the free gas, i.e.

$$E=2\pi K/L, \tag{4.7.1}$$

where $K$ is an integer.

Indeed, take a product of eqns. (A) in §§4.2–4.6 for all $j$ and the product of eqns. (B) in §§4.2.–4.6 for all $\alpha$. Then one finds that at $g=0$

$$\exp(iEL)=1. \tag{4.7.2}$$

In the cases of $S=1/2$ Kondo hamiltonian and degenerate exchange hamiltonians one gets a non-interacting gas also in the strong-coupling limit $g^{-1}=0$. The net effect of the impurity is an increase by unity of the exponent of the free gas factor. This results in a replacement $L\to L[(N+1)/N]$ in (4.7.1) and (4.7.2) and, consequently, in a decrease of the particle density by $1/L$. In other words, in the strong coupling

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

limit the impurity compensates one particle, and the system has the Fermi-liquid behaviour at low energies (Nozieres 1974).

For our purposes a conventional consideration of 1/2 spin free particles as subsets of spin-up and spin-down particles is inadequate. In our approach the $S$ matrix contains the permutation operator and convenient subsystems are the spin and charge ones.

Equations (A) in §§4.2–4.6 describe the 'scattering' of the charge subsystem particles with momenta $k_j$ on the spin subsystem particles having rapidities $\lambda_\alpha$. Equation (B) of the same section describes the spin–spin scattering. Both subsystems are fermionic since from an analysis of the normalization of the eigenvector $\Omega(\alpha, \{\lambda_\beta\})$ it follows that the wavefunction vanishes if any two values of either $\lambda_\beta$ or $k_j$ coincide. The number of particles in the spin subsystem is equal to the number of flipped spins $M$. In the s–d exchange model a natural definition of the momentum of spin excitations is

$$p(\lambda) = 2\tan^{-1} 2\lambda, \tag{4.7.3}$$

whilst for the Anderson model it is

$$p(\lambda) = \frac{1}{L}\sum_{j=1}^{N} 2\tan^{-1} 2(\lambda - g(k_j)). \tag{4.7.4}$$

Taking the log of eqns. (A) and (B) in §§4.2–4.6 we obtain

$$k_j L = 2\pi N_j - \sum_{\alpha=1}^{M} (\pi + p(\lambda_\alpha)) - \delta_c(k_j) \tag{4.7.5 a}$$

$$Np(\lambda_\alpha) = 2\pi J_\alpha + \sum_{\beta=1}^{M} \Phi(\lambda_\alpha - \lambda_\beta) - \delta_s(\lambda_\alpha), \tag{4.7.5 b}$$

where $\Phi(\lambda) = 2\tan^{-1}\lambda$ is the two-particle scattering phase of the spin density waves; and $\delta_s(\lambda)$ and $\delta_c(k)$ are the one-particle phases corresponding to the scattering of spin and charge excitations by an impurity.

For the s–d exchange model we have

$$\delta_c(k) = -IS/2, \qquad \delta_s(\lambda) = 2\tan^{-1}[(\lambda + 1/g)/S]. \tag{4.7.6}$$

For the Anderson model

$$\delta_c(k) = 2\tan^{-1}\left(\frac{k - \epsilon_d}{\Gamma}\right), \qquad \delta_s(\lambda) = 0. \tag{4.7.7}$$

The integers $2N_j$ and $2J_\alpha$ are quantum numbers of a system.

In the exchange models the phases of scattering on the impurity do not depend on the momentum of the incident particle. As a result the spin and charge excitations do not interact. In the Anderson model both subsystems are interconnected.

Add eqns. (4.7.5 *a*, *b*). Then:

$$E = E_h + E_i/L; \qquad E_h = E^{ch} + E^{sp}$$

$$E^{ch} = \frac{2\pi}{L}\sum_{j=1}^{N} N_j$$

$$E^{sp} = -\frac{2\pi}{L}\sum_{\alpha=1}^{M} J_\alpha - \frac{N\pi M}{L}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

are the energies of the charge and spin subsystems in the absence of the impurity and

$$E_{\mathrm{i}}=\sum_{\alpha=1}^{M}\delta_{\mathrm{s}}(\lambda_{\alpha})+\sum_{j=1}^{N}\delta_{\mathrm{c}}(k_j)$$

is an impurity contribution to the energy.

As we see, in the exchange models the impurity contribution to the energy depends only on the spin subsystem. This can be seen explicitly in the bosonic representation approach § 3.1.1.

As mentioned in § 4.2.2, for the free particles with the linear spectrum the scattering matrix can be chosen arbitrarily†. This freedom is eliminated once the interaction with impurity is fixed. In the s–d model the particle–particle $S$ matrix is a permutation operator $\mathbf{P}$, whereas in the Anderson model it is of a more general form (4.5.19).

A traditional choice of the unity $S$ matrix corresponds to a conventional perturbation theory. The choice of a permutation operator as the $S$ matrix corresponds, on the contrary, to the strong coupling limit.

Let us consider, for example, the $S$ matrix (4.5.10). It is known that in the Schrieffer–Wolf limit of $U\to\infty$ the Anderson model is equivalent to the s–d exchange model. Therefore, the relevant $S$ matrix coincides with the permutation operator

$$\lim_{U\to\infty}\mathbf{S}=\mathbf{P}$$

It is far from well known how far from the perturbation theory this limit is at any small exchange amplitude $I=8\Gamma/\pi U$. On the other hand, at either $\Gamma\to 0$ or $U\to 0$ the perturbation theory holds and the $S$ matrix is close to the unity matrix

$$\lim_{U\to 0}\mathbf{S}(k,p)=\lim_{\Gamma\to 0}\mathbf{S}(k,p)=\mathbf{I}.$$

In § 8 we show in detail how transition from the strong coupling to the perturbation-theory domain takes place.

For free particles the freedom in the choice of the $S$ matrix stems from the linearity of the spectrum. The linear kinetic energy operator

$$-i\sum_{n=1}^{N}\frac{\partial}{\partial x_n}\Psi=E\Psi \tag{4.7.8}$$

approximates the energy of the near Fermi-surface conduction electrons.

$$-\sum_{n=1}^{N}\left(\frac{\partial^2}{\partial x_n^2}+\epsilon_{\mathrm{F}}\right)\Psi=E\Psi. \tag{4.7.9}$$

Equation (4.7.9) has, however, just one solution with the unity $S$ matrix, which can never take the form (4.2.24). The origin of solution (4.2.24) can be understood as follows.

† The ambiguity in the equations with linear dispersion was discussed by Sutherland and Mattis (1981) and Lai and Shi (1981).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Consider the gas of 1/2-spin fermions with the delta-function interaction (4.1.20)

$$-\sum_{n=1}^{N}\frac{\partial^2}{\partial x_n^2}\Psi+c\sum_{i>j}\delta(x_i-x_j)\Psi=E\Psi. \tag{4.7.10}$$

As mentioned above in § 4.1, this is a completely integrable model (Yang 1967) with the $S$ matrix of the form

$$\mathbf{S}(k,p)=\frac{k-p+ic\mathbf{P}}{k-p+ic}. \tag{4.7.11}$$

As known in the limit of a large number of particles $N\to\infty$, $L\to\infty$, $\pi N/L=k_{\mathrm{F}}$ and $c\ll 1$ one can study only a small range of momenta near the Fermi surface and assume the spectrum to be linear. Introduce the creation and annihilation operators for electrons near the right-hand and left-hand Fermi points $\Psi^{+}_{+,\sigma}\Psi_{+,\sigma}$ and $\Psi^{+}_{-,\sigma}\Psi_{-,\sigma}$. The hamiltonian (4.1.20) can be rewritten as

$$\mathscr{H}=\int\left[i\left(\Psi^{+}_{+,\sigma}\frac{\partial}{\partial x}\Psi_{+,\sigma}-\Psi^{+}_{-,\sigma}\frac{\partial}{\partial x}\Psi_{-,\sigma}\right)+\kappa(\Psi^{+}_{+,\sigma}\Psi_{+,\sigma}+\Psi^{+}_{-,\sigma}\Psi_{-,\sigma})^2\right]dx.$$

This hamiltonian is relativistically invariant in the $1+1D$ spacetime ($\Psi_{\pm}$ is a two-component spinor) and has a background. It was first studied by Anselm (1959) and Vaks and Larkin (1961) and, later, by Luther and Emery (1974) (see also Wiegmann and Larkin 1977). It is also known as the $SU(2)$-isospin Thirring model and the chiral Gross–Neveu model. The two-particle $S$ matrix is of the form

$$\mathbf{S}(\tau,\tau')=\frac{\tau-\tau'+i\kappa\mathbf{P}}{\tau-\tau'+i\kappa}, \tag{4.7.12}$$

where $\tau=\pm 1$ are particle chiralities (Belavin 1979, Andrei and Lowenstein 1979) and can be obtained directly from (4.7.10) if one puts $k=k_{\mathrm{F}}\tau$. If in (4.7.10) $\kappa\to 0$, we set $\mathbf{S}\to\mathbf{I}$. However, in (4.7.12) the $S$ matrix tends to unity at $\kappa\to\infty$ only for particles of different chirality, whereas at $\tau=\tau'$ irrespective of $\kappa$

$$\mathbf{S}(\tau,\tau)=\mathbf{P}.$$

Indeed, two particles with identical chirality, say $\tau=1$, obey the Schrödinger equation

$$-i\left(\frac{\partial}{\partial x_1}+\frac{\partial}{\partial x_2}\right)\Psi_{\sigma_1,\sigma_2}(x_1,x_2)+\kappa\delta(x_1-x_2)\boldsymbol{\sigma}_{\sigma_1\sigma_1'}\boldsymbol{\sigma}_{\sigma_2\sigma_2'}\Psi_{\sigma_1',\sigma_2'}(x_1,x_2)$$
$$=E\Psi_{\sigma_1,\sigma_2}(x_1,x_2) \tag{4.7.13}$$

which, unlike the free Schrödinger equation (4.2.20) has *only one solution* (4.2.24). Therefore, solution (4.2.24) can be considered as a $\Psi$ function of two interacting particles in the limit of identical momenta. At identical velocities the interaction vanishes, so that both (4.7.13) and the free Schrödinger equation have identical solutions.

It has been observed repeatedly that the spin-1/2 s–d exchange model and the $SU(2)$ isotopic Thirring model are closely related to each other. This observation was employed by Andrei (1980) to diagonalize the s–d exchange hamiltonian.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Indeed, the numbers of both the left-hand and right-hand particles are conserved. Putting them equal to

$$N_+ = \sum_\sigma \int \Psi^+_{+,\sigma}\Psi_{+,\sigma}\,dx = N, \qquad N_- = \sum_\sigma \int \Psi^+_{-,\sigma}\Psi_{-,\sigma}\,dx \tag{4.7.14}$$

we obtain the Schrödinger equation

$$\begin{aligned}\left(-i\sum_{i=1}^N \frac{\partial}{\partial x_i} + i\frac{\partial}{\partial y} - E\right)\Psi_{\sigma_1\ldots\sigma_N,\sigma}(x_1,\ldots,x_N,y)\\ +\kappa\sum_{i=1}^N \delta(x_i-y)\boldsymbol{\sigma}_{\sigma_i\sigma_i'}\boldsymbol{\sigma}_{\sigma\sigma'}\Psi_{\ldots\sigma_i'\ldots\sigma'}(x_1,\ldots,x_N,y)\\ +\kappa\sum_{i>j}^N \delta(x_i-x_j)\boldsymbol{\sigma}_{\sigma_i\sigma_i'}\boldsymbol{\sigma}_{\sigma_j\sigma_j'}\Psi_{\ldots\sigma_i'\ldots\sigma_j'\ldots\sigma}(x_1,\ldots,x_N,y)=0.\end{aligned} \tag{4.7.15}$$

If one substitutes $x_N \to x_N + y$ and $\kappa \to I/4$, (4.7.15) coincides with (4.2.9) with exception of the last term in eqn. (4.7.15). As stated above, this last term does not contribute, since, according to (4.2.10) and (4.2.24), $\delta(x_i - x_j)\Psi(x_1,\ldots,x_N)=0$. However, it helps to eliminate the ambiguity and to get the solution of (4.2.10).

The equivalence of the Kondo model and $SU(2)$ isotopic Thirring model at condition (4.7.14) is still more obvious, if one uses Abrikosov's (1965) pseudofermions and replaces the $S=1/2$ impurity spin operator by an equivalent operator:

$$\mathbf{S} = d^+_\sigma \mathbf{S}_{\sigma\sigma'} d_{\sigma'}.$$

Note that the delta-function interaction of one-dimensional particles moving in one direction with coinciding velocities does not contribute to the energy provided only the interaction is isotropic. In the anisotropic case it results in the renormalization of the magnetic field and chemical potential (see § 5.2).

Equation (4.7.5 *b*) with the omitted phase $\delta_s$ of the scattering on an impurity coincides with eqns. (4.1.4) and (4.1.42) for the Haisenberg model (4.1.1) but differs in the form of the energy functional. This list can be continued: eqns. (4.4.B) coincide with Bethe's equations for the generalized Haisenberg ferromagnet (4.1.36) and (4.1.37): eqns. (4.5 A–B) for the Anderson model are similar to Bethe's equations for the Hubbard model (4.1.22) and (4.1.23) if one replaces $g(k) \to t/U \sin k$. The above analogy enables one to exploit the technique developed for the Haisenberg and Hubbard models to study the integrable models in the theory of dilute magnetic alloys.

Particles with rapidities satisfying eqns. (4.2–6 (A, B)) are bare excitations above the ferromagnetic state in which $M \sim 1$ and the spin is close to maximal $S^z \sim N/2$. The energy of this state (the 'bare' vacuum) is maximal, too. The ground state of free electrons is, of course, antiferromagnetic: $S^z = 0$ and $M = N/2$. The relevant excitations are real renormalized particles. Hence the ground state is always the many-particle state at $N \to \infty$ is described by an infinite set of equations.

In the § 5 we shall study the ground-state energy of the s–d exchange model as a function of the spin projection.

*Appendix to § 4.3.1. Solution of the factorization equation*

We find the solution of the triangle equations

$$\mathbf{r}_{ij}(\alpha)\mathbf{r}_{i0}(\alpha+\alpha')\mathbf{r}_{j0}(\alpha') = \mathbf{r}_{j0}(\alpha')\mathbf{r}_{i0}(\alpha+\alpha')\mathbf{r}_{ij}(\alpha) \tag{1}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

with the unitarity conditions

$$\mathbf{r}_{ij}(\alpha)\mathbf{r}_{ij}(-\alpha)=\mathbf{I} \tag{2}$$

and the initial condition

$$\mathbf{r}_{ij}(0)=\mathbf{P}_{ij}. \tag{3}$$

The $U(1)$-symmetric solution should have the following form:

$$\mathbf{r}_{ij}(\alpha)=a(\alpha)(\mathbf{1}\otimes\mathbf{1}+\boldsymbol{\sigma}_i^z\otimes\boldsymbol{\sigma}_j^z)+b(\alpha)(\mathbf{1}\otimes\mathbf{1}-\boldsymbol{\sigma}_i^z\otimes\boldsymbol{\sigma}_j^z)+\frac{1}{2}c(\alpha)(\boldsymbol{\sigma}_i^+\otimes\boldsymbol{\sigma}_j^-+\boldsymbol{\sigma}_i^-\otimes\boldsymbol{\sigma}_j^+). \tag{4}$$

Using eqns. (2) and (4) one obtains

$$b(\alpha)b(-\alpha)+c(\alpha)c(-\alpha)=1, \tag{5 a}$$

$$b(\alpha)c(-\alpha)+c(\alpha)b(-\alpha)=0. \tag{5 b}$$

The triangle equation (1) in terms of (4) is

$$\left.\begin{aligned} a(\alpha)b(\alpha+\alpha')c(\alpha')&=c(\alpha)c(\alpha+\alpha')b(\alpha')+b(\alpha)a(\alpha+\alpha')c(\alpha'),\\ a(\alpha)c(\alpha+\alpha')a(\alpha')&=(b(\alpha)c(\alpha+\alpha')b(\alpha')+c(\alpha)a(\alpha+\alpha')c(\alpha'). \end{aligned}\right\} \tag{6}$$

Let us introduce the ratios

$$g(\alpha)=a(\alpha)/c(\alpha); \qquad h(\alpha)=b(\alpha)/c(\alpha) \tag{7}$$

Then eqn. (6) takes the form

$$\left.\begin{aligned} g(\alpha)h(\alpha+\alpha')&=h(\alpha')+h(\alpha)g(\alpha+\alpha'),\\ g(\alpha)g(\alpha')&=h(\alpha)h(\alpha')+g(\alpha+\alpha'). \end{aligned}\right\} \tag{8}$$

Setting $\alpha'=0$ in (8) one obtains

$$h(0)=0, \qquad g(0)=1. \tag{9}$$

Therefore condition (3) is valid for $a(0)=1$. Furthermore, differentiating eqns (8) with respect to $\alpha'$ and then setting $\alpha'=0$, one obtains

$$\left.\begin{aligned} g(\alpha)\frac{\partial}{\partial\alpha}h(\alpha)&=u+h(\alpha)\frac{\partial}{\partial\alpha}g(\alpha),\\ g(\alpha)v&=h(\alpha)u+\frac{\partial}{\partial\alpha}g(\alpha), \end{aligned}\right\} \tag{10}$$

where $u=h'(0)$, $v=g'(0)$.

The solution of eqn. (10) is

$$g(\alpha)=-i\frac{\sinh(i\mu+f\alpha)}{\sin\mu}; \qquad h(\alpha)=-i\frac{\sinh f\alpha}{\sin\mu}. \tag{11}$$

Quantities $\mu$ and $f$ parametrically determine $v$ and $u$. The unitarity conditions (5 *b*) are automatically satisfied and (5 *a*) yields the equation

$$a(\alpha)a(-\alpha)=1. \tag{12}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

To diagonalize the matrix $\mathbf{T}_j$ we need only the functions $g(\alpha)$ and $h(\alpha)$ and the quantity $a(1)$. Therefore function $a(\alpha)$ may be an arbitrary solution of eqn. (14), for example, $a(\alpha)=1$.

## § 5. Exact solution of the s–d exchange model at $T=0$

The subject of this section is the zero temperature magnetic properties of the s–d exchange model. We find the solution of Bethe-Ansatz equations for a large number of particles, describing the ground state of the system in the presence of a magnetic field.

### 5.1. *Isotropic s–d exchange model with an arbitrary impurity spin*

#### 5.1.1. *The continuous limit*

In general, the solutions of eqns. (4.2.A) and (4.2.B) lie in a complex plane of $\lambda$. However, in § 6 we shall show that the ground state with a given spin projection $S^z$ is formed by the real solutions of eqns. (4.2.A) and (4.2.B). Putting off the exact proof of this statement let us return to eqns. (4.2.A) and (4.2.B). Taking the logarithm of these equations one obtains:

$$k_j L = 2\pi N_j - \sum_{\alpha=1}^{M} (p(\lambda_\alpha)+\pi), \tag{5.1.1 a}$$

$$N p(\lambda_\alpha) + \delta_s(\lambda_\alpha) = 2\pi J_\alpha + \sum_{\beta=1}^{M} \Phi(\lambda_\alpha - \lambda_\beta), \tag{5.1.1 b}$$

where

$$\left.\begin{array}{l} p(\lambda)=2\tan^{-1}2\lambda, \quad \delta_s(\lambda)=p[(\lambda+1/g)/2S], \quad \Phi(\lambda)=p(\lambda/2), \\ J_\alpha \text{ integer, if } M \text{ is odd}, \quad J_\alpha+1/2 \text{ integer, if } M \text{ is even}, \quad |2J_\alpha|\leqslant N-M \end{array}\right\} \tag{5.1.1 c}$$

First, we should determine the configuration of the integers $\{N_j\}$ and $\{J_\alpha\}$ corresponding to the ground state. This configuration does not depend on the impurity state and is determined by the state of free fermions only. The following propositions play a principal role in our theory. We quote them without proof:

(i) For any set of $J_\alpha$s, $N_j$s satisfying (5.1.1 *c*), no two of which are identical, there is a unique set of real $\lambda$'s, $k$'s satisfying (5.1.1 *a*, *b*), with no two $\lambda$'s, $k$'s being identical. With this set of $\lambda$'s, $k$'s only a unique eigenfunction of $\mathscr{H}$ of Bethe's form, can be constructed (Yang and Yang 1969).

(ii) The solutions of eqn. (5.1.1 *b*) are monotonous functions of the integers $J_\alpha$.

(iii) The integers $J_\alpha$ are bounded by the interval $((-N+M)/2, (N-M)/2)$. The boundaries correspond to $\lambda=\mp\infty$.

The energy of the free particles is the sum of energies associated with spin and charge degrees of freedom

$$\left.\begin{array}{l} E^{\mathrm{ch}} = \dfrac{2\pi}{L}\displaystyle\sum_{j=1}^{N} N_j \\[2ex] E^{\mathrm{sp}} = -\dfrac{2\pi}{L}\displaystyle\sum_{\alpha=1}^{M} J_\alpha - \dfrac{\pi}{L} MN. \end{array}\right\} \tag{5.1.2}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The sum of these quantities is the energy of free Fermi gas with a constant density of states. In the ground state it should be equal to

$$E^{(0)}=E^{\mathrm{ch}}+E^{\mathrm{sp}}=-\frac{\pi N^2}{2L}+\frac{2\pi S^{z^2}}{L}. \tag{5.1.3}$$

We have already noted that free particles with a constant density of states may be represented by independent spin and charge excitations. Therefore, we should minimize the charge and spin parts of the energy independently.

According to (iii) the spin part of the energy is bounded. Therefore, the integers $J_\alpha$ should begin with the highest: $J_1=J_{\max}=(N-M)/2$ and go successively with unit step:

$$J_{\alpha+1}=\frac{N-M}{2}-\alpha, \qquad \alpha=0,1,\ldots,M-1. \tag{5.1.4}$$

Furthermore, according to (ii) the solutions of eqn. (5.1.1 *b*) form, for a large $N$, $M$, a non-uniform dense distribution between a maximal $\lambda=+\infty$ and minimal $\lambda=-B$. The value $\lambda=-B$ corresponds to the lowest integer $J_M=(N-3M)/2$ (fig. 5.3 *a*). When $S^z=0$ $(M=N/2)$ the integer $J_M=-N/4$ and coincides with the lowest boundary of the allowed interval. Therefore, when $S^z=0$ we have $B=\infty$. The spin part of the ground-state energy is

$$E^{\mathrm{sp}}=-\frac{2\pi}{L}\left[\sum_{\alpha=0}^{M-1}\left(\frac{N-M}{2}-\alpha\right)+\frac{MN}{2}\right]=-\frac{\pi N^2}{2L}+\frac{S^{z^2}}{2\chi_{\mathrm{host}}}, \tag{5.1.5}$$

where $\chi_{\mathrm{host}}=L/4\pi$ is the Pauli susceptibility of a Fermi gas with a constant density of states. Comparing (5.1.5) and (5.1.3) we see that $E^{\mathrm{sp}}$ coincides with the whole ground-state energy. Here we encounter difficulty with a linear spectrum of initial particles.

The charge energy of particles with a linear spectrum is bounded from below. It is interesting to note that this ambiguity does not affect the impurity properties because they depend only on the spin subsystem. The unboundedness of the spectrum reveals itself in the charge channel which does not influence the impurity. To maintain mathematical rigour we must describe more carefully the charge subsystem. We assume that all charge energies should not exceed the Fermi energy $\epsilon_{\mathrm{F}}=\pi N/L$. It means that the minimum integer should be

$$N_1=-N/2$$

Therefore, $N_j$ are successive integers from $-N/2$ to $N/2$ and $E^{\mathrm{ch}}=0$.

This choice of $N_j$s may be illustrated by the following speculation. Let $M=0$. Then all spins align, the interaction vanishes and $k_j$s are ordinary momenta of free spinless particles. According to the Pauli principle these particles fill all states beginning from the bottom of the band $-\epsilon_{\mathrm{F}}$:

$$N_j=-N/2+j \qquad (j=1,\ldots,N)$$

It must be emphasized once more that charge excitations do not influence the impurity properties.

Following Yang and Yang (1969) we shall name the solutions of eqn. (5.1.1 *b*) 'particle' rapidities and we define 'hole' rapidities as follows.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Let us consider a function

$$h(\lambda)=\frac{1}{2\pi}\left(Np(\lambda)+\delta_s(\lambda)-\sum_{\beta=1}^{M}\Phi(\lambda-\lambda_\beta)\right), \tag{5.1.6}$$

where the summation is performed over the rapidities of particles. We shall name 'hole' rapidities all those values of $\lambda=\tilde{\lambda}_\beta$ ($\beta=1,\ldots,N-2M$) at which $h(\tilde{\lambda}_\beta)$ is equal to an integer belonging to the lattice of the permissible integer numbers and not coinciding with any quantum number $J_\alpha$. For the given case, $\tilde{J}_\beta=((N-3M)/2)-\beta$. Thus, for a large system $N\to\infty$, $L\to\infty$, $\pi N/L=\epsilon_F$ there exists a density distribution of holes as well as of particles:

$$N\rho(\lambda)d\lambda=\text{number of } \lambda\text{s in } d\lambda,$$

$$N\tilde{\rho}(\lambda)d\lambda=\text{number of holes in } d\lambda.$$

It is obvious that for the ground state with a given spin $S^z$, the rapidities of holes take their values on $(-\infty, -B)$. Therefore, $\tilde{\rho}=0$ when $\lambda>-B$ and $\rho=0$ when $\lambda<-B$.

By definition, the number of particles and holes in the interval $d\lambda$ is the number of times $h(\lambda)$ ranges over values $J_\alpha$ and $\tilde{J}_\beta$ in this interval. Thus,

$$\frac{1}{N}\frac{dh(\lambda)}{d\lambda}=\rho(\lambda)+\tilde{\rho}(\lambda). \tag{5.1.7}$$

Equation (5.1.6) in the continuous limit gives

$$\frac{2\pi}{N}h(\lambda)=p(\lambda)-\int_{-B}^{\infty}\Phi(\lambda-\lambda')\rho(\lambda')d\lambda'+\frac{1}{N}\delta_s(\lambda). \tag{5.1.8}$$

Differentiation with respect to $\lambda$ gives

$$\rho(\lambda)+\tilde{\rho}(\lambda)=a_1(\lambda)+\frac{1}{N}a_{2S}(\lambda+1/g)-\int_{-B}^{\infty}a_2(\lambda-\lambda')\rho(\lambda')\,d\lambda', \tag{5.1.9}$$

where

$$a_n(\lambda)=\frac{2}{\pi}\frac{n}{4\lambda^2+n^2}. \tag{5.1.10}$$

According to (4.2.C) and (5.1.1) the energy per particle for the ground state is

$$\frac{1}{N}E^{sp}=-\frac{N}{L}\int_{-B}^{\infty}(p(\lambda)+\pi)\rho(\lambda)\,d\lambda. \tag{5.1.11}$$

The spin per particle is

$$\frac{1}{N}S^z=\frac{1}{2}+\frac{S}{N}-\int_{-B}^{\infty}\rho(\lambda)\,d\lambda. \tag{5.1.12}$$

Equations (5.1.9)–(5.1.12) describe all the magnetic properties of the impurity. They were derived by Andrei (1980) and Wiegmann (1980 a).

To find the impurity magnetic moment it is convenient to use the following trick. We have shown above that eqns. (5.1.9)–(5.1.11) without the $1/N$ term in (5.1.9)

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

describe the free Fermi gas. Because of linearity the solution of eqn. (5.1.9) contains two terms

$$\rho = \rho_{\mathrm{h}} + \frac{1}{N}\rho_{\mathrm{i}} \tag{5.1.13}$$

corresponding to the host metal and impurity.

These functions satisfy the following equations

$$\rho_{\mathrm{h}}(\lambda) = a_1(\lambda) - \int_{-B}^{\infty} a_2(\lambda-\lambda')\rho_{\mathrm{h}}(\lambda')\,d\lambda'; \qquad \lambda > -B, \tag{5.1.14 a}$$

$$\rho_{\mathrm{i}}(\lambda) = a_{2S}(\lambda + 1/g) - \int_{-B}^{\infty} a_2(\lambda-\lambda')\rho_{\mathrm{i}}(\lambda')\,d\lambda'; \qquad \lambda > -B. \tag{5.1.14 b}$$

One may decompose the spin in the same way:

$$\frac{1}{N}S_{\mathrm{h}}^z = \frac{1}{2} - \int_{-B}^{\infty} \rho_{\mathrm{h}}(\lambda)\,d\lambda, \tag{5.1.15 a}$$

$$M_{\mathrm{i}} = S - \int_{-B}^{\infty} \rho_{\mathrm{i}}(\lambda)\,d\lambda. \tag{5.1.15 b}$$

In § 6 we shall show that $B$ is really independent of the impurity state. Formulae (5.1.15 *a*, *b*) describe the total magnetization of the host metal and impurity magnetization. In the leading order with respect to $1/N$ the total spin of the system is determined by the magnetism of the conduction band. Therefore,

$$\frac{1}{N}S^z = H/4\epsilon_{\mathrm{F}}. \tag{5.1.16}$$

Let us now determine the dependence of $B$ on the magnetic field in the leading order with respect to $1/N$, i.e. using only the solution of eqns. (5.1.15 *a*) and (5.1.16), and then find the impurity magnetization using the solution of eqn. (5.1.14 *b*). In other words, the eqns. (5.1.14 *a*), (5.1.15 *a*) and (5.1.16) determine the function $B(H)$ and eqns. (5.1.14 *b*) and (5.1.15 *b*) determine the impurity magnetization.

### 5.1.2. *The ground state and magnetic susceptibility at zero magnetic field $H=0$*

The characteristic feature of eqns. (5.1.14), as well as other equations which appear in problems related to the magnetic impurities, is that the region of definition of these equations is a semiaxis. Often it is possible to find the solution of such equations in an analytical form with the help of the Wiener–Hopf method. We briefly outline it in the Appendix to 5.1.3.

However, before solving eqns. (5.1.14) it is appropriate to study the character of the ground state. We have already mentioned that for $M = N/2$ holes are absent and $B = \infty$ ($\tilde{\rho} = 0$). Assuming $B = \infty$ and integrating eqn. (5.1.14 *a*) over $\lambda$ we obtain $S_{\mathrm{h}}^z = 0$ as it should be. But the integration of eqn. (5.1.14 *b*) gives the *2S-fold degenerate impurity ground state*

$$\lim_{H\to 0} M_{\mathrm{i}} = S - 1/2. \tag{5.1.17}$$

This result was conjectured by Mattis (1967) who used qualitative arguments. Thus, the conduction electrons cannot quench the impurity spin $S$ completely, and the

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

impurity spin is decreased only by 1/2. If the spin of an impurity is equal to 1/2, as can be the case in real alloys (§ 2.1), there is total compensation of the impurity spin, so that *the impurity ground state is a singlet state.*

To make further conclusions more clear let us introduce the following transformations. It is convenient to express all physical quantities in terms of the distribution function of holes, i.e. to count the physical quantities from their ground-state values.

Let now $H \neq 0$ and $B \neq \infty$. To count rapidities from the Fermi point let us make the following shift:

$$r(\lambda) = \rho(\lambda - B),$$
$$\tilde{r}(\lambda) = \tilde{\rho}(\lambda - B).$$

Let us define the functions $\rho^{\pm}(\omega)$ analytically in the upper (lower) half-plane of $\omega$:

$$\left.\begin{aligned} \rho^{+}(\omega) &= \int_0^{\infty} \exp(i\omega\lambda) r(\lambda)\, d\lambda \\ \rho^{-}(\lambda) &= \int_{-\infty}^{0} \exp(i\omega\lambda) \tilde{r}(\lambda)\, d\lambda. \end{aligned}\right\} \tag{5.1.18}$$

Making the Fourier transformation of eqn. (5.1.9) we obtain

$$\left.\begin{aligned} \rho^{-}(\omega) + (1 + \exp(-|\omega|))\rho^{+}(\omega) &= \exp(i\omega B)\Big(\exp(-|\omega|/2) \\ &\qquad + \frac{1}{N}\exp(-S|\omega| - i\omega/g)\Big); \\ \frac{1}{N} S^{z} &= \frac{1}{2} + \frac{S}{N} - \rho^{+}(0). \end{aligned}\right\} \tag{5.1.19}$$

Dividing eqn. (5.1.19) by $(1 + \exp(-|\omega|))$ and returning to the $\lambda$ space we obtain

$$\tilde{r}_{\mathrm{h}}(\lambda) + r_{\mathrm{h}}(\lambda) - \int_{-\infty}^{0} R(\lambda - \lambda')\tilde{r}_{\mathrm{h}}(\lambda')d\lambda' = (2\cosh \pi(\lambda - B))^{-1}, \tag{5.1.20 a}$$

$$\tilde{r}_{\mathrm{i}}(\lambda) + r_{\mathrm{i}}(\lambda) - \int_{-\infty}^{0} R(\lambda - \lambda')\tilde{r}_{\mathrm{i}}(\lambda')d\lambda' = \mathscr{S}_{2S}(\lambda - B + 1/g), \tag{5.1.20 b}$$

$$H/2\epsilon_{\mathrm{F}} = \int_{-\infty}^{0} \tilde{r}_{\mathrm{h}}(\lambda)\, d\lambda, \tag{5.1.20 c}$$

$$M_{\mathrm{i}} = S - \frac{1}{2} + \frac{1}{2}\int_{-\infty}^{0} \tilde{r}_{\mathrm{i}}(\lambda) d\lambda, \tag{5.1.20 d}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where

$$\left.\begin{aligned} R(\lambda) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \exp(-i\omega\lambda)(1+\exp(|\omega|))^{-1}\,d\omega, \\ \mathscr{S}_{2S}(\lambda) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \exp(-i\omega\lambda)\frac{\exp(-(2S-1)|\omega|/2)}{2\cosh\omega/2}\,d\omega. \end{aligned}\right\} \tag{5.1.21}$$

This form of equation is more convenient because all the characteristics of the system are expressed in terms of the excited states only.

One may evaluate the 1/2-spin impurity magnetic susceptibility for $H=0$ without using the exact solution of (5.1.20). To do so one must note how Nozières' (1974) (§ 3.1.3) correspondence between the low-energy behaviour of the 1/2-spin impurity and Fermi liquid shows up in eqns. (5.1.20). When $H\to 0$ and $B\to\infty$ one should retain only the leading terms in the right-hand side of (5.1.20 *a*, *b*):

$$(2\cosh\pi(\lambda-B))^{-1} \simeq \exp(-\pi B+\pi\lambda)$$

$$\mathscr{S}_1(\lambda-B+1/g) \simeq \exp(-\pi B+\pi\lambda)\exp(\pi/g).$$

In this approach the host metal distribution $\tilde{r}_{\mathrm{h}}(\lambda)$ and impurity distribution $\tilde{r}_{\mathrm{i}}(\lambda)$ differ from each other only by the factor $\exp(\pi/g)$. Therefore, one obtains

$$\frac{M_{\mathrm{i}}}{H/4\epsilon_{\mathrm{F}}} = \exp\left(\frac{\pi}{g}\right). \tag{5.1.22}$$

Equations (5.1.16) and (5.1.22) give the finite 1/2-spin impurity magnetic susceptibility at zero temperature

$$\chi_{\mathrm{i}} = \frac{1}{4\epsilon_{\mathrm{F}}}\exp\left(\frac{\pi}{g}\right).$$

Defining the Kondo temperature as

$$T_{\mathrm{K}} = \frac{2\epsilon_{\mathrm{F}}}{\pi}\exp\left(\frac{-\pi}{g}\right) \tag{5.1.23 a}$$

we have

$$\chi_{\mathrm{i}} = (2\pi T_{\mathrm{K}})^{-1}. \tag{5.1.23 b}$$

We shall often employ the Fermi-liquid analogy below.

We deal with a magnetic field small in comparison with the Fermi energy. The condition $H \ll \epsilon_{\mathrm{F}}$ or $S^z/N \ll 1$ means that $B \gg 1$, and it is only sufficient to solve eqn. (5.1.20 *a*) in the first order of $\exp(-\pi B)$. Thus,

$$H(B)/2\epsilon_{\mathrm{F}} = \exp(-\pi B)\int_{-\infty}^{0} \tilde{r}^{(0)}(\lambda)\,d\lambda. \tag{5.1.24}$$

Now $\tilde{r}^{(0)}$ is the solution of the equation

$$\tilde{r}^{(0)}(\lambda) + r^{0}(\lambda) - \int_{-\infty}^{0} R(\lambda-\lambda')\tilde{r}^{(0)}(\lambda')\,d\lambda' = \exp(\pi\lambda). \tag{5.1.25}$$

The corrections due to the omitted terms in the right-hand side of eqn. (5.1.20 *a*) are of the order of $((H/\epsilon_{\mathrm{F}})^3)$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

5.1.3. *Impurity magnetic susceptibility at arbitrary magnetic fields*

Equations (5.1.20) may be solved by the Wiener–Hopf method. The solution is constructed with the use of the analytical in the upper (lower) half-plane functions $G^{(+)}(\omega)\,(G^{(-)}(\omega))$ having no zeros and factorizing the kernel

$$(1-R(\omega))^{-1}=G^{(+)}(\omega)G^{(-)}(\omega), \qquad G(\infty)=1. \tag{5.1.26}$$

These functions have the form

$$G^{(-)}(\omega)=G^{(+)}(-\omega)=\sqrt{(2\pi)}f_-\left(\frac{\omega}{2\pi}\right)\Big/\Gamma\left(\frac{1}{2}+\frac{i\omega}{2\pi}\right), \tag{5.1.27}$$

where the functions

$$f_\mp(\omega)=\left(\frac{\pm i\omega+0}{e}\right)^{\pm i\omega} \tag{5.1.28}$$

factorize the function

$$\exp(-\pi|\omega|)=f_-(\omega)f_+(\omega).$$

The solution of eqn. (5.1.25) is

$$r_-^{(0)}(\omega)=\frac{G^{(-)}(\omega)G^{(+)}(i\pi)}{i\omega+\pi} \tag{5.1.29}$$

(see the Appendix to § 5.1.3).

Using (5.1.24) and (5.1.29) we find the relation between $B$ and $H$:

$$\frac{H}{2\epsilon_F}=\exp(-\pi B)\left(\frac{2}{\pi e}\right)^{1/2}. \tag{5.1.30}$$

Let us define the new scale which is correct for the perturbation theory (at $H\gg T_K$):

$$B-\frac{1}{g}=\frac{1}{\pi}\ln\frac{T_H}{H}. \tag{5.1.31}$$

This scale is related to the Kondo temperature (5.1.23) as follows:

$$T_H=\left(\frac{2\pi}{e}\right)^{1/2}T_K. \tag{5.1.32}$$

Then using eqns. (5.1.20*b*) and (5.1.31) we obtain the *universal formula* for the *impurity magnetization* at $T=0$ (Wiegmann 1980, Fateev and Wiegmann (1981 a, b):

$$M_i(H)=S-\frac{1}{2}+\frac{i}{8\sqrt{\pi}}\int_{-\infty}^{+\infty}d\omega$$
$$\times\exp(-2i\omega\ln H/T_H)\frac{\Gamma(1/2+i\omega)f_+^{2S}(\omega)}{\omega+i0}f_-^{2S-1}(\omega). \tag{5.1.33}$$

The integral (5.1.33) has two different representations and asymptotic expansions for different ratios of $H/T_H$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

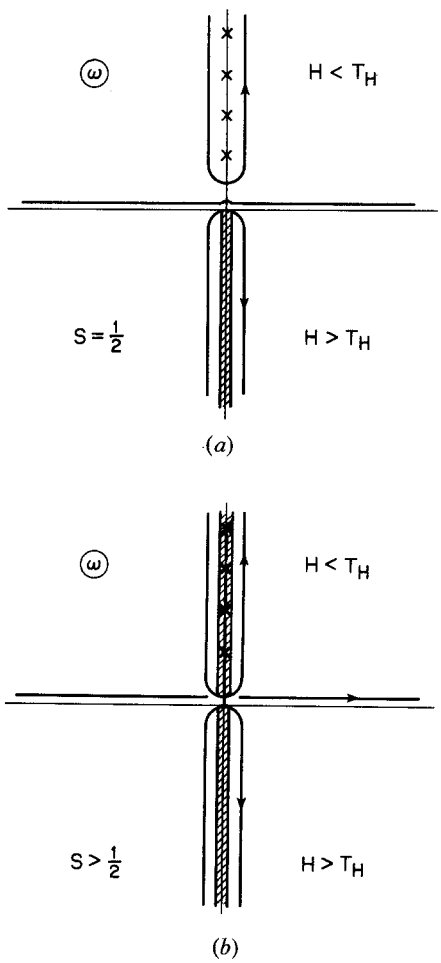
If $H > T_H$, the contour of integration envelops the lower half-plane and one should calculate the integral over the contour encircling the cut $f_+(\omega)$ and pole $\omega = -i0$ (see fig. 5.1):

$$M_i(H > T_H) = S - \frac{1}{2\pi^{3/2}} \int_0^\infty d\omega \frac{\sin 2\pi S\omega}{\omega} \Gamma(1/2+\omega) \left(\frac{\omega}{e}\right)^{-\omega} \times \exp(-2\omega \ln H/T_H). \quad (5.1.34)$$

Using the 'invariant charge' (§ 2.2) $z(H/T_H)$:

$$1/z - \frac{1}{2} \ln z = \ln H/T_H$$

Fig. 5.1




The complex plane of the integrand (5.1.33) for (*a*) $S = 1/2$ and (*b*) $S > 1/2$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

we have

$$M_{\mathrm{i}}(H>T_H)=S-\frac{1}{2\pi^{3/2}}\int_0^\infty dt\frac{\sin 2\pi Szt}{t}\Gamma(1/2+zt)\left(\frac{t}{e}\right)^{-zt}\exp(-2t) \tag{5.1.35}$$

and obtain from (5.1.35) a power-series expansion in $z$

$$M_{\mathrm{i}}(H>T_H)=S\left(1+\sum_{n=1}^{\infty}a_n(S)z^n(H/T_H)\right). \tag{5.1.36}$$

The first term in this expansion $a_1=-1/2$ coincides with the term obtained by means of the perturbation theory (Abrikosov and Migdal 1970).

The most interesting region $H<T_H$ is inaccessible by perturbation theory. The properties of the integral (5.1.34) in the cases of $S=1/2$ and $S\neq 1/2$ are quite different. If $H<T_H$ the integration contour could be deformed to encircle the positive part of the imaginary axis.

If $S=1/2$ the only singularities of the integrand in the upper half-plane are the poles, leading to the power series in $(H/T_H)$:

$$M_{\mathrm{i}}^{(1/2)}(H<T_H)=\frac{2}{\sqrt{\pi}}\sum_{n=0}^{\infty}\left(\frac{n+1/2}{e}\right)^{(n+1/2)}\frac{(-1)^n}{n!(n+1/2)}\left(\frac{H}{T_H}\right)^{2n+1} \tag{5.1.37}$$

(Wiegmann 1980 a). This expansion is absolutely convergent. If $S=1/2$, $H<T_H$ all physical functions are analytical in the complex $H$ plane. On the other hand the series (5.1.36) is asymptotical. It means that perturbation theory does not define the physical quantities unambiguously. For example, functions differing from each other by an arbitrary analytical function of $z^{1/2}\exp(-1/z)\equiv H/T_H$ have identical expansions in $z$. Yet as follows from (5.1.37) such a function determines the behaviour of the physical quantities at a low magnetic field. This is one more piece of evidence that perturbation theory is principally incomplete.

Let us consider the case $S\neq 1/2$. In this case the integration over the cut $f_-(\omega)$ in the upper half-plane contributes to the low magnetic-field behaviour. The poles of the $\Gamma$ function now give only the exponentially small contribution to the impurity magnetization:

$$M_{\mathrm{i}}^{(s)}(H<T_H)=S-1/2+\frac{1}{2\pi^{3/2}}\int_0^\infty dt\frac{\sin\pi(2S-1)tz}{t}\left(\frac{t}{e}\right)^{tz}$$
$$\times\Gamma(1/2-zt)\exp(-2t)+O\left(\frac{\exp(-1/|z|)}{\sqrt{|z|}}\right). \tag{5.1.38}$$

With exponential accuracy we have

$$M_{\mathrm{i}}^{(s)}(H<T_H)=(S-1/2)\left(1+\sum_{n=1}^{\infty}a_n(S-1/2)z^n\right)+O\left(\frac{\exp(-1/|z|)}{\sqrt{|z|}}\right). \tag{5.1.39}$$

Note a remarkable 'duality' of the low and high magnetic-field series (5.1.36) and (5.1.39). The coefficients $a_n(S)$ in these series after substitution $S\leftrightarrow S-1/2$.

The conduction electron cannot quench the impurity spin $S$ completely. The dressed impurity remains magnetic.

The ground state with the moment $S-1/2$ can be chosen as a zeroth order approximation in perturbation theory which would be correct in the low energy region. It follows from (5.1.39) that the coupling in this region is ferromagnetic (for a

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

discussion see § 2) and the approach to this strong coupling fixed point is still logarithmic. The logarithmic behaviour was predicted by Nozières and Blandin (1980) and observed by Cragg and Lloyd (1979), who treated the problem numerically.

The 'dual' logarithmic character of the low and high energy behaviour is a general feature of the problem. In particular, in § 6 below it will be shown that the temperature dependence of the thermodynamics quantities is dual in the cases $T \gg T_K$ and $T \ll T_K$. The impurity magnetization is plotted in fig. 5.2.

5.1.4. *The scattering phase*

In this subsection we shall calculate the $S$-matrix element for the scattering of electrons on the impurity in an arbitrary magnetic field as a function of energy†. Note that the scattering phase is related to measurable quantities only at $\varepsilon = 0$. For instance, it determines the magnetoresistance. On the other hand, via the Friedel sum rule the scattering phase is related to the impurity magnetization which has already been calculated. Still we deemed it appropriate to present here the calculations of the scattering phase because it illustrates the Nozières theory.

The methods developed above are quite sufficient to compute the scattering phase. However, we shall employ a much more general and unified approach below. It can be applied directly to the continuous limit and enables us to calculate simultaneously the bound state energy and the spectrum of elementary excitations. In the next section its extension will be used to study the equilibrium properties at finite temperature. Only the scattering phase of the electron with spin projection parallel to magnetic field $\Delta^{\uparrow\uparrow}(z, H)$, will be calculated below.

The scattering phase $\Delta(\varepsilon)$ in general differs from the phase shift $\eta(\omega)$ defined by eqn. (3.2.8). The scattering phase $\Delta(\varepsilon)$ is the log of the $S$-scattering matrix element and describes the real scattering processes, in contrast to the phase shift $\eta(\omega)$ related to the Green function, which also takes into account virtual processes. This is a reason, for example, why $\Delta(\varepsilon)$ cannot be controlled by perturbation theory in contrast to $\eta(\omega)$. These quantities, however, coincide only at low energies and both can be found using the Fermi-liquid approach. So $\Delta(\varepsilon)$ correctly describes the low energy part of the Abrikosov–Suhl narrow many-body resonance.

Consider elementary excitations in the system of odd number of electrons $N$ and the impurity in the ground state and with spin projection $S^z$. Add to the system one more spin-down electron retaining the number of spin-up particles. Now the system is characterized by quantum numbers $(N+1, S^z+1/2)$. The excitation can be decomposed into spin and charge components. The charge subsystem is now described by $N+1$ half-integer quantum numbers $N_j = -N+j+1/2$ $(j=1, \ldots, N)$ and $N_0 > 0$. The latter describes the excitation:

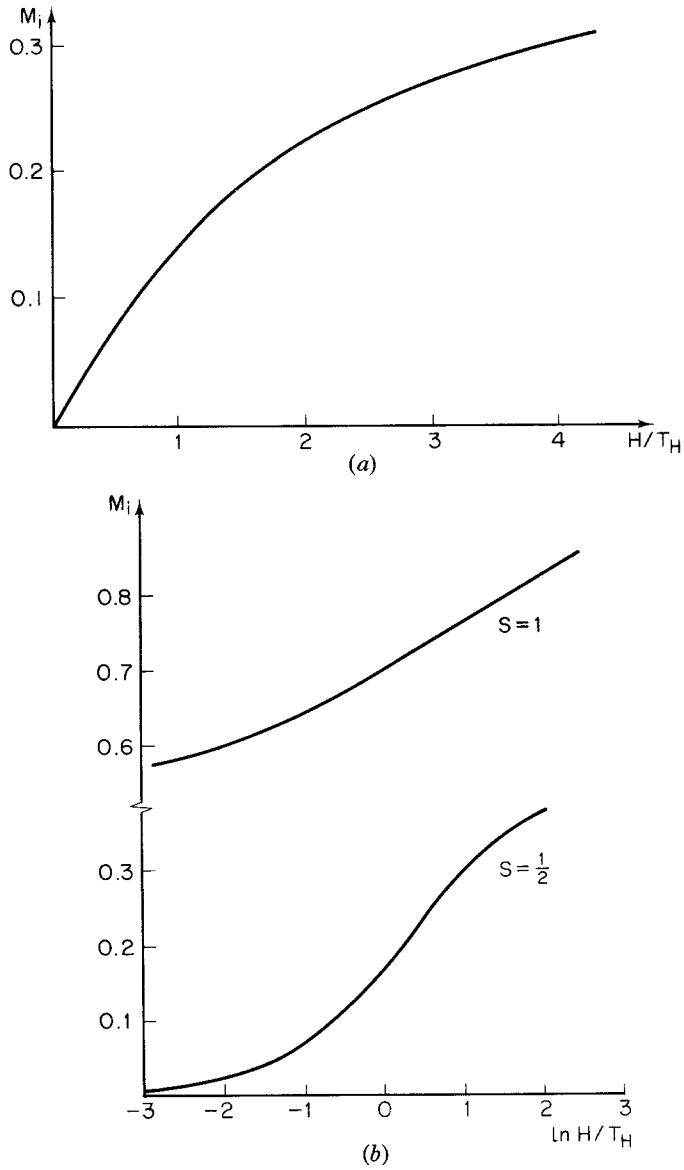
$$k_0 L = 2\pi N_0 + \delta_c + \sum_{\alpha=1}^{M} (p(\lambda_\alpha) + \pi). \tag{5.1.40}$$

In the spin subsystem the rapidities $\lambda_\alpha$ do rearrange. The new electron added to the in-box system gets the phase shift $k_0 L$ as it propagates through the system. In the

† For the scattering on the Fermi level, the phase in the framework of the Bethe Ansatz was calculated by Andrei (1982).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 5.2




Magnetic field dependence of the impurity magnetization for the impurity spin: (*a*) $S=1/2$ and (*b*) $S=1/2$, 1 (after Melnicov 1982 b).

absence of an impurity the phase shift equals

$$\pi+2\pi\times(\text{integer})=2\pi(N_0-1/2)+2\pi J_\alpha+\pi$$

as follows from eqn. (5.1.40). In the presence of the impurity one gets rather

$$-k_0L=2\Delta^{\uparrow\uparrow}(\varepsilon) \qquad (\text{mod}\,2\pi),$$

where $\Delta_1^{\uparrow\uparrow}(\varepsilon)$ $(0<\Delta^{\uparrow\uparrow}<\pi)$ is a phase shift for the scattering of the 1/2-spin elementary excitations with energy $\varepsilon$ and spin directed along the total spin of the system.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The total phase shift is related to energy via the obvious equation

$$k_0 L = L(E(N+1, S^z+1/2) - E(N, S^z)), \tag{5.1.41}$$

where $E(N+1, S^z+1/2)$ and $E(N, S^z)$ are energies of states with corresponding quantum numbers.

Since the energy of the free electron gas $E_{\text{host}}$ is a multiple of $2\pi/L$, only the variation of the impurity part of the energy contributes to the phase shift:

$$\Delta^{\uparrow\uparrow}(\varepsilon) = -\frac{L}{2N}(E_{\text{i}}(N+1, S^z+1/2) - E_{\text{i}}(N_0 S^z)). \tag{5.1.42}$$

In leading order in $1/N$ the excitation energy equals the integer part of the total phase shift (5.1.41):

$$\varepsilon = E_{\text{host}}(N+1, S^z+1/2) - E_{\text{host}}(N, S^z). \tag{5.1.43}$$

The excitation energy as well as the scattering phase can be decomposed into spin and charge components:

$$\left.\begin{aligned} \Delta &= \Delta_{\text{c}} + \Delta_{\text{s}}, \\ \varepsilon &= \varepsilon_{\text{c}} + \varepsilon_{\text{s}}, \end{aligned}\right\} \tag{5.1.44}$$

where $\Delta_{\text{c}} = IS/2$ is the potential scattering phase shift which is a non-universal quantity,

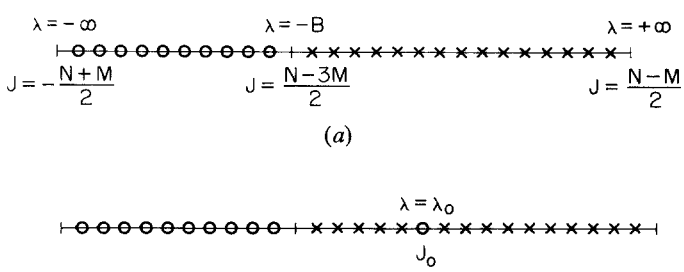
$$\varepsilon_{\text{c}} = 2\pi N_0/L,$$

and $\Delta_{\text{s}}$ is a phase shift for the scattering of the spin excitation with energy $\varepsilon_{\text{s}}$.

Thus, a calculation of the scattering phase reduces to the problem of elementary excitations. In what follows we confine ourselves to the spin excitations responsible for the Kondo singularities.

In (5.1.40)–(5.1.42) $E(N, S^z)$ is an energy of the ground state of the system with quantum numbers $N$, $S^z$. In the ground state the integers $J_\alpha$ are distributed in consecutive order as shown by the crosses in fig. 5.3 (*a*). The circles show the distribution of quantum numbers of holes. As $N$ is increased by 1, the size of the lattice of integers also expands by one more site. This new site corresponds to a hole $J_0 \geqslant (N-3M)/2$ and $\lambda_0 \leqslant -B$. The excited configuration is presented in fig. 5.3 (*b*).

Fig. 5.3




Schematic sketch of the distribution integers $J_\alpha$ and rapidities $\lambda_\alpha$ in (*a*) the ground state and (*b*) the excited state. The integers $J_\alpha$ are shown by crosses. The circles show the holes.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Its energy differs from the ground-state energy by an amount $\varepsilon(\lambda_0)$. Of course, as $\varepsilon \to 0$ the excitations rapidity coincides with the Fermi surface: $\lambda_0 - B$. Then the quantity $E(N+1, S^z+1/2)$ in (5.1.41) is also the ground-state energy and, in particular, from (5.1.43) one immediately obtains the Friedel sum rule:

$$\left.\begin{aligned} &\Delta_s^{\uparrow\uparrow}(H/2) = \pi(1/2 - M_i) \\ \text{i.e.} \quad & \\ &dE_i/dS^z = M_i \chi_h. \end{aligned}\right\} \tag{5.1.45}$$

Now we turn to a general approach to elementary excitations in the Bethe-Ansatz framework, the basic idea of which goes back to a remarkable paper by Yang and Yang (1969). In our presentation we shall follow the paper by Japaridze *et al.* (1982). Let $\rho(\lambda)$ and $\tilde{\rho}(\lambda)$ be equilibrium particle and hole distributions, i.e. those which minimize the energy functional. Consider small deviations $\delta\rho$ and $\delta\tilde{\rho}$ from the equilibrium distributions. Then, as the energy function (5.1.11)

$$N^{-1}(E - HS^z) = \int (b(\lambda) - H)\rho(\lambda)\, d\lambda, \tag{5.1.46}$$

where

$$b(\lambda) = -\frac{N}{L}(p(\lambda) + \pi)$$

is a linear one, the energy will change by an amount

$$\delta E/N = -\int (\delta\tilde{\rho}(\lambda)\varepsilon^+(\lambda) - \varepsilon^-(\lambda)\delta\rho(\lambda) + (b(\lambda) - H)\delta\rho(\lambda))\, d\lambda,$$

where $\varepsilon^+(\lambda) > 0$ and $\varepsilon^-(\lambda) < 0$ are as yet unknown functions describing the linear response of the system to variations of the particle and hole distributions. The constraint (5.1.9) implies

$$\frac{\delta\tilde{\rho}(\lambda)}{\delta\rho(\lambda')} = \delta(\lambda - \lambda') + a_2(\lambda - \lambda').$$

Now we can derive an equation for the energy spectrum, putting the variation $\delta E$ respective to $\rho(\lambda)$ equal to zero:

$$\varepsilon^+(\lambda) + \varepsilon^-(\lambda) + \int a_2(\lambda - \lambda')\varepsilon^-(\lambda')d\lambda' = b(\lambda) - H. \tag{5.1.47}$$

This equation determines the continuous function $\varepsilon = \varepsilon^+ + \varepsilon^-$. Then we can expand the energy of an arbitrary state in terms of $\varepsilon^+$ and $\varepsilon^-$. Namely, substituting $b(\lambda)$ (5.1.46) via (5.1.47) and using that $\varepsilon^+(\lambda) > 0$ and $\varepsilon^-(\lambda) < 0$, we obtain:

$$E/N = \int [\varepsilon^+(\lambda)\rho(\lambda) - \varepsilon^-(\lambda)\tilde{\rho}(\lambda)]d\lambda + E^{(0)}/N, \tag{5.1.48}$$

where $E^{(0)} = E_h^{(0)} + (1/N)E_i^{(0)}$,

$$E_h^{(0)}/N = \int a_1(\lambda)\varepsilon^-(\lambda)\, d\lambda \tag{5.1.49}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

and

$$E_{\mathrm{i}}^{(0)}=\int a_1(\lambda+1/g)\varepsilon^-(\lambda)\,d\lambda. \tag{5.1.50}$$

The formula (5.1.48) is a principal one in the determination of the ground state and elementary excitations. Indeed, the first two terms in (5.1.48) are always positive and the ground state should obey

$$\varepsilon^+(\lambda)\rho(\lambda)=0; \qquad \varepsilon^-(\lambda)\tilde{\rho}(\lambda)=0. \tag{5.1.51}$$

Therefore, in order to find the ground state it is sufficient to solve the basic equation (5.1.47). Evidently, as $b(\lambda)$ is continuous and monotonous the same is also true for $\varepsilon(\lambda)$. $\varepsilon(\lambda)$ intercepts zero at a certain value of $\lambda=-B$, so that:

$$\varepsilon^+(\lambda)=\begin{cases}\varepsilon(\lambda) & \text{at } \lambda<-B,\\ 0 & \text{at } \lambda>-B,\end{cases} \qquad \varepsilon^-(\lambda)=\begin{cases}0 & \text{at } \lambda<-B,\\ \varepsilon(\lambda) & \text{at } \lambda>-B.\end{cases}$$

Then equations (5.1.51) imply that

$$\rho(\lambda)=0 \quad \text{at } \lambda<-B, \qquad \tilde{\rho}(\lambda)=0 \quad \text{at } \lambda>-B$$

so that eqn. (5.1.47) may be rewritten as

$$\varepsilon(\lambda)+\int_{-B}^{\infty} a_2(\lambda-\lambda')\varepsilon(\lambda')d\lambda'=b(\lambda)-H \qquad (-\infty<\lambda<-\infty),$$

$$\varepsilon(-B)=0. \tag{5.1.52}$$

The resulting ground-state energy is

$$E^{(0)}=E_{\mathrm{h}}^{(0)}+E_{\mathrm{i}}^{(0)},$$

where $E_{\mathrm{h}}^{(0)}$ and $E_{\mathrm{i}}^{(0)}$, given by eqns. (5.1.49) and (5.1.50), are the Fermi gas and impurity energies.

From (5.1.47) and (5.1.49) it can easily be shown that

$$E_{\mathrm{h}}^{(0)}=(S^z)^2/2\chi_{\mathrm{h}}, \tag{5.1.53}$$

whilst the impurity magnetization, calculated in § 5.1.3, equals

$$M_{\mathrm{i}}=-\partial E_{\mathrm{i}}^{(0)}/\partial H \tag{5.1.54}$$

Equations (5.1.47) and (5.1.52) give the elementary excitation energy as a function of rapidity. Indeed, let there be a hole with rapidity $\lambda_0>-B$ in the rapidity distribution:

$$\rho(\lambda)=\rho_0(\lambda)-\frac{1}{N}\delta(\lambda-\lambda_0); \qquad \tilde{\rho}(\lambda)=\tilde{\rho}_0(\lambda)=\tilde{\rho}_0(\lambda)+\frac{1}{N}\delta(\lambda-\lambda_0), \tag{5.1.55}$$

where $\rho_0$ and $\tilde{\rho}_0$ are certain implicit functions which possess the continuous limit. Inserting (5.1.55) into (5.1.48), we see that, in view of (5.1.48), the energy variation is given by $-\varepsilon^-(\lambda_0)$. We emphasize that one cannot insert (5.1.55) directly into (5.1.45), since $\rho_0$ differs from the ground-state distribution by a term of the order $1/N$, which must also be included in the excitation energy. Thus, $\varepsilon(\lambda_0)$ is the energy of the elementary excitation with rapidity $\lambda_0$. The rapidity dependence of the

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

scattering phase $\Delta_s(\lambda_0)$ can be determined in a similar way. Namely, $\Delta_s(\lambda_0)$ satisfies the equation

$$\Delta_s(\lambda)+\int_{-B}^{\infty} a_2(\lambda-\lambda')\Delta_s(\lambda')\,d\lambda'=\delta_s(\lambda_0), \tag{5.1.56}$$

where $\delta_s(\lambda)=2\tan^{-1}[(\lambda+1/g)/S]$ is the bare phase shift. Indeed according to (5.1.9) and (5.1.11)

$$E_i=\frac{N}{L}\int \delta_s(\lambda)\rho(\lambda)\,d\lambda. \tag{5.1.57}$$

Substituting $\delta_s(\lambda)$ in (5.1.57) by the left-hand side of eqn. (5.1.56) one obtains:

$$E_i=\frac{N}{L}\int(\Delta_s^+(\lambda)\rho(\lambda)=\Delta_s^-(\lambda)\tilde{\rho}(\lambda))\,d\lambda+E_i^{(0)}, \tag{5.1.58}$$

where

$$E_i^{(0)}=\frac{N}{L}\int \Delta_s^-(\lambda)a_1(\lambda)\,d\lambda \tag{5.1.59}$$

is the energy of the impurity's ground state which, obviously, coincides with (5.1.50) and $\Delta_s^{\pm}(\lambda)=\Delta_s(\lambda)\theta(\pm(\lambda+B))$. Consider once more a configuration (5.1.52). Inserting (5.1.52) into (5.1.58) one gets

$$E_i(N+1,S^z+1/2)-E_i(N,S^z)=\Delta_s(\lambda_0) \tag{5.1.60}$$

and according to (5.1.41) and (5.1.43) $\Delta_s^{\uparrow\uparrow}(\lambda)=\Delta_s^-(\lambda)$. Hence, eqns. (5.1.52) and (5.1.56) are parametric definitions of the scattering phase as a function of energy. Note that there exists a simple relationship between $\varepsilon^{\pm}$ and the characteristic of the Fermi gas with uniform density of states:

$$-\frac{1}{2\epsilon_F}\frac{\partial\varepsilon^-(\lambda)}{\partial\lambda}=\rho_h(\lambda); \qquad -\frac{1}{2\epsilon_F}\frac{\partial\varepsilon^+(\lambda)}{\partial\lambda}=\tilde{\rho}_h(\lambda). \tag{5.1.61}$$

The similar relation reads

$$-\frac{\partial}{\partial\lambda}\Delta_s^-(\lambda)=\rho_i(\lambda); \qquad -\frac{\partial}{\partial\lambda}\Delta_s^+(\lambda)=\tilde{\rho}_i(\lambda), \tag{5.1.62}$$

where $\rho_h$ and $\rho_i$ are defined by eqns. (5.1.13) and (5.1.14). Equations (5.1.61) and (5.1.62) provide the most simple formulae for the scattering phase and excitation energy. Indeed, $\Delta_s(+\infty)=0$ so that

$$\left.\begin{aligned}\Delta_s^{\uparrow\uparrow}&=\pi\int_{\lambda}^{\infty}\rho_i(\lambda)\,d\lambda,\\ -\varepsilon^-(\lambda)&=2\epsilon_F\int_{-B}^{\lambda}\rho_h(\lambda)\,d\lambda,\end{aligned}\right\}\quad(\lambda>-B).$$

The Friedel sum rule follows immediately from here; taking $\varepsilon=0$, i.e. $\lambda=-B$, one gets (5.1.44) in view of (5.1.15 *b*) (Andrei 1982).

Now compare the results obtained for $S=1/2$ with Nozières' theory. Of course, it may well be done using explicit formulae. Still it is simple and more instructive to use

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

only eqns. (5.1.52) and (5.1.56) which, for $S=1/2$, are very much alike. Rewrite them in the form:

$$\left.\begin{aligned}\varepsilon(\lambda)-\int_{-\infty}^{-B}R(\lambda-\lambda')\varepsilon(\lambda')d\lambda'&=-\frac{2\epsilon_F}{\pi}\tan^{-1}\exp(\pi\lambda)+H,\\ \Delta_s(\lambda)-\int_{-\infty}^{-B}R(\lambda-\lambda')\Delta_s(\lambda')d\lambda'&=\tan^{-1}\exp(\pi(\lambda+1/g))-\pi M_i/2.\end{aligned}\right\}\quad(5.1.63)$$

(*a*) At $\varepsilon\to 0$, $H\to 0$ ($\lambda\to-\infty$) the right-hand sides of equations (5.1.63) can be expounded in powers of $\exp(\pi\lambda)$. Therefore, $\Delta_s(\varepsilon_s, H)$ is an analytic function of $\varepsilon_s$ and $H$, i.e. can be expanded in powers of $\varepsilon_s/T_K$ and $H/T_K$:

$$\Delta_s(\varepsilon_s,H)=\Delta(0,0)-k_1\frac{\varepsilon_s}{T_K}-k_2\frac{H}{T_K}+O\left(\frac{\varepsilon^2}{T_K{}^2},\frac{H^2}{T_K^2}\right).\quad(5.1.64)$$

(*b*) At $1/g=0$ both equations coincide. Indeed, in this case the Bethe-Ansatz equations describe the Fermi gas with one particle less than for the case of $g=0$. Hence, slopes $k_1$ and $k_2$ should be identical to those for the Fermi liquid.

$$k_1=1/4,\qquad k_2=1/2.$$

However, in the Fermi liquid, the charge sector contributes to the specific heat as much as the scattering in the spin channel:

$$\Delta=\Delta_c^h+\Delta_s^h=\frac{\pi}{2}-\frac{\pi}{8\epsilon_F}(\varepsilon_s+\varepsilon_c)-\frac{H\pi}{4\epsilon_F}.$$

Obviously, the charge sector does not contribute to the impurity specific heat. Hence,

$$\frac{C^i}{C^h}=\frac{\partial\Delta_s}{\partial\varepsilon_s}\bigg/\left(\frac{\partial\Delta_c^h}{\partial\varepsilon_c}+\frac{\partial\Delta_s^h}{\partial\varepsilon_s}\right)=\frac{1}{2}\exp\left(\frac{\pi}{g}\right)$$

As to the susceptibility, both for the impurity and the Fermi liquid it is solely determined by the spin channel, so that

$$\frac{\chi^i}{\chi^h}=\left(\frac{\partial\Delta_s}{\partial\varepsilon_s}\right)\bigg/\left(\frac{\partial\Delta_s^h}{\partial\varepsilon_s}\right)=\exp\left(\frac{\pi}{g}\right)\quad\text{and}\quad\frac{C^i}{C^h}=\frac{1}{2}\frac{\chi^i}{\chi^h}.$$

Comparing (5.1.64) with (3.1.26) we find Nozières' phenomenological coefficient

$$\alpha=\frac{1}{4T_K}.$$

In doing so one must keep in mind that $\varepsilon$ is an energy respective to the Fermi level in the magnetic field, so that

$$\left.\begin{aligned}z&=-\varepsilon^--H/2\quad\text{in (3.1.26)},\\ \Delta^{\uparrow\uparrow}(z)&=\Delta^-(-\varepsilon^--H/2).\end{aligned}\right\}\quad(5.1.65)$$

The explicit forms of the functions $-\varepsilon^-(\lambda)$ and $\Delta_s^{\uparrow\uparrow}(\lambda,H)$ are given in §3.1.3 (see eqn. (3.1.36)).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

At $H=0$ in the vicinity of the Fermi energy $\varepsilon \ll \epsilon_F$

$$\varepsilon(\lambda)=\frac{2\epsilon_F}{\pi}\exp(\pi\lambda) \qquad (\lambda\to-\infty)$$

and

$$\Delta(\lambda)=\pi/2-\tan^{-1}\exp(\pi(\lambda+1/g)).$$

Combining these equations we have the simple result

$$\Delta(\varepsilon)=\pi/2-\tan^{-1}(\varepsilon/T_K). \tag{5.1.66}$$

Note the quantity $d\Delta(\varepsilon)/d\varepsilon$ can be considered as the impurity part of one-particle density of state. At $\varepsilon=0$ there is a narrow many-body peak, the width of which is $T_K$. This is the well-known Abrikosov–Suhl resonance.

It is clear that functions $\varepsilon^+(\lambda)$ and $\Delta^+(\lambda)$ defined by eqns. (5.1.52) and (5.1.56) at $\lambda<-B$ parametrically define the scattering phase of the particle, the spin projection of which is opposite to the magnetic field, i.e.

$$\Delta^+(\varepsilon^+)=\Delta^{\uparrow\uparrow}(z-H/2),$$

where $z=H/2-\varepsilon^+$. Using the eqns. (5.1.52) and (5.1.56) we obtain the Friedel sum rule for $\Delta^{\uparrow\downarrow}$:

$$\Delta^{\uparrow\downarrow}(-H/2)=\Delta^+(H)=\Delta^+(\varepsilon^+(-\infty))=\pi/2+\pi M_i(H).$$

The functions $\Delta^{\uparrow\uparrow}(z)$ and $\Delta^{\uparrow\downarrow}(z)$ form two parts of the continuous function $\Delta(\varepsilon)$. In the region $-\infty<\varepsilon<H$ this function is defined by eqns. (5.1.52) and (5.1.56). The energy $\varepsilon=H$ is the threshold of the creation of higher excitation, namely, the 'spin complex' or '2-string'. These excitations will be discussed in § 6.

### 5.1.5. *Scales in the Kondo phenomenon*

The energy scale in the Kondo effect is the so-called Kondo temperature $T_K$. Usually one only bears in mind the order of magnitude of this temperature, determined by the exponential factor

$$T_K\sim\epsilon_F\exp(-1/I\rho(\epsilon_F)).$$

One can specify the scale for the 'Kondo temperature' in a unique way by adopting a certain definition of $T_K$. Throughout this paper $T_K$ implies the quantity related to the magnetic susceptibility at $H=T=0$:

$$T_K=(2\pi\chi_i)^{-1}.$$

In his classical paper, Wilson (1975) uses another definition of the Kondo temperature, related to the perturbation theory at $T\gg H$ and $T\gg T_K$:

$$\ln\frac{T}{T_W}=\frac{1}{z}-\frac{1}{2}\ln z \qquad (z>0), \tag{5.1.67}$$

where $z(T)$ is an 'invariant charge' (see § 2.5). We denote $T_K$ as defined by Wilson as $T_W$. Recall that by definition all the physical quantities are represented as a series in

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

powers of the 'invariant charge'. For instance, at $T \gg T_K$

$$T\chi_i(T) - 1/4 = z + \sum_{n=2}^{\infty} a_n z^n,$$

where $a_n$ are as yet unspecified numbers. This definition fixed $T_W$ in a unique way. In another domain of perturbation theory $H \gg T$, $H \gg T_K$ the invariant charge is different. Hence a new scale $T_H$ is given by

$$\ln H/T_H = \frac{1}{z} - \frac{1}{2}\ln z. \tag{5.1.68}$$

It is this scale $T_H$ which enters the formula (5.1.33).

Different constructions of the model may lead to different dependences of $T_K$, $T_H$ and $T_W$ on the bare parameters. However, their ratios are universal numbers independent of how the ultraviolet cut-off is introduced and can be calculated. It was done numerically by Wilson (1975), who used the renormalization group numerical approach and analytically by Andrei and Lowenstein (1981), on the basis of the exact solution. The ratio $T_W/T_H$ is a regular function of $I$ and can be calculated by comparing the perturbation theories in the domains $T \gg H$ and $T \ll H$ but $\max(T, H) \gg T_K$. The other ratios $T_K/T_H$ or $T_K/T_W$ relate scales measured far above and below the Kondo temperature and, hence, require a non-perturbative treatment of the crossover. Wilson's numerical result is (see eqn. (3.1.24))

$$\frac{T_W}{T_K} = 2\pi(0{\cdot}1032 \pm 0{\cdot}0005). \tag{5.1.69}$$

In § 5.1.3 another ratio (5.1.32) was calculated:

$$\frac{T_H}{T_K} = \left(\frac{2\pi}{e}\right)^{1/2}.$$

Andrei and Lowenstein (1981) combined it with $T_W/T_H$ calculated in perturbation theory and compared it with Wilson's value (5.1.69). They found that the impurity magnetization in second-order perturbation theory is

$$M_i = \frac{1}{2}\left(1 - \frac{1}{2}I\rho - \frac{1}{2}(I\rho)^2 \ln\left(\frac{De}{2H}\right) + O(I^3)\right) \tag{5.1.70}$$

at $T/H \to 0$ and

$$M_i = \frac{H}{4T}(1 - I\rho - (I\rho)^2 \ln(\beta\gamma e^{-7/4} D/T) + O(I^3)) \tag{5.1.71}$$

at $H/T \to 0$, where $D$ is an ultraviolet cut-off and

$$\ln\beta = \int_0^1 dx \frac{x^3(1-x)^2}{\pi^2 x^2 \operatorname{cosec}^2 \pi x - 1} \simeq 0{\cdot}662122,$$

and $\ln\gamma = 0{\cdot}577216$ is Euler's constant. Comparing the log terms in (5.1.70) and (5.1.71) we find:

$$T_W/T_H = 2\beta\gamma e^{-7/4}. \tag{5.1.72}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Now from the two universal numbers $T_K/T_H$ and $T_W/T_H$ one may deduce a third one:

$$\frac{T_W}{T_K}=\frac{T_W}{T_H}\frac{T_H}{T_K}=2\beta\gamma\pi^{1/2}e^{-9/4}=2\pi\times 0{\cdot}102676. \tag{5.1.73}$$

An agreement with Wilson's numerical answer is found (see (5.1.69)).

The general relation between high- and low-temperature dimensional scales (5.1.72) for an arbitrary impurity spin was found by Furuya and Lowenstein (1982).

$$\frac{T_W}{T_K}=2\beta\gamma\pi^{1/2}\alpha^{(1/10)(1-(4/3)S(S+1))},$$

where

$$\alpha=\int_0^1 x(\pi^2\operatorname{cosec}\pi x-x^{-2}-(1-x)^{-2})\,dx\simeq 0{\cdot}841166.$$

The theory we discuss is not free from difficulties. As we have seen, the universal dependence of magnetization on $H/T_H$ corresponds well to the perturbation theory results:

$$M_i(H)=S\left(1-\frac{1}{2}z(H)+\ldots\right)=S\left(1-\frac{1}{2\ln H/T_H}-\frac{1}{4}\frac{\ln\ln H/T_H}{\ln^2 H/T_H}+\ldots\right). \tag{5.1.74}$$

Unfortunately, this is not the case for the coupling constant dependence of $T_K$ or $T_H$. Indeed, we have found (see (5.1.23) and (5.1.32))

$$T_H=\text{const}\,D\exp(-1/I\rho). \tag{5.1.75}$$

Inserting (5.1.75) into (5.1.74) we find a non-analytic dependence of the physical value of the invariant charge in the normalization point $Z(H=D)$

$$M_i(D)=S\left(1-\frac{1}{2}I\rho-\frac{1}{4}(I\rho)^2\ln I\rho+\ldots\right), \tag{5.1.76}$$

$$1/I\rho=\frac{1}{z(D)}-\frac{1}{2}\ln z(D)+\text{const}. \tag{5.1.77}$$

Of course, this has nothing in common with the perturbation theory. We have already discussed in §2.5 that the normalization point $D$ depends on $I$ in a non-universal way. But this dependence must be analytic at $I\ll 1$. On the other hand formulae (5.1.76), (5.1.77) and (5.1.75) require the substitution

$$D\to D(I\rho)^{1/2}.$$

This trouble is an artefact of the linear spectrum and point-like interaction approximations. To be more precise, its origin is in the momentum independence of the scattering phase. In order to get the correct pre-exponential factor in $T_K$ as a function of $I$ one must regularize the theory preserving its integrability. For the s–d-exchange hamiltonian this problem is not yet solved, whereas for the Anderson model in the Schrieffer–Wolf limit such a regularization was constructed by Wiegmann *et al.* (1982). In §8 on the exact solution of the Anderson model we shall demonstrate in detail how, in the Schrieffer–Wolf limit, the Bethe-Ansatz equations (4.5.A)–(4.5.C) for the Anderson model transform into those for the s–d model,

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

subject to substitution of $N$ in eqn. (4.3.B) by $L(U\Gamma)^{1/2}$. The latter substitution leads to the known result (Abrikosov and Migdal 1970, Fowler and Zawadowski 1971): $T_K = D(\rho I)^{1/2} \exp(-1/I\rho)$.

We conclude by emphasizing that the approximations of § 4.1.1, though yielding the wrong pre-exponential factor for $T_K$, are still the most adequate if one is interested in universality properties of physical quantities as a function of $H/T_K$, $T/T_K$.

### 5.2. *The anisotropic exchange model*

This section is closely connected to §3.1.1. On calculating the impurity magnetization we try to illustrate Anderson's 'poor man scaling', Toulouse limit, the equivalency to the resonant-level model (see the Supplement section), etc., in the framework of the exact solution. We investigate, below, the magnetic properties of the anisotropic exchange model only at $I_\perp < I_\parallel$.

#### 5.2.1. *Scaling picture*

Using only the structure properties of eqns. (4.3.A)–(4.3.C) and the parametrization (4.3.8) the scaling behaviour of the system may be established without the direct solution of eqns. (4.3.A)–(4.3.C). Indeed, in leading order in $1/N$, eqn. (4.3.B) depends only on one parameter $\mu$. Another parameter $f/\mu$ defining the physical properties of our system determines the energy scale of the impurity. As will be shown below, the Kondo temperature

$$T_K \sim D \exp(-\pi f/\mu), \tag{5.2.1}$$

where the proportionality coefficient $D$ is a slowly varying function of $\mu$. Therefore, motion along the lines of the constant $\mu$ on the plane $(I_\parallel, I_\perp)$ affects the energy scale of the system conserving the form of the interaction. This plane is given in fig. 5.4. The arrows on the trajectories indicate the scale time increase $f \to 0$. The behaviour of the trajectories in the region $|I_\perp|, |I_\parallel| \ll 1$ is well known. It corresponds to the scaling procedure calculated by the perturbation theory (Anderson *et al.* 1970). If $|I_\perp|, |I_\parallel| \ll 1$ expression (4.3.8) gives

$$I_\perp^2 - I_\parallel^2 = 4\mu^2. \tag{5.2.2}$$

One may obtain the renormalization group equations. Let us assume that $f$ is a function of $D$, $T_K$ being independent from $D$. Differentiating eqn. (5.2.1) with respect to $D$ one obtains

$$\frac{df}{d\ln D} = \frac{\mu}{\pi}. \tag{5.2.3}$$

If $|I_\parallel|, |I_\perp| \ll 1$ eqn. (4.3.8) gives

$$\coth f = I_\parallel / 2\mu. \tag{5.2.4}$$

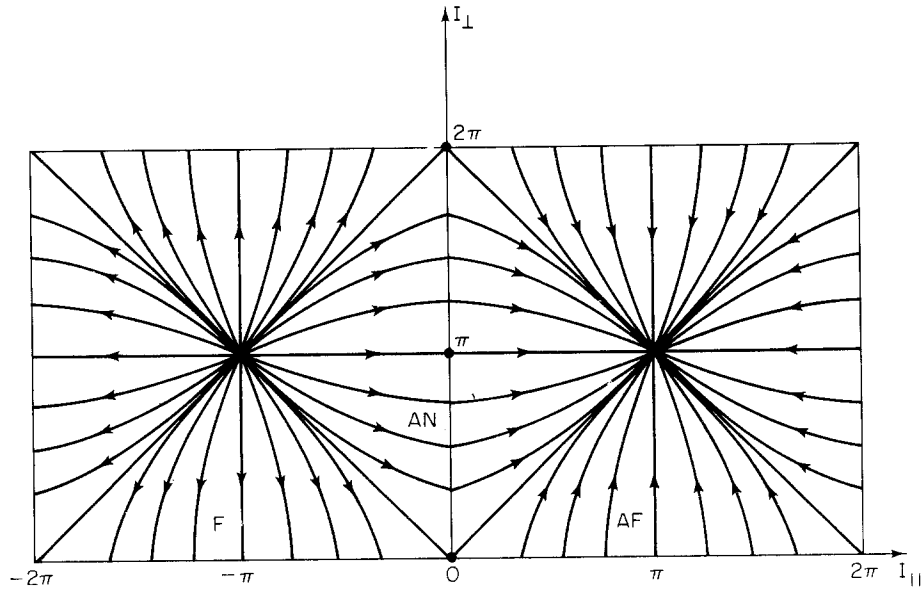
Combining eqns. (5.2.3) and (5.2.4) we obtain

$$\frac{dI_\parallel}{d\ln D} = \frac{1}{2\pi}(-I_\parallel^2 + 4\mu^2).$$

This equation together with the relation (5.2.2) coincides with the renormalization group equations of (3.1.5).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 5.4




The renormalization-group flow diagram: $\mu(I_{||}, I_\perp) = \text{const}$. Trajectories depict the flow of the hamiltonian with decreasing energy scale (or decreasing $f \to 0$). The fixed points $I_\perp = \pm I_{||} = \pi$ are the strong-coupling limits. At $I_\perp > I_{||}$ only the strong-coupling fixed point is stable. The lines $I_{||} = \pm\pi$ are the Toulouse limits. The region $|I_{||}, I_\perp| \ll 1$ is known as a 'poor man scaling' (Anderson 1970).

Let us continue the analysis of the scaling picture. It is evident that the lines $I_{||} = \pm I_\perp$ $(\mu = 0)$ and $\pm I_{||} + I_\perp = 2\pi (\mu = \pi)$ are separatrices. On the intersections of these lines there are fixed points. One of them is attractive and another is repulsive.

Thus, for $I_\perp > -I_{||}$ and for any interrelation between $I_{||}$ and $I_\perp$ the system has only one attractive fixed point. This point corresponds to the strong coupling limit: $\mu/f \to \infty$ ($g \to \infty$ for an isotropic case). For the value $\mu = \pi/2$ the two-particle scattering phase

$$\Phi(\lambda) = 2\tan^{-1}(\cot\mu \tanh\lambda\mu)|_{\mu=\pi/2} = 0.$$

At this point eqns. (4.3.A) and (4.3.B) are decoupled, the interaction is absent and we have a free theory. This was discovered by Anderson *et al.* (1970). A brief review of their paper can be found in § 3.1.1.

The line $I_{||} = \pi$ $(\mu = \pi/2)$ is known as the Toulouse limit. It is surprising that there exists a similar line at the ferromagnetic region $I_{||} = -\pi$.

According to the hypothesis of Anderson *et al.* (1970) the exchange amplitude $I(D)$ in the isotropic s–d model, which is small at a large energy and increases when the energy scale decreases, achieves the Toulouse limit by a finite number of recursion steps. We see, however, this is not quite true. Actually, starting from small $I_\perp$ and $I_{||} > 0$ the Toulouse limit (i.e. the line $\mu = \pi/2$) can be achieved by an infinite number of steps because the scaling trajectories intersect each other only in the fixed

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

point. Nevertheless, the conclusion made by Anderson *et al.* on the magnetic susceptibility at $T=0$ retains its validity. The low energy properties of the theory are determined by the fixed hamiltonian. In the isotropic case the strong coupling leads to essential renormalization of the hamiltonian. However, in the Toulouse limit on the one hand the theory corresponds to the case of the free particles and there is no renormalization; but on the other hand both theories have coinciding fixed points. We shall continue this discussion in the next section. Here we should note that the numerical investigations performed by Melnicov (1982 a) and Oliveira and Wilkins (1981) showed that the strong coupling limit determines the behaviour of the system not only at $T=0$ but (perhaps due to some numerical reasons) also describes the thermodynamics up to $T \lesssim 0{\cdot}5 T_K$ within 1% accuracy.

5.2.2. *The ground state of the anisotropic exchange model at $I_\perp < I_\parallel$*

The statements of § 5.1.1 concerning the quantum numbers $J_\alpha$ and $N_j$ in eqn. (5.1.1) are also valid for the anisotropic Bethe-Ansatz equations:

$$k_j L = 2\pi N_j - \sum_{\alpha=1}^{M} (p(\lambda_\alpha) + \pi - \mu), \tag{5.2.5 a}$$

$$N p(\lambda_\alpha) + \delta_s(\lambda_\alpha) = 2\pi J_\alpha + \sum_{\beta=1}^{M} \Phi(\lambda_\alpha - \lambda_\beta), \tag{5.2.5 b}$$

where

$$\left.\begin{aligned} p(\lambda) &= 2\tan^{-1}(\cot \mu/2 \tanh \mu\lambda), \\ \delta_s(\lambda) &= p(\lambda + f/\mu), \\ \Phi(\lambda) &= 2\tan^{-1}(\cot \mu \tanh \mu\lambda). \end{aligned}\right\} \tag{5.2.6}$$

As well as in the isotropic case the ground state is formed by real rapidities $\lambda_\alpha$ and $k_j$. The charge numbers are again equal to

$$N_j = -N/2 + j \qquad (j = 1, \ldots, N).$$

However, the spin numbers $J_\alpha$ now form a uniform lattice between

$$-(1/2\pi)[N(\pi-\mu) - M(\pi - 2\mu)] \text{ and } (1/2\pi)[N(\pi-\mu) - M(\pi-2\mu)].$$

This leads to the incorrect formula for the ground-state energy:

$$\begin{aligned} LE^{(0)} &= -NM(\pi-\mu) - 2\pi \sum_{\alpha=1}^{M} \left\{ -\alpha + \frac{1}{2\pi}[N(\pi-\mu) - M(\pi-2\mu)] \right\} \\ &= L\left(1 - \frac{\mu}{\pi}\right)\left(-\frac{\pi N^2}{2L} + \frac{2\pi S^{z^2}}{L}\right). \end{aligned} \tag{5.2.7}$$

Formula (5.2.7) shows that eqns. (4.3.A)–(4.3.C), described at $f=0$, describe non-interacting fermions with a renormalized density of states of spin excitations $\rho_s = (1/2\pi)(1-\mu/\pi)^{-1}$, while we started from the density of states $\rho_s = 1/2\pi$. This difficulty has a general character and appears in many models with linear spectrum (Japaridze *et al.* 1983). To understand the cause of this difficulty let us recall that for the construction of the coordinate Bethe Ansatz we factually added the contact interaction between the particles, which was of the same type as the interaction between particles and the impurity (see § 4.6). This interaction has been supposed to

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

be non-essential because it cannot change the spectrum of the particles moving to only one side with the same velocities.

The additional interaction proves not to influence the scattering kinematics but it may lead to the renormalization of the density of states in the limit of a large number of particles. This situation seems to take place only in the solution of the anisotropic s–d model. Indeed, the effective hamiltonian of 'free fermions' has the following form:

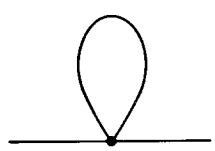
$$\mathscr{H}=\int\left\{\sum_{\sigma}-i\hat{C}_{\sigma}^{+}(x)\frac{\partial}{\partial x}\hat{C}_{\sigma}(x)+\sum_{\alpha,\alpha',\beta,\beta'}\hat{C}_{\alpha}^{+}(x)\hat{C}_{\alpha'}(x)\right.$$
$$\left.\times\frac{1}{4}(I_{\parallel}\sigma_{\alpha\alpha'}^{z}\sigma_{\beta\beta'}^{z}+I_{\perp}(\sigma_{\alpha\alpha'}^{x}\sigma_{\beta\beta'}^{x}+\sigma_{\alpha\alpha'}^{y}\sigma_{\beta\beta'}^{y}))\hat{C}_{\beta}^{+}(x)\hat{C}_{\beta'}(x)\right\}dx. \quad (5.2.8)$$

Consider, for example, the correction to the $g$-factor of the electron due to the interaction (5.2.8) for $I_{\perp}=0$. That correction already arises in the first order of perturbation theory. The corresponding diagram is shown in fig. 5.5. It gives

$$g_{\text{eff}}=g(1+I_{\parallel}/4\pi).$$

Thus the 'interaction' leads to the additional magnetization of the conduction electrons. It is clear that for the isotropic case the additional magnetization corrections at $H\to 0$ are absent because of the rotational symmetry. This fact has been observed in §5.1., where the additional interaction did not lead to any renormalizations. For the anisotropic case, however, renormalization takes place. It seems to be the cause of the appearance of the factor $(1-\mu/\pi)$ in formula (5.2.7).

Fig. 5.5



The first-order correction to the density of states.

It is obvious that the influence of this 'interaction' is reduced to the renormalization of the density of states because the other diagrams having cuts with more than one fermionic propagator are equal to zero. Therefore, the simplest way to remove this artefact is to treat an electronic Lande-factor as

$$g=(1-\mu/\pi), \quad (5.2.9)$$

which will always be implied below. The same renormalization factor also takes place for compressibility.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

5.2.3. *Magnetic susceptibility*

We can now approach the limit $N\to\infty$, $M\to\infty$, $L\to\infty$ proportionally, obtaining from eqns. (5.2.6) the integral equations (see § 5.1.1 for the details):

$$\rho_h(\lambda)+\int_{-B}^{\infty} a_2(\lambda-\lambda')\rho_h(\lambda')d\lambda'=a_1(\lambda); \qquad \lambda>-B, \tag{5.2.10 a}$$

$$\rho_i(\lambda)+\int_{-B}^{\infty} a_2(\lambda-\lambda')\rho_i(\lambda')d\lambda'=a_1(\lambda+f/\mu); \qquad \lambda>-B, \tag{5.2.10 b}$$

where now

$$a_n(\lambda)=\frac{1}{2\pi}\frac{\sin\mu n}{\cosh 2\mu\lambda-\cos\mu n}=\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega\exp(-i\omega\lambda)\frac{\sinh(\pi/\mu-n)\,\omega/2}{\sinh(\pi/2\mu)\omega}.$$

Functions $\rho_h$ and $\rho_i$ parametrically determine the impurity magnetization:

$$\left.\begin{aligned} H/4\epsilon_F&=1/2-\int_{-B}^{\infty}\rho_h(\lambda)\,d\lambda,\\ M_i&=1/2-\int_{-B}^{\infty}\rho_i(\lambda)\,d\lambda \end{aligned}\right\} \tag{5.2.11}$$

Further calculations are quite analogous to those for the isotropic case. Multiplying (5.2.10) by $(1+a_2)^{-1}$ we go to the hole distributions $\tilde\rho_h$ and $\tilde\rho_i$ (for the definition of these functions, see § 5.1.1).

$$\tilde\rho_h(\lambda)-\int_{-\infty}^{-B} R(\lambda-\lambda')\tilde\rho_h(\lambda')d\lambda'=s(\lambda)\simeq\exp(\pi\lambda); \qquad \lambda<-B, \tag{5.2.12 a}$$

$$\tilde\rho_i(\lambda)-\int_{-\infty}^{-B} R(\lambda-\lambda')\tilde\rho_i(\lambda')d\lambda'=s(\lambda+f/\mu); \qquad \lambda<-B, \tag{5.2.12 b}$$

where

$$R(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \times\exp(-i\omega\lambda)\frac{\sinh(\pi/2\mu-1)\omega}{2\cosh\omega/2\sinh(\pi/2\mu-1/2)\omega}; \qquad s(\lambda)=(2\cosh\pi\lambda)^{-1}.$$

Assuming $H\ll\epsilon_F$ we restrict ourselves to the asymptotic of $s(\lambda)$ in (5.2.12 *a*) for $\lambda\to-\infty$. If $H\ll T_K$ one may rewrite the right-hand side of eqn. (5.2.12 *b*) as $\exp(\pi\lambda+\pi f/\mu)$. Comparing eqns. (5.2.12 *a*) and (5.2.12 *b*) we obtain

$$\frac{\chi_{imp}}{\chi_{host}}=\exp(\pi f/\mu). \tag{5.2.13}$$

Therefore, according to the definition of $T_K$ (5.1.23), we have

$$T_K=\frac{2\epsilon_F}{\pi}\exp\left(-\frac{\pi f}{\mu}\right). \tag{5.2.14}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

When $I_\perp \ll I_\parallel \ll 1$

$$T_K = (I_\perp/2I_\parallel)^{2\pi/I_\parallel} \frac{2\epsilon_F}{\pi} \tag{5.2.15}$$

and for $I_\perp \simeq I_\parallel = I \ll 1$

$$T_K = \frac{2\epsilon_F}{\pi} \exp\left(-\frac{2\pi}{I}\right). \tag{5.2.16}$$

These expressions coincide with the perturbation theory results.

Before proceeding to solve the equations for arbitrary magnetic fields we should make the following remark. For the isotropic case there is an essential difference between the distribution functions of bare particles (the right-hand side of eqn. (5.1.14)) and that of physical particles (the right-hand side of eqn. (5.1.20)). The cause of this difference is the strong renormalization accompanying the transition from the high-energy to low-energy scale. In terms of Bethe-Ansatz equations 'to account for the interaction' means to consider the distribution function of the holes $\tilde{\rho}$ instead of the distribution function of the particles $\rho$. In the anisotropic case the difference mentioned above is not too large. In the infrared region one has:

$$\text{r.h.s. eqn. (5.2.12)} \simeq \exp(\pi\lambda), \tag{5.2.17 a}$$

$$\text{r.h.s. eqn. (5.2.10)} \simeq \exp(2\mu\lambda). \tag{5.2.17 b}$$

In the Toulouse limit $\mu = \pi/2$ this difference vanishes as the kernel of eqns. (5.2.10) tends to zero and the theory becomes free. It is interesting that the presence of the anisotropy changes only the distribution of bare particles. The distribution of physical particles at $H \to 0$ does not depend on the anisotropy.

This circumstance is reflected in fig. 5.4. All trajectories with $-I_\parallel < I_\perp$ have a common fixed point. Therefore, the hamiltonians (4.3.1) for different $\mu$ have a common fixed hamiltonian. With a decrease in the energy scale the renormalization of the hamiltonian with $\mu = \pi/2$ does not occur and, therefore, the Toulouse hamiltonian (3.1.6) is fixed for any s–d hamiltonian:

$$\mathscr{H}_{\text{s–d}} \to \mathscr{H}_T \quad \text{at 'energy scale'} \to 0.$$

The solution of eqns. (5.2.12) is given by the formulae of the Appendix to 5.1.3, but now

$$G^{(+)}(\omega)G^{(-)}(\omega) = 1 + \frac{\sinh(\pi/2\mu - 1)\omega}{\sinh \pi\omega/2\mu} \tag{5.2.18}$$

and

$$\left.\begin{aligned} G^{(-)}(\omega) = G^{(+)}(-\omega) &= \frac{(2(\pi-\mu))^{1/2}\Gamma(1+i\omega/2\mu)\exp(i\omega a)}{\Gamma(1+(i\omega/2)(1/\mu - 1/\pi))\Gamma(1/2 + i\omega/2\pi)} \\ a &= \frac{1}{2\mu}\ln\left(1-\frac{\mu}{\pi}\right) - \frac{1}{2\pi}\ln\left(\frac{\pi}{\mu}-1\right). \end{aligned}\right\} \tag{5.2.19}$$

The impurity magnetization is given by the formulae (Wiegmann 1981):

$$M_i(H) = \frac{i}{4\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{d\omega}{\omega + i0} \exp\left(-2i\omega\left(\ln\frac{H}{T_H} + \pi a\right)\right) \Gamma\left(1 - \frac{i\pi\omega}{\mu}\right) \times \Gamma(1/2 + i\omega)/\Gamma(1 - i\omega(\pi/\mu - 1)); \tag{5.2.20}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$T_H = 2\sqrt{\pi}\frac{\Gamma(1+\pi/2\mu)}{\Gamma(1/2+\pi/2\mu)}\exp(\pi a)T_K. \tag{5.2.21}$$

The integrand in (5.2.20) only has poles placed in the imaginary axis of $\omega$ (fig. 5.6).

In the lower half-plane the positions of the poles are

$$\operatorname{Im}\omega = -n\mu/\pi \qquad (n=1,2,\ldots) \tag{5.2.22}$$

and in the upper half-plane

$$\operatorname{Im}\omega = n+1/2 \qquad (n=0,1,\ldots). \tag{5.2.23}$$

If $H<T_H$ the contour of integration presumably envelops the upper half-plane and the poles (5.2.23) give the power-series expansion of $M_i(H)$:

$$M_i(H<T_H) = \frac{1}{\sqrt{\pi}}\sum_{n=0}^{\infty}\frac{(-1)}{n!}\left(\frac{H}{T_H}\right)^{2n+1} \times \frac{\exp(\pi a(2n+1))\Gamma(1+\pi/2\mu(2n+1))}{(2n+1)\Gamma(1/2+\pi/2\mu(2n+1))}. \tag{5.2.24}$$

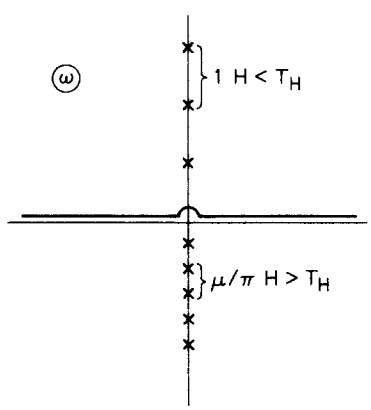
Thus, at low energies the local moment is frozen out by the conduction electrons. The anisotropy does not affect the character of the power-series expansion determining only the coefficients.

If $H>T_H$ the contour of integration envelops the lower half-plane and the poles are important (5.2.22):

$$M_i(H>T_H) = \frac{1}{2} - \frac{1}{2\sqrt{\pi\mu}}\sum_{n=1}^{\infty}\frac{\sin\mu n}{n!}\Gamma\left(\frac{1}{2}+\frac{\mu n}{\pi}\right) \times \Gamma(n(1-\mu/\pi))\left(\frac{T_H}{H}\right)^{2\mu n/\pi}\exp(-2\mu a n). \tag{5.2.25}$$

The expansion in powers of $(T_H/H)^{2\mu/\pi}$ was predicted by Luther and Emery (1974) in the perturbation-theory framework.

Fig. 5.6




The complex plane of the integrand (5.2.20).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

At $H < T_H$ the known expansion in integer powers of $H/T_H$ for the isotropic case may be obtained directly if $\mu \to 0$ is taken in each term of the series (5.2.24). Yet, the limit $\mu \to 0$ at $H > T_H$ is not so simple. The poles (5.2.22) converge forming a cut along the negative part of the imaginary axis and one should calculate the integral over the contour enveloping the cut.

In the Toulouse limit $\mu = \pi/2$, $T_H = 2T_K$ and

$$\chi_i = \frac{T_H}{H^2 + T_H^2}.$$

It is interesting to consider one more case: $\mu \simeq \pi$. Substituting $\mu = \pi$ into (5.2.20) and (5.2.21) we obtain

$$\begin{aligned} M_i(H) &= \frac{i}{4\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{d\omega}{\omega + i0} \exp(i\omega \ln H/\pi T_K) \Gamma(1 - i\omega) \Gamma\left(\frac{1}{2} + i\omega\right) \\ &= \frac{1}{2} \frac{(H/\pi T_K)}{(1 + (H/\pi T_K)^2)^{1/2}}. \end{aligned} \tag{5.2.26}$$

The point $\mu = \pi$ corresponds to $I_\perp = 2\pi - I_\parallel$, where $T_K \approx 2\epsilon_F(\pi - \mu) \to 0$. Such a situation has no physical meaning. However, the formula (5.2.26) is approximately valid when $\pi - \mu \ll 1$. When $\pi - (I_\parallel + I_\perp)/2 \ll 1$ eqns. (4.3.8) may be approximately rewritten as

$$(\pi - \mu)^2 \simeq 2\left(\pi - \frac{I_\parallel + I_\perp}{2}\right) \tan I_\perp/2, \qquad f \to 0. \tag{5.2.27}$$

From (5.2.27) one sees that for validity of the formula (5.2.26) it is necessary that $(2\pi - I_\parallel - I_\perp) \tan I_\perp/2 \ll 1$. Then

$$T_K(\mu \to \pi) = \frac{2\epsilon_F}{\pi^2} [(2\pi - I_\parallel - I_\perp) \tan I_\perp/2]^{1/2}.$$

*Appendix to §5.1.3. The Wiener–Hopf method*

Let us consider the equation

$$\left.\begin{aligned} \psi_-(x) &= \int_0^\infty V(x - x')\psi_+(x')dx' + g(x) \qquad (x < 0); \\ \psi_+(x) &= \int_0^\infty V(x - x')\psi_+(x')dx' + g(x) \qquad (x > 0). \end{aligned}\right\} \tag{1}$$

The functions $g(x)$, $V(x)$ are assumed to be integrable and regular on the real axis.

Let us perform the Fourier-transformation of eqn. (1):

$$\psi_+(\omega) + \psi_-(\omega) = V(\omega)\psi_+(\omega) + g(\omega). \tag{2}$$

Here the functions with argument $\omega$ are the Fourier-transforms, for example,

$$g(\omega) = \int_{-\infty}^{+\infty} \exp(i\omega x) g(x)\, dx.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

In the following we shall use the fact that any function $f(\omega)$ may be represented as the sum of two summands $[f]_+(\omega)$ and $[f]_-(\omega)$ which are analytical in the upper and lower half-planes, respectively:

$$\left.\begin{aligned} f(\omega) &= [f]_+(\omega)+[f]_-(\omega), \\ [f]_+(\omega) &= \frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{f(\omega')}{\omega-\omega'+i0}\,dw', \\ [f]_-(\omega) &= -\frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{f(\omega')}{\omega-\omega'-i0}\,dw'. \end{aligned}\right\} \tag{3}$$

In particular, using formulae (3) with $f(\omega)=\ln(1-V(\omega))$ one may represent the function $1-V(\omega)$ as the product $G^{(+)}(\omega)G^{(-)}(\omega)$, where $G^{(+)}(\omega)$ is analytical in the upper (lower) half-plane.

Rewrite eqn. (2) as

$$\psi_+(\omega)G^{(+)}(\omega)+\psi_-(\omega)/G^{(-)}(\omega)=g^{(\omega)}/G^{(-)}(\omega)=[g/G^{(-)}]_+(\omega)+[g/G^{(-)}]_-(\omega) \tag{4}$$

and

$$\psi_+G^{(+)}-[g/G^{(-)}]_+=-\psi_-/G^{(-)}+[g/G^{(-)}]_-. \tag{5}$$

The left-hand side of eqn. (5) is analytical at $\operatorname{Im}\omega\geqslant 0$, the right-hand side is analytical at $\operatorname{Im}\omega\leqslant 0$. Both these have a common region of analyticity ($\operatorname{Im}\omega=0$) where they are equal to each other. Therefore, one may say that the right-hand side is the analytical continuation of the function $F=\psi_+G^{(+)}-[g/G^{(-)}]_+$ to the lower half-plane.

So defined, the function $F(\omega)$ is analytical in the whole complex plane and is an entire function:

$$F(\omega)=P(\omega).$$

The above speculation is not sufficient to find the function $F(\omega)$. It is necessary to remember its behaviour at large $\omega$. From the integrability of $\psi(x)$ at $x\to 0$ it follows that $\psi_+(\omega\to\infty)\to 0$. Analogously, we have

$$[g/G^{(-)}]_+(\omega)\simeq\frac{i}{2\pi\omega}\int_{-\infty}^{+\infty}g(\omega')\,d\omega'=\frac{i}{\omega}g(x=0)\to 0, \qquad \omega\to\infty.$$

So, $F(\omega)$ is an entire function and tends to zero at large $\omega$. Therefore, $F(\omega)=0$ at all $\omega$.

The solution of eqn. (2) is

$$\left.\begin{aligned} \psi_+(\omega) &= \frac{i}{2\pi G^{(+)}(\omega)}\int_{-\infty}^{+\infty}\frac{g(\omega')}{G^{(-)}(\omega')}\,\frac{d\omega'}{\omega-\omega'+i0}, \\ \psi_-(\omega) &= -\frac{i}{2\pi}G^{(-)}(\omega)\int_{-\infty}^{+\infty}\frac{g(\omega')}{G^{(-)}(\omega')}\,\frac{d\omega'}{\omega-\omega'-i0}. \end{aligned}\right\} \tag{6}$$

For a review of the Wiener–Hopf method see, for example, Krein (1962).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

## § 6. Thermodynamics of the exchange models

In this section we apply the Bethe-Ansatz equations (4.2.A)–(4.2.C) and (4.3.A)–(4.3.C) to study the thermodynamics of s–d exchange models (4.2.1) and (4.3.1). At finite temperatures we cannot derive such closed expressions for physical quantities as has been done for $T=0$ (see § 5). The thermodynamical properties are described by a set of non-linear integral equations. They can hardly be solved exactly. However, it is possible to study the analytical properties of their solutions and understand the character of the temperature dependence of physical quantities in the most interesting cases. As was the case above, all the mathematical intricacies will be exposed in detail for the example of the isotropic s–d exchange model (§ 6.1). They are then applied to other models in less detail. The proper mathematical approach to the thermodynamics of systems described by the Bethe-Ansatz equations was developed in the pioneering paper by Yang and Yang (1969) and applied to the Haisenberg model by Takahashi (1971 a, 1973), Gaudin (1971 a), Johnson and McCoy (1972) and Takahashi and Suzuki (1972). Many of the technical tricks used below are borrowed from the above papers.

### 6.1. *Thermodynamics of the s–d exchange model*

#### 6.1.1. *Solutions with complex rapidities*

If $T\neq 0$ one should consider all possible solutions of eqns. (4.2.B):

$$\left(\frac{\lambda_\alpha+i/2}{\lambda_\alpha-i/2}\right)^N\left(\frac{\lambda_\alpha+1/g+iS}{\lambda_\alpha+1/g-iS}\right)=-\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta+i}{\lambda_\alpha-\lambda_\beta-i}.$$

Obviously, apart from real solutions eqns. (4.2.B) admit some complex ones. Bethe (1931) suggested the so-called '*string*' *hypothesis*, according to which the solutions of (4.2.B), as well as other closely-related equations which arise in other models, consist, in the thermodynamic limit, solely of strings, i.e. families

$$\lambda_\alpha^{(n,j)}=\lambda_\alpha^n+i\left(\frac{n+1}{2}-j\right)+O(\exp(-\delta N);\qquad j=1,\ldots,n. \tag{6.1.1}$$

which are depicted in fig. 6.1. In (6.1.1) $\lambda_\alpha^n$ is real and $n$ is order of a string. Here $\delta N$ is a number of excitations (Destri and Lowenstein 1982). The proof will be given in Appendix to 6.2.1 where we also discuss what the thermodynamic limit means.

The string's classification is defined by the right-hand side of eqn. (4.2.B). Therefore, the classification for the s–d exchange model coincides with that for the isotropic 1/2-spin Haisenberg ring, characterizing by the same symmetry group $SU(2)$. It is easy to derive the Bethe-Ansatz equations for the real parts $\lambda_\alpha^n$. Let us consider a state with $M_n$ strings of $n$th order ($n=1,\ldots$). Substituting (6.1.1) into eqns. (4.2.B) and taking the product of eqns. (4.2.B) for $j$th components of a string, we get the following equations for the real parts $\lambda_\alpha^n$:

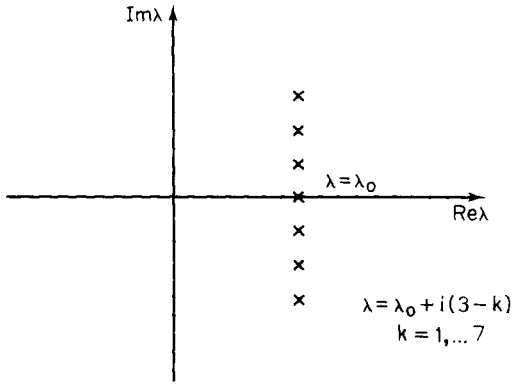
$$[e_n(\lambda_\alpha^n)]^N e_{n,2S}(\lambda_\alpha^n+1/g)=\prod_{m=1}^{\infty}\prod_{\beta=1}^{M_m}E_{nm}(\lambda_\alpha^n-\lambda_\beta^m), \tag{6.1.2}$$

where

$$e_n(\lambda)=\frac{\lambda+in/2}{\lambda-in/2} \tag{6.1.3}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 6.1




An $n$-string solution in the complex rapidity plane.

$$e_{n,2S}(\lambda)=\prod_{j=1}^{n}\frac{\lambda+i\left(\dfrac{n+1}{2}-j+S\right)}{\lambda+i\left(\dfrac{n+1}{2}-j-S\right)} \tag{6.1.4}$$

and

$$E_{nm}(\lambda)=e_{|n-m|}(\lambda)e^2_{|n-m|+2}(\lambda)\ldots e^2_{n+m-2}(\lambda)e_{n+m}(\lambda). \tag{6.1.5}$$

Each string contains $nM_n$ spins up, the whole spin being equal to

$$S^z=N/2-\sum_{n=1}^{\infty}nM_n. \tag{6.1.6}$$

Equation (4.2.A) rewritten through real parts of $\lambda^n_\alpha$ is

$$\exp(ik_jL)=\exp(iIS/2)\prod_{n=1}^{\infty}\prod_{\alpha=1}^{M_n}e_n(\lambda^n_\alpha). \tag{6.1.7}$$

Taking the logarithm of (6.1.2) and (6.1.7) we obtain

$$k_jL=2\pi N_j-IS/2-\sum_{n=1}^{\infty}\sum_{\alpha=1}^{M_n}(\pi+p_n(\lambda^n_\alpha)), \tag{6.1.8 a}$$

$$Np_n(\lambda^n_\alpha)+\delta_{n,2S}(\lambda^n_\alpha)=2\pi J^n_\alpha+\sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m}\Xi_{nm}(\lambda^n_\alpha-\lambda^m_\beta), \tag{6.1.8 b}$$

where $2N_j$, $2J^n_\alpha$ are integers and functions $p_n(\lambda), \delta_{n,2S}(\lambda), \Xi_{nm}$ characterize a two-particle scattering. $p_n(\lambda)$ is the momentum of a string with spin $n/2$, which provides scattering on the impurity and other strings with phase shifts $\delta_{n,2S}(\lambda)$ and $\Xi_{nm}(\lambda^n_\alpha-\lambda^m_\beta)$, respectively. It is convenient to define the functions $p_n$, $\delta_{n,2S}$ and $\Xi_{nm}$ as

$$\left.\begin{aligned}
p_n(\lambda)&=i\ln e_n(\lambda)=2\tan^{-1}2\lambda/n \qquad (-\pi<p_n\leqslant\pi)\\
\delta_{n,2S}(\lambda)&=\sum_{j=1}^{\min(n,2S)}p_{n+1+2S-2j}(\lambda+1/g);\\
\Xi_{nm}(\lambda)&=p_{|n-m|}(\lambda)+2\sum_{k=1}^{\min(n,m)-1}p_{|n-m|+2k}(\lambda)+p_{n+m}(\lambda).
\end{aligned}\right\} \tag{6.1.9}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Equation (6.1.6) and (6.1.8) constrain the admittable set of integers

$$|J_\alpha^n| \leqslant \frac{1}{2}(N+M_n+\min(n,2S)-1)+n-\sum_{m=1}^{\infty}\min(n,m)M_m \equiv D_n; \quad \sum_{n=1}^{\infty} nM_n \leqslant N/2. \tag{6.1.10}$$

It may be proven that for any set of $J_\alpha^n$s satisfying (6.1.10), no two of which with the same $n$ are identical, there is a unique set of real $\lambda_\alpha^n$s satisfying (6.1.8 *b*), with no two $\lambda_\alpha^n$s with the same $n$ being identical.

Hence, the numbers $J_\alpha^n$ as well as $N_j$ are precisely quantum numbers of the system. Therefore, the number of possible states is determined by the number of possible sets of integers $\{J_\alpha^n\}$ satisfying (6.1.10). Bethe showed (1931) that at $S=0$ this number is exactly $2^N$, as it must be (see also Takahashi 1971 a) and Takhtajan and Faddeev (1981 a, b). We give below another proof of this statement calculating the entropy of our system for high temperatures (see § 6.1.6). It should be equal to $\mathscr{S}=2N\ln 2+\ln(2S+1)$†.

### 6.1.2. *Thermodynamic limit*

Thus any state of the system is characterized by $M_n$ sets of integers $J_\alpha^n$ filling in a lattice with omitted values $\tilde{J}_\alpha^n$ ('holes'). The notion of a 'hole', introduced by us in § 5.1.1 while studying the ground state with the fixed magnetic moment, can easily be generalized to arbitrary state.

Following Yang and Yang (1969), consider the function

$$h^n(\lambda)=\frac{1}{2\pi}\left[Np_n(\lambda)+\delta_{n,2S}(\lambda)-\sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m}\Xi_{nm}(\lambda-\lambda_\beta^m)\right]. \tag{6.1.11}$$

Those values of $\lambda$ where $h^n(\lambda)=J_\alpha^n \epsilon D_n$ are the rapidities of particles $\lambda_\alpha^n$. Those values of $\lambda$ where $h^n(\lambda)=\tilde{J}_\alpha^n \epsilon D_n$ are the rapidities of holes.

Thus, for a large system one may introduce a density distribution of holes as well as of particles:

$$\begin{aligned} N\rho_n(\lambda)d\lambda &= \text{number of } \lambda^n\text{s in } d\lambda, \\ N\tilde{\rho}_n(\lambda)d\lambda &= \text{number of holes of order } n \text{ in } d\lambda. \end{aligned} \tag{6.1.12}$$

This definition is a generalization of that given in § 5.1.1.

By definition, the number of particles and holes in the interval $d\lambda$ is the number of times $h^n(\lambda)$ ranges over values $J_\alpha^n$ and $\tilde{J}_\alpha^n$ in this interval. Thus

$$\frac{1}{N}\frac{dh^n(\lambda)}{d\lambda}=\rho_n(\lambda)+\tilde{\rho}_n(\lambda). \tag{6.1.13}$$

Equations (6.1.8 *a* and *b*) give

$$Lk_j=2\pi N_j-N\sum_{n=1}^{\infty}\int(p_n(\lambda)+\pi)\rho_n(\lambda)\,d\lambda, \tag{6.1.14}$$

$$\frac{2\pi h^n(\lambda)}{N}=p_n(\lambda)+\frac{1}{N}\delta_{n,2S}(\lambda)-\sum_{m=1}^{\infty}\int\Xi_{nm}(\lambda-\lambda')\rho_m(\lambda')\,d\lambda', \tag{6.1.15}$$

† The generalization of the direct combinatorial proof for arbitrary $S$ was made by Furuya and Lowenstein (1982).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where boundaries of all integrals here and through this section are equal to $\pm\infty$. Differentiation with respect to $\lambda$ gives

$$a_n(\lambda)+\frac{1}{N}a_{n,2S}(\lambda+1/g)=\tilde{\rho}_n(\lambda)+\sum_{m=1}^{\infty}\int A_{nm}(\lambda-\lambda')\rho_m(\lambda')\,d\lambda', \tag{6.1.16}$$

where

$$a_n(\lambda)=\frac{2}{\pi}\frac{n}{4\lambda^2+n^2}; \tag{6.1.17}$$

$$A_{nm}(\lambda)=\delta_{nm}\delta(\lambda)+(1-\delta_{nm})a_{|n-m|}(\lambda)+a_{n+m}(\lambda)+2\sum_{k=1}^{\min(n,m)-1}a_{|n-m|+2k}(\lambda); \tag{6.1.18}$$

$$a_{n,2S}(\lambda)=\sum_{j=1}^{\min(n,2S)}a_{n+2s+1-2j}(\lambda). \tag{6.1.19}$$

The energy of the system is

$$E=\sum_{j=1}^{N}k_j=\frac{2\pi}{L}\sum_{j=1}^{N}N_j+E^{\mathrm{sp}}, \tag{6.1.20}$$

$$\frac{1}{N}E^{\mathrm{sp}}=-\frac{N}{L}\sum_{n=1}^{\infty}\int(p_n(\lambda)+\pi)\rho_n(\lambda)\,d\lambda. \tag{6.1.21}$$

The spin is

$$\frac{1}{N}S^z=\frac{1}{2}-\sum_{n=1}^{\infty}n\int\rho_n(\lambda)\,d\lambda. \tag{6.1.22}$$

The formulae (6.1.16) and (6.1.20)–(6.1.22) describe all states of a spin subsystem in the continuous limit.

For the sake of simplicity we do not pass to the continuous limit in a charge subsystem. As has been discussed above, the charge subsystem is a gas of free spinless fermions and does not demand additional treatment.

In conclusion we cite the important relation between functions $\delta_{n,2s}$ and $A_{nm}$:

$$\frac{1}{2\pi}\frac{d\delta_{n,2S}(\lambda-1/g)}{d\lambda}=s*A_{n,2S}(\lambda). \tag{6.1.23}$$

The symbol $s*f(\lambda)$ denotes the convolution of $s(\lambda)$ and $f(\lambda)$ as follows:

$$s*f(\lambda)=\int_{-\infty}^{+\infty}(2\cosh\pi(\lambda-\lambda'))^{-1}f(\lambda')\,d\lambda'.$$

The validity of relation (6.1.23) can easily be proved by comparing Fourier-transforms of corresponding functions. For instance, we have

$$A_{nm}(\omega)=\coth\frac{|\omega|}{2}(\exp(-|(n-m)\omega|/2)-\exp(-(n+m)|\omega|/2)). \tag{6.1.24}$$

Further, we shall often use the inverse matrix $A^{-1}$. It has the following form:

$$(A^{-1})_{nm}(\lambda)=\delta_{nm}\delta(\lambda)-s(\lambda)(\delta_{n,m+1}+\delta_{n,m-1}). \tag{6.1.25}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Using eqn. (6.1.16) one may rewrite eqn. (6.1.25) as follows

$$\rho_n(\lambda)+\tilde{\rho}_n(\lambda)=s*(\tilde{\rho}_{n-1}(\lambda)+\tilde{\rho}_{n+1}(\lambda))+\delta_{n1}s(\lambda)+\frac{1}{N}\delta_{n,2S}s(\lambda+1/g) \tag{6.1.26}$$

and express the energy and the total spin through the density of holes:

$$\frac{1}{N}S^z=\lim_{n\to\infty}\int\tilde{\rho}_n(\lambda)\,d\lambda, \tag{6.1.27}$$

$$E^{\mathrm{sp}}-E^{(0)}=2N^2/L\int\tan^{-1}\exp(\pi\lambda)\tilde{\rho}_1(\lambda)\,d\lambda. \tag{6.1.28}$$

Here $E^{(0)}$ is the ground-state energy:

$$E^{(0)}=\frac{N^2}{L}\left\{\int_{-\infty}^{+\infty}\frac{A_{11}(\omega)}{2\cosh\omega/2}\frac{d\omega}{\omega+i0}+\frac{1}{N}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i0}\right.$$
$$\left.\times\exp(i\omega/g)A_{1,2S}(\omega)/2\cosh\omega/2\right\}. \tag{6.1.29}$$

Note that the energy is completely determined by the distribution of the holes in the first string ($n=1$). We have already said that in the ground state all $\rho_n=0$ at $n\neq 1$. It follows from (6.1.28) that there are no holes with $n=1$ in the ground state.

Calculating the first integral in (6.1.29) it is easy to prove that it is equal to $-\pi N^2/2L$, i.e. the free-gas energy. The second term in (6.1.29) is the impurity correction to the ground-state energy. This correction is not a universal function of a coupling constant and we do not evaluate it.

### 6.1.3. *Equilibrium distribution*

At finite temperature $T$, we should maximize the contribution to the partition function from the states described by $\rho_n$ and $\tilde{\rho}_n$. In other words, given $\rho_n$, $\tilde{\rho}_n$ is defined by (6.1.16) (or (6.1.26)). One then computes the contribution to the partition function

$$\exp\left(-\frac{E-HS^z}{T}\right)e^S, \tag{6.1.30}$$

where $E$ is given by (6.1.21) or (6.1.28) and $S$ is the entropy of the state. The equilibrium $\rho$ is then obtained by maximizing this contribution when $\rho_n$s, $\tilde{\rho}_n$s are varied subject to condition (6.1.16).

The entropy of the 'state' does not vanish since the existence of the omitted quantum numbers $\tilde{J}^n_\alpha$ allows many wavefunctions of approximately the same energy to be described by the same $\rho_n$ and $\tilde{\rho}_n$. In fact, for given $\rho_n$ and $\tilde{\rho}_n$, the number of particles and holes in $d\lambda$ is $N(\rho_n+\tilde{\rho}_n)\,d\lambda$, of which $N\rho_n\,d\lambda$ are particles and $N\tilde{\rho}_n\,d\lambda$ are holes. Thus, the number of possible choices of states in $d\lambda$ consistent with given $\rho_n$ and $\tilde{\rho}_n$ is

$$\frac{[N(\rho_n+\tilde{\rho}_n)\,d\lambda]!}{(N\rho_n\,d\lambda)!\,(N\tilde{\rho}_n\,d\lambda)!}.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Its logarithm gives the contribution to the entropy from $d\lambda^n$. Thus, the total entropy is,

$$S=N\sum_{n=1}^{\infty}\int d\lambda[(\rho_n+\tilde{\rho}_n)\ln(\rho_n+\tilde{\rho}_n)-\rho_n\ln\rho_n-\tilde{\rho}_n\ln\tilde{\rho}_n]. \tag{6.1.31}$$

In what follows one must remember that functions $\rho_n$ and $\tilde{\rho}_n$ are not independent. From eqn. (6.1.16) one obtains the relation between the variations of $\rho_n$ and $\tilde{\rho}_n$:

$$\frac{\delta\tilde{\rho}_n(\lambda)}{\delta\rho_m(\lambda')}=A_{nm}(\lambda-\lambda'). \tag{6.1.32}$$

Varying the partition function with respect to $\delta\rho_n$ and defining the fundamental functions†

$$\varepsilon_n(\lambda)=T\ln[\tilde{\rho}_n(\lambda)/\rho_n(\lambda)].$$

We obtain the following non-linear integral equations:

$$T\ln(1+\exp(\varepsilon_n/T))=A_{nm}*T\ln(1+\exp(-\varepsilon_m/T))+H_n-\frac{\epsilon_F}{\pi}(p_n+\pi). \tag{6.1.33}$$

These equations together with (6.1.16) define the equilibrium distributions $\rho_n(\lambda)$, $\tilde{\rho}_n(\lambda)$.

It may be proved that the solution of (6.1.16) and (6.1.33) indeed leads to a minimum of the free energy, i.e. a maximum of the partition function (6.1.30) (Yang and Yang 1969). The functions $\varepsilon_n(\lambda)$ are the fundamental quantities describing the thermodynamics of integrable systems. Let us return to eqn. (6.1.33). Another form of these equations appears when one inverts matrix $A$:

$$\varepsilon_n(\lambda)=Ts*\ln(1+\exp(\varepsilon_{n-1}(\lambda)/T))(1+\exp(\varepsilon_{n+1}(\lambda)/T)$$
$$-\frac{2\epsilon_F}{\pi}\tan^{-1}\exp(\pi\lambda)\delta_{n1},\qquad \lim_{n\to\infty}\frac{\varepsilon_n}{n}=H. \tag{6.1.34}$$

The free energy may be expressed through $\varepsilon_n$s only. According to (6.1.21) and (6.1.31) we have

$$\frac{1}{N}\mathscr{F}^{\mathrm{sp}}=\sum_{n=1}^{\infty}\int d\lambda\left\{\rho_n\left[H_n-\frac{\epsilon_F}{\pi}(p_n+\pi)-T\ln(1+\exp(\varepsilon_n/T))\right]\right.$$
$$\left.+\tilde{\rho}_nT\ln(1+\exp(-\varepsilon_n/T))\right\}-H\left(\frac{1}{2}+S/N\right). \tag{6.1.35}$$

Using eqn. (6.1.16) we eliminate $\tilde{\rho}_n$ and obtain

$$\frac{1}{N}\mathscr{F}^{\mathrm{sp}}=\sum_{n=1}^{\infty}\int d\lambda\left\{\rho_n(\lambda)[\ldots]-\left(a_n(\lambda)+\frac{1}{N}a_{n,2s}(\lambda+1/g)\right)\right.$$
$$\left.\times T\ln(1+\exp(-\varepsilon_n(\lambda)/T)\right\}-H\left(\frac{1}{2}+S/N\right). \tag{6.1.36}$$

† In § 5.1.4 we defined the functions $\varepsilon\equiv\varepsilon_1$ for $T=0$. We shall show below that for $T\to0$ eqns. (6.1.33) and (5.1.52) do coincide.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The term in square brackets is precisely the left-hand side of eqn. (6.1.33). Therefore, we have

$$\frac{1}{N}\mathscr{F}^{\mathrm{sp}} = -T\sum_{n=1}^{\infty}\int d\lambda\left(a_n(\lambda)+\frac{1}{N}a_{n,2S}(\lambda+1/g)\right)$$
$$\times\ln(1+\exp(-\varepsilon_n(\lambda)/T)-H\left(\frac{1}{2}+S/N\right). \qquad (6.1.37)$$

Another useful expression for the free energy may be obtained from (6.1.35) removing $\rho_n$s. The term with $\tilde{\rho}_n$ vanishes because of condition (6.1.34). Using the relation (6.1.23) we obtain:

$$\frac{1}{N}\mathscr{F}^{\mathrm{sp}} = -T\int d\lambda s(\lambda)\ln(1+\exp(\varepsilon_1(\lambda)/T)$$
$$-\frac{T}{N}\int d\lambda s(\lambda+1/g)\ln(1+\exp(\varepsilon_{2S}(\lambda)/T)). \qquad (6.1.38)$$

As has been discussed above, the spectrum of the *charge* subsystem is unbounded from below. In § 5.1.1 we considered this problem and showed that one should consider only $k \geqslant -\epsilon_{\mathrm{F}}/2$. Therefore, the chemical potential of the charge subsystem computed from $\epsilon_{\mathrm{F}}$ is equal to $\epsilon_{\mathrm{F}}/2$. According to this we have

$$\frac{1}{N}\mathscr{F}^{\mathrm{ch}} = -\frac{T}{2\epsilon_{\mathrm{F}}}\int_{-\epsilon_{\mathrm{F}}}^{\infty}\ln(1+\exp(-k/T))\,dk+\frac{\epsilon_{\mathrm{F}}}{4} = -\frac{\pi^2}{12}\frac{T^2}{\epsilon_{\mathrm{F}}}. \qquad (6.1.39)$$

Hence the heat capacity of the charge subsystem is just a half of that free Fermi gas.

### 6.1.4. *Non-interacting electron gas and the Bethe-Ansatz technique*

A correct description of the behaviour of an impurity requires a very unusual way of representing the gas of non-interacting particles. Instead of studying free fermions with spin 'up' and 'down', we deal with the different types of fermions. One type transports charge but not spin, while the other does the opposite, i.e. does not change the local distribution of charges. Moreover, excitations in the spin subsystem are linear combinations of different strings.

The fact that the non-linear equations (6.1.34), whose solution is analytically impossible, together with the first terms in (6.1.18) describe free particles is remarkable and requires proof (Filyov *et al.* 1981).

In eqns. (6.1.8) we drop the term with $1/N$ or simply put $S=0$:

$$a_n(\lambda) = \tilde{\rho}_n(\lambda) + A_{nm} * \rho_m(\lambda). \qquad (6.1.40)$$

Comparing (6.1.42) with (6.1.34) and taking into account that $a_n = p_n'/2\pi$, we find that in the absence of an impurity the $\rho_n$ and $\tilde{\rho}_n$ are linked by simple formulae characteristic of a free system:

$$\rho_n(\lambda) = -\frac{1}{2\epsilon_{\mathrm{F}}}\frac{\partial\varepsilon_n(\lambda)}{\partial\lambda}n(\varepsilon_n(\lambda)), \qquad (6.1.41)$$

$$\tilde{\rho}_n(\lambda) = -\frac{1}{2\epsilon_{\mathrm{F}}}\frac{\partial\varepsilon_n(\lambda)}{\partial\lambda}(1-n(\varepsilon_n(\lambda))), \qquad (6.1.42)$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where

$$n(\varepsilon)=(1+\exp(\varepsilon/T))^{-1} \tag{6.1.43}$$

is the Fermi distribution function.

This means, for one thing, that the average number of strings at a given temperature $T$ is

$$\frac{\langle M_n\rangle}{N}=\frac{T}{2\epsilon_F}\ln\left[\frac{1+\exp(-\varepsilon_n(-\infty)/T)}{1+\exp(-\varepsilon_n(+\infty)/T)}\right]. \tag{6.1.44}$$

Formula (6.1.43) also implies that the $\varepsilon_n$ are monotonically increasing functions since, by their very meaning, $\rho_n$, $\tilde{\rho}_n \geqslant 0$.

Let us take the free energy in the absence of an impurity:

$$\frac{1}{N}\mathscr{F}_{\mathrm{h}}^{\mathrm{sp}}=T\sum_{n=1}^{\infty}\int d\lambda a_n(\lambda)\ln(1-n(\varepsilon_n(\lambda)))-H/2. \tag{6.1.45}$$

Differentiating eqn. (6.1.34) with respect to $\lambda$ and combining the result with (6.1.45), we obtain

$$\frac{1}{N}\mathscr{F}_{\mathrm{h}}^{\mathrm{sp}}=-\frac{T}{2\epsilon_F}\sum_{n=1}^{\infty}\int d\lambda\ln(1-n(\varepsilon_n))\left[\frac{d\varepsilon_n}{d\lambda}-\Xi''_{nm}*T\ln(1-n(\varepsilon_m))\right]-H/2. \tag{6.1.46}$$

The second term inside the brackets yields zero because $\Xi_{nm}$ is an odd continuous function, hence

$$\frac{1}{N}\mathscr{F}_{\mathrm{h}}^{\mathrm{sp}}=\frac{T}{2\epsilon_F}\sum_{n=1}^{\infty}\int_{\min\varepsilon_n}^{\max\varepsilon_n}d\varepsilon\ln(1-n(\varepsilon))-\frac{H}{2}. \tag{6.1.47}$$

The easiest way to establish the limits of (6.1.47) is to employ eqn. (6.1.34). Indeed, sending $\lambda$ to $-\infty$, we have a self-consistent system of equations in $\bar{\varepsilon}_n\equiv\max\varepsilon_n(\lambda)$:

$$\bar{\varepsilon}_n=-\frac{T}{2}\ln[n(\bar{\varepsilon}_{n+1})n(\bar{\varepsilon}_{n-1})];\quad \lim_{n\to\infty}\frac{\bar{\varepsilon}_n}{n}=H,\qquad \bar{\varepsilon}_0=-\infty\qquad n=1,2,\ldots. \tag{6.1.48}$$

It is easy to find the solution to these equations (Takahashi 1971 *a*):

$$\bar{\varepsilon}_n=T\ln(\Phi_n^2-1) \tag{6.1.49}$$

with

$$\Phi_n=\sinh(\alpha_n+\beta)/\sinh\alpha.$$

To find $\alpha$ and $\beta$ one must use the boundary conditions for (6.1.48). As a result $\alpha=\beta=H/2T$ and

$$\Phi_n=\frac{\sinh(H/2T)(n+1)}{\sinh H/2T}. \tag{6.1.50}$$

In the other limit $\lambda\to+\infty$ we have $\varepsilon_1\to-\epsilon_F\ll-T$. Therefore, if we assume that $n(\varepsilon_1)=1$, we have an equation for $\tilde{\varepsilon}_n\equiv\min\varepsilon_n(\lambda)$:

$$\tilde{\varepsilon}_n=-\frac{T}{2}\ln[n(\tilde{\varepsilon}_{n+1})n(\tilde{\varepsilon}_{n-1})];\qquad n=2,3,\ldots,\qquad \lim_{n\to\infty}\tilde{\varepsilon}_n/n=H. \tag{6.1.51}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Comparing (6.1.48) with (6.1.51), we find that

$$\bar{\varepsilon}_n = \tilde{\varepsilon}_{n+1} = T \ln\left[\left(\frac{\sinh(H/2T)(n+1)}{\sinh H/2T}\right)^2 - 1\right] \qquad n=1,2,\ldots. \tag{6.1.52}$$

The behaviour of the functions $\varepsilon_n(\lambda)$ derived from the numerical calculation (Melnicov 1982 a) is depicted in fig. 6.2.

Using eqn. (6.1.52) one can rewrite the expression for the free energy (6.1.47) as

$$\frac{1}{N}\mathscr{F}_{\mathrm{h}}^{\mathrm{sp}} = -\frac{T}{2\epsilon_{\mathrm{F}}}\int_{-\epsilon_{\mathrm{F}}}^{\infty} \ln(1+\exp(-\varepsilon/T)d\varepsilon = -\frac{\epsilon_{\mathrm{F}}}{4} - \frac{\pi^2 T^2}{12\epsilon_{\mathrm{F}}}. \tag{6.1.53}$$

Here the magnetic field is supposed to be equal to zero. It is convenient to calculate the magnetic part of the energy by calculating the magnetization. According to (6.1.27), (6.1.43) and (6.1.52)

$$S^z = \lim_{n\to\infty} \frac{T}{2\epsilon_{\mathrm{F}}} \ln\left[\frac{1+\exp(\varepsilon_n(-\infty)/T)}{1+\exp(\varepsilon_n(+\infty)/T)}\right] = H/4\epsilon_{\mathrm{F}} \tag{6.1.54}$$

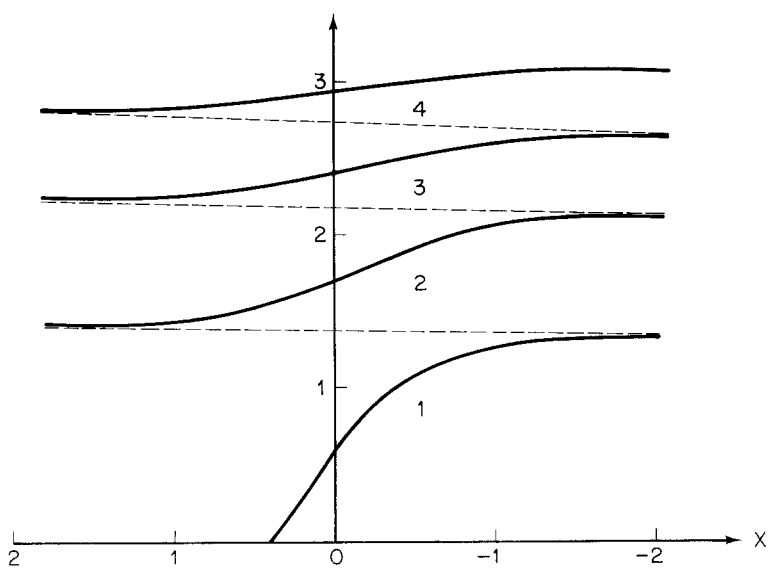
and we obtain, for the spin part of the host free energy,

$$\frac{1}{N}\mathscr{F}_{\mathrm{h}}^{\mathrm{sp}} = -\frac{\epsilon_{\mathrm{F}}}{4} - \frac{\pi^2 T^2}{12\epsilon_{\mathrm{F}}} - \frac{H^2}{8\epsilon_{\mathrm{F}}}. \tag{6.1.55}$$

Here is an important point. The magnetic susceptibilities of the host spin subsystem, $\chi^{\mathrm{sp}}$, and the electron gas, $\chi_{\mathrm{h}}$, coincide, while the heat capacities differ by a factor of two:

$$\frac{C^{\mathrm{sp}}}{T\chi^{\mathrm{sp}}} = \frac{1}{2}\frac{C_{\mathrm{h}}}{T\chi_{\mathrm{h}}} = 2\pi^2/3. \tag{6.1.56}$$

Fig. 6.2




Plots of the solutions of the universal equations (6.1.60). $\ln(1+\exp(\varphi_n(\lambda)))$ versus $\lambda$ at $H=0$ describes the thermodynamics of the s–d exchange model (after Melnikov 1982 a).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

We discussed this connection earlier in § 5.1.4. This result will be used below.

6.1.5. *Universality*

According to the general conditions for renormalizability, the impurity parts of thermodynamic functions must be universal functions of $T/T_K$ and $H/T_K$ or functions of the invariant charge $z(T/T_K)$ and $H/T$ at $I\to 0$, $\epsilon_F\to\infty$, $T_K=\text{const}$.

Equations (6.1.34) are the simplest for eliminating non-universal terms. Let us substitute everywhere $\lambda+1/\pi\ln\pi T/2\epsilon_F$ in place of $\lambda$

$$\varepsilon_n'(\lambda)=\frac{1}{T}\varepsilon_n\left(\lambda+\frac{1}{\pi}\ln\frac{\pi T}{2\epsilon_F}\right). \tag{6.1.57}$$

In the process the absolute term of (6.1.34) becomes

$$\frac{2\epsilon_F}{\pi}\tan^{-1}\left(\frac{\pi T}{2\epsilon_F}\exp(\pi\lambda)\right)$$

and the free energy is

$$\frac{1}{N}\mathscr{F}_h^{sp}=-T\int_{-\infty}^{+\infty}s\left(\lambda+\frac{1}{\pi}\ln\frac{\pi T}{2\epsilon_F}\right)\ln(1+\exp(\varepsilon_i'(\lambda)))\,d\lambda, \tag{6.1.58 a}$$

$$\mathscr{F}_i=-T\int_{-\infty}^{+\infty}s\left(\lambda+\frac{1}{\pi}\ln\frac{T}{T_K}\right)\ln(1+\exp(\varepsilon_{2S}'(\lambda)))\,d\lambda, \tag{6.1.58 b}$$

$$T_K=\frac{2\epsilon_F}{\pi}\exp\left(\frac{-\pi}{g}\right). \tag{6.1.59}$$

At $T\ll\epsilon_F$ the main contribution to the integral in (6.1.58 *b*) is provided by the region

$$|\lambda|\sim+1/\pi\ln T/T_K\ll 1/\pi\ln\epsilon_F/T.$$

Therefore, for the term $2\epsilon_F/\pi\tan^{-1}(\pi T/2\epsilon_F\exp(\pi\lambda))$ in eqn. (6.1.34) we must substitute $T\exp(\pi\lambda)$. But this can only be done if we wish to calculate the impurity part, $\mathscr{F}_i$. For the function $\mathscr{F}_h^{sp}$ the important region is only $|\lambda|\sim 1/\pi\ln\epsilon_F/T$. Performing such an approximation in (6.1.58 *a*) we obtain, instead of (6.1.54) for $\mathscr{F}_h^{sp}$, a complete series in powers $(H/\epsilon_F)^2$ and $(T/\epsilon_F)^2$. However, the first term in this series are just the same as in (6.1.55).

The dimensionless functions

$$\varphi_n(\lambda)=\varepsilon_n'(\lambda)/\epsilon_F=\infty$$

depend on $H/T$ only as a parameter and satisfy the universal set of equations

$$\varphi_n(\lambda)=-\delta_{n1}\exp(\pi\lambda)+s*\ln(1+\exp(\varphi_{n+1}(\lambda)))$$
$$\times(1+\exp\varphi_{n-1}(\lambda)));\quad \lim_{n\to\infty}\varphi_n/n=H/T. \tag{6.1.60}$$

Here $\mathscr{F}_i$ is a universal function of $H/T$ and $T/T_K$.

$$\mathscr{F}_i=-\frac{T}{2\pi}\int_{-\infty}^{+\infty}d\omega\exp\left(-\frac{i\omega}{\pi}\ln\frac{T}{T_K}\right)\frac{C_{2S}(\omega,H/T)}{2\cosh\omega/2}, \tag{6.1.61}$$

where

$$C_{2S}(\omega,H/T)=\int_{-\infty}^{+\infty}\exp(-i\omega\lambda)\ln(1+\exp(\varphi_{2S}(\lambda)))\,d\lambda. \tag{6.1.62}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Equations (6.1.60)–(6.1.62) determine the thermodynamics of an impurity in the entire region of universality. These equations were derived for $S=1/2$ by Andrei and Lowenstein (1981) and Filyov *et al.* (1981) and for an arbitrary $S$ by Fateev and Wiegmann (1981 b). They were numerically solved by Melnicov (1982 a), Desgrange and Schotte (1982) and Rajan *et al.* (1982). The plot of $\ln(1+\exp(\varphi_n))$ at $H=0$ is depicted in fig. 6.2. (Melnicov 1982 a). The temperature dependence of the impurity magnetic susceptibility, entropy and heat capacity are represented in fig. 6.3.

6.1.6. *The limits of strong and weak coupling*

Let us send $T/T_K$ to $\infty$ in eqn. (6.1.58 *b*). Since $\ln(1+\exp(\varepsilon'_{2s}))$ is bounded, we have

$$\mathscr{F}_i \to -\frac{T}{2}\ln\left(1+\exp\left(\frac{\bar{\varepsilon}_{2S}}{T}\right)\right)$$

and according to (6.1.52), we have

$$\mathscr{F}_i(T \gg T_K) = -T\ln\left[\frac{\sinh(H/2T)(2S+1)}{\sinh H/2T}\right]. \tag{6.1.63}$$

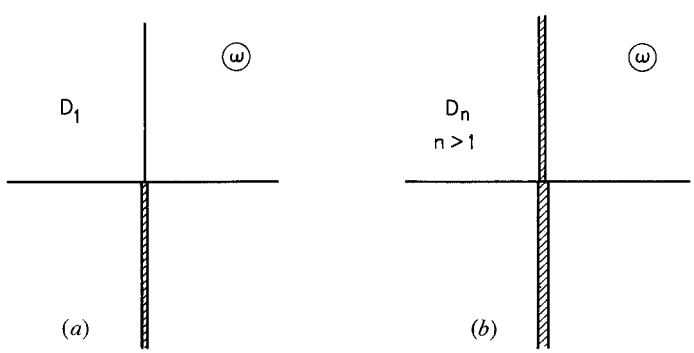
At high temperatures the interaction of an impurity with the conduction electrons vanishes, as expected. Therefore, (6.1.63) describes the behaviour of a free magnetic moment $S$, and we are dealing with the *weak-coupling limit*. Note that the high temperature limit of the host entropy is proved to be

$$S^{ch} = N\ln 2 \quad \text{and} \quad S^{sp}(T\to\infty) = \ln(1+\exp(\bar{\varepsilon}_1/T)) = N\ln 2.$$

This shows a completeness of the states determined by eqn. (6.1.8). Now let us consider the case of *strong coupling*, i.e. $T/T_K \to 0$. According to (6.1.52), we have

$$\mathscr{F}_i(T \ll T_K) = -T\ln\left[\frac{\sinh HS/T}{\sinh H/2T}\right]. \tag{6.1.64}$$

Fig. 6.3




The singularities of $D_{2s}(\omega)$ defined by eqn. (6.1.73) in the complex plane $\omega$ for (*a*) $S=1/2$ and (*b*) $S>1/2$. $D_n(\omega)$ at $n>1$ has a cut in the lower and upper half-planes with dual discontinuities at this cut. $D_1(\omega)$ is analytic everywhere in the upper half-plane except at $\omega=\infty$, and has a cut in lower half-plane.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

We can therefore conclude that at $T=0$ the impurity ground state is $2S$-fold degenerate. The impurity entropy and the magnetic moment are $\ln 2S$ and $S-1/2$, according to (6.1.64) (Fateev and Wiegmann (1981 b). The conduction electrons cannot compensate for the impurity spin and decrease it by 1/2. On the basis of quantitative arguments, Mattis arrived at this result as long ago as 1967.

In the following we shall show that when $S$ is not 1/2, the strong-coupling limit is approached logarithmically and the coefficients of inverse powers of $\ln[\max(H, T)/T_K]$ can be found by a perturbation-theory technique. But if $S=1/2$ at $T \ll T_K$ the impurity part of the free energy can be expanded in a power-series in $T/T_K$, $H/T_K$, as noted before. It has been proved for $T=0$ in § 5. Now we show it for another limit $T \gg H$ (Filyov *et al.* 1981). It suffices to prove that $C_1(\omega)$ is analytic in the upper half-plane. Indeed, eqns. (6.1.60) imply that $\varphi_1 \to -\exp(\pi\lambda)$ as $\lambda \to +\infty$, and the integral

$$C_1(\omega) = \int_{-\infty}^{+\infty} \exp(-i\omega\lambda) \ln(1+\exp(\varphi_1(\lambda)))\, d\lambda \tag{6.1.65}$$

is finite at $\operatorname{Im}\omega > 0$.

Then, at $T \ll T_K$ we can bend the integration contour in (6.1.61) into the upper half-plane and determine the integral via the sum of residues of $(\cosh \omega/2)^{-1}$:

$$\mathscr{F}_i^{(S-1/2)} = -T \sum_{n=0}^{\infty} (-1)^n C_1(i\pi(n+1/2), H/T)(T/T_K)^{2n+1}. \tag{6.1.66}$$

Knowing the behaviour of $\varphi_1(\lambda)$ at $\lambda \to +\infty$ one can derive the asymptotics of $C_1(i\pi(n+1/2))$ at large $n \gg 1$. Indeed, substituting $\varphi_1(\lambda) = -\exp(\pi\lambda)$ into (6.1.65) we find

$$C_1(i\pi(n+1/2)) \to n!. \tag{6.1.67}$$

The expansion (6.1.66) is an asymptotic one in contrast to the analogous expansion for the impurity magnetic moment at $T=0$ (5.1.37).

### 6.1.7. *The Fermi-liquid picture*

To determine the expansion coefficients in (6.1.66), we must know the $\varphi_1$ versus $\lambda$ dependence over the entire range for $\lambda$. Nevertheless, the heat capacity at $T \to 0$ can be determined by simple reasoning (Filyov *et al.* (1981). Note that the formulae for the free energy of the spin subsystem (6.1.58 *a*) and of an impurity with spin $S=1/2$ (6.1.58 *b*) are very similar. In the strong coupling limit $g \to \infty$ they coincide completely, hence

$$\frac{C_i}{C^{sp}} = \frac{2\epsilon_F}{\pi T_K}. \tag{6.1.68}$$

From the same reasoning we have already derived the expression for the magnetic susceptibility (5.1.23). These formulae, together with (6.1.56), yield

$$\frac{C_i}{T\chi_i} = \frac{C^{sp}}{T\chi^{sp}} = \frac{1}{2}\frac{C_h}{T\chi_h} = \frac{2\pi^2}{3} \tag{6.1.69}$$

and

$$C_i = \frac{\pi}{3}\frac{T}{T_K}, \tag{6.1.70}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\chi_i = (2\pi T_K)^{-1}, \tag{6.1.71}$$

$$C_1(i\pi/2, H/T) = \pi/6 + \frac{1}{4\pi}(H/T)^2. \tag{6.1.72}$$

It goes without saying that this method can be used only to find the first term in expansion (6.1.66). The point is that the temperature dependence in (6.1.58 *a*, *b*) lies not only in $s(\lambda)$ but in $\varepsilon_1'(\lambda)$ as well. Therefore, the formula for the free energy of an impurity (6.1.58 *b*) contains integral powers of $T/\epsilon_F$ as well as integral powers of $T/T_K$. But since $\varepsilon_1' = \varphi_1 + O(T^2/\epsilon_F^2)$, terms with $T/\epsilon_F$ appear only in the fourth- and higher-order terms.

### 6.1.8. *Thermodynamics of the impurity*

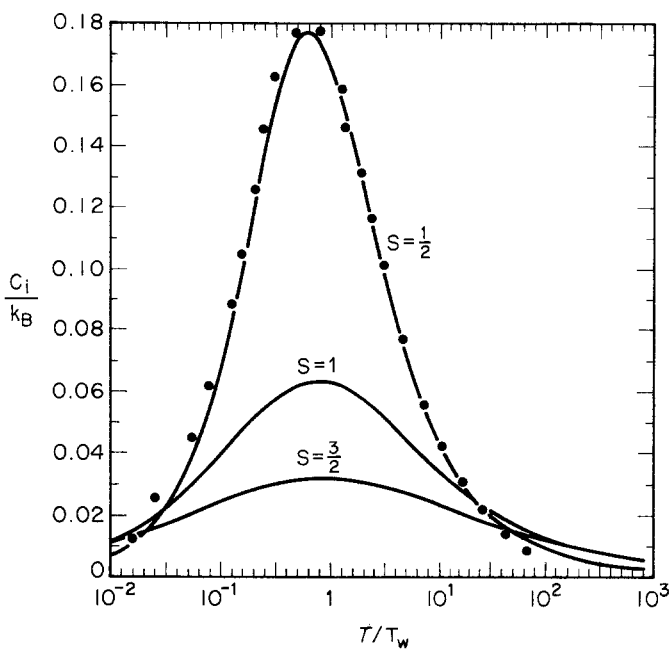
For further studies we shall list the analytic properties of $C_{2S}(\omega, H/T)$. These will be partly proved below. We start with the asymptotics as $\lambda \to \pm\infty$:

$$C_n(\omega) = 2i\frac{\ln \Phi_n}{\omega + i0} - 2i\frac{\ln \Phi_{n+1}}{\omega - i0} + D_n(\omega), \tag{6.1.73}$$

where $\Phi_n$ is defined in (6.1.50), and $D_n(\omega)$ is finite at $\omega = 0$ and has the following properties:

(i) $D_n(\omega)$ has a cut in the lower half-plane and, for $n > 1$, also in the upper half-plane. These cuts start from $\omega = 0$ and are supposed to go along the imaginary axis (fig. 6.3).

Fig. 6.4.




The specific heat $C/k_B$ versus $\log_{10} T/T_K$ plot for impurity spin $S = 1/2, 1, 3/2$. The points are the renormalization group calculation results by Oliveira and Wilkins (1981) (see §3.1.1) (after Rajan *et al.* 1982, Melnicov 1982 a, Desgranges and Schotte 1982). The figure is taken from Rajan *et al.* (1982).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

(ii) The discontinuities at these cuts are dual:

$$\operatorname{Disc} D_{n+1}(i|\omega|) = \operatorname{Disc} D_n(-i|\omega|). \tag{6.1.74}$$

(iii) $D_1(\omega)$ is analytic everywhere in the upper half-plane except at $\omega = \infty$, a point where the function has an essential singularity at $T \gg H$.

(iv)
$$\operatorname{Disc} D_n(-i|\omega|) = B_n(|\omega|, T/H)\left(\frac{|\omega|}{2\pi}\right)^{-|\omega|/2\pi}, \tag{6.1.75}$$

where $B_n(\omega)$ is analytic everywhere except at the cuts and seems to have zeros in $\omega = -i\pi(2k+1)$ $(k = 0, 1 \ldots)$.

At arbitrary $T/H$ the functions $C_n(\omega)$ cannot be expressed explicitly. However, at $T=0$ eqns. (6.1.60) become linear and the functions $\varepsilon_n = \lim_{T\to 0} T\varphi_n$ will be found analytically in §6.1.9 to illustrate the above properties. Comparing (6.1.61) with (5.1.33) we shall show in §6.1.9 that

$$\lim_{T/H\to 0}\left[C_n\left(2\pi\omega, \frac{H}{T}\right)\exp\left(2i\omega \ln\frac{H}{T}\right)\frac{T}{H}\right]$$
$$= \frac{\pi^{1/2}}{(i\omega+0)^2}\,\frac{f_+^{2S}(\omega) f_-^{2S-1}(\omega)}{\Gamma(1/2+i\omega)}\exp\left(-i\omega\ln\frac{e}{2\pi}\right), \tag{6.1.76}$$

where

$$f_\mp(\omega) = \left(\frac{\pm i\omega + 0}{e}\right)^{\pm i\omega}.$$

The above properties of $C_n(\omega)$ determine the dependence of free energy on temperature and magnetic field both at $T \gg H$ and at $T \ll H$. Indeed, at $H \ll T$ and $T \gg T_K$, bending the integration contour into the lower half-plane and by-passing the cut yields.

$$\mathscr{F}_i = -T\ln\left[\frac{\sinh(H/2T)(2S+1)}{\sinh H/2T}\right] + T\int_0^\infty \frac{B_{2S}(2\pi t, T/H)}{\cos \pi t}\, t^{-t}$$
$$\times \exp(-2t\ln T/T_K)\, dt \tag{6.1.77}$$

at $\ln T/T_k \gg 1$ and we arrive at the well-known perturbation-theory expansion in inverse powers of $\ln T/T_K$ (see §2.4.2). According to item (iv), the poles of $(\cosh\omega/2)^{-1}$ are compensated for by zeros of $B_{2S}(\omega)$.

Formula (6.1.77) implies that $\mathscr{F}_i$ can be expanded in a power-series in the invariant charge (2.4.22) for $0 < z \ll 1$:

$$1/z(T) - \frac{1}{2}\ln z(T) = \ln T/T_K. \tag{6.1.78}$$

Changing variables in the integral in (6.1.77), we have

$$z\int_0^\infty \frac{B_{2S}(2\pi z t, T/H)}{\cos \pi t z}\exp(-2t - zt\ln t)\, dt = \sum_{n=1}^{\infty} b_n(T/H, S) z^n. \tag{6.1.79}$$

We shall find below the first terms of the expansion in $z$ and compare the result with the perturbation-theory expansion. As usual, (6.1.79) is an asymptotic expansion

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

and its coefficients grow like $n!$ as $n \to \infty$. This readily follows from the fact that the integrand has a finite radius of convergence in $t$, which is determined by the position of the pole of $(\cos \pi t z)^{-1}$.

Now let us turn to the region $T \ll T_K$ and $S \neq 1/2$. Bending the integration contour into the upper half-plane, we again encounter a cut and poles of $(\cosh \omega/2)^{-1}$. At $|z| \ll 1$ the cut plays the main role, while the poles are exponentially small. Therefore, according to (6.1.52), at $T \ll T_K$ the free energy of the s–d model with $S \neq 1/2$ is given by an asymptotic expansion in inverse logarithms whose coefficients coincide with those of the expansion at $T \gg T_K$ with $S = 1/2$ substituted for $S$ (Fateev and Wiegmann 1981):

$$\mathscr{F}_i(T \ll T_K) = -T \ln\left[\frac{\sinh SH/T}{\sinh H/2T}\right] + \sum_{n=1}^{\infty} b_n(T/H, S-1/2) z^n + TO(T/T_K). \tag{6.1.80}$$

The logarithmic behaviour of the free energy in the strong-coupling limit $g = \infty$ was discovered by Cragg *et al.* (1980) in the numerical investigation of hamiltonian (2.4.7).

The duality of the logarithmic expansions in the low- and high-temperature regions can be qualitatively explained in the following way. In each interaction act of a conduction electron with the impurity, the configuration with the electron spin opposite to the impurity spin is the most favourable. At high temperatures, when the effective interaction is small, the correlation between the impurity spin and the spin of the electron that has just interacted with the impurity drops off over a long time interval compared with the interaction time but which is still logarithmically small. In the strong-coupling limit (i.e. at $T \to 0$) the spins of the impurity and electron 'remember' their mutual position after interaction for an infinitely long time. Therefore, the actual magnetic moment of the impurity is $S - 1/2$, and we can speak of a ground state of the impurity that is $2S$-fold degenerate.

The interaction of the electron-impurity system whose spin is now $S - 1/2$ with other conduction electrons can proceed in two ways. First, this may again be by the exchange interaction, which produces a 'reverse' Kondo effect and leads to logarithmic corrections in (6.1.80), but, as (6.1.80) shows, the interaction is now ferromagnetic, i.e. increases with energy. Indeed, an electron whose spin is opposite to that of the impurity does not interact with the impurity since its energy level is occupied by the bound electron. But if its spin is parallel to that of the impurity, a spin–flip process is possible. Since this is a second-order process, it leads to a decrease in energy, i.e. the interaction is ferromagnetic (Nozières and Blandin 1980).

The other possible interaction mechanism is connected with polarization of the electron-impurity system. This mechanism leads to power contributions made by the poles of $(\cosh \omega/2)^{-1}$ in (6.1.79). These contributions are exponentially small compared to the contribution provided by integration around the cut.

The situation differs drastically at $S = 1/2$. As has been shown in § 6.1.5 $C_1(\omega)$ and, hence, $D_1(\omega)$ are in this case analytic in the upper half-plane, and the logarithmic contribution at $T \ll T_K$ vanishes, $b_n(S=0) = 0$. Only the poles of $(\cosh \omega/2)^{-1}$ contribute, leading to an expansion in integral powers of $T/T_K$ (6.1.66). We arrive at the same result in the region $H \gg T$; but here the power-series in $H$ ($H \ll T_K$, $S = 1/2$) converges.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

6.1.9. *Zero-temperature limit*

Let us show that eqns. (6.1.60) for $T \to 0$, but keeping $H$ finite, coincide with eqns. (5.1.52).

We introduce the notations

$$\varepsilon_n^+ = \begin{cases} \varepsilon_n & \text{at} \quad \varepsilon_n \geqslant 0 \\ 0 & \text{at} \quad \varepsilon_n < 0 \end{cases}, \qquad \varepsilon_n^- = \begin{cases} 0 & \text{at} \quad \varepsilon_n > 0 \\ \varepsilon_n & \text{at} \quad \varepsilon_n \leqslant 0 \end{cases}.$$

Equation (6.1.34) implies that at $n > 1$ all the $\varepsilon_n$ are positive, therefore $\varepsilon_n^- = 0$ at $n > 1$. Only $\varepsilon_1$ changes sign, and since it is monotonic, it vanishes at only one point $\lambda = -B$, i.e.

$$\varepsilon_1(-B) = 0. \tag{6.1.81}$$

As $T \to 0$

$$T \ln(1 + \exp(\pm \varepsilon_n / T)) \Rightarrow \pm \varepsilon_n^{\pm} \tag{6.1.82}$$

and eqns. (6.1.33) become linear:

$$\varepsilon_n^+ = -nH - \frac{\epsilon_F}{\pi}(\pi + p_n) - A_{n1} * \varepsilon_1^- \tag{6.1.83}$$

and for $n = 1$ coincide with (5.1.52). The fact that all the $\varepsilon_n^-$ are zero at $n > 1$ implies that the ground state is a linear combination of only the real solutions of eqns. (4.2.B). Indeed, according to (6.1.44),

$$\frac{\langle M_n \rangle}{N} = -\delta_{n1} \frac{\varepsilon_1^{(-)}(+\infty)}{2\epsilon_F} \tag{6.1.84}$$

as $T \to 0$. It is expedient to rewrite eqn. (6.1.83) in such a way that $\varepsilon_n$ and $\varepsilon_1^-$ are expressed in terms of $\varepsilon_1^+$:

$$\varepsilon_n = (n-1)H + A_{n1} * A_{11}^{-1} * \varepsilon_1^+, \tag{6.1.85}$$

$$\varepsilon_1^- = H/2 - A_{11}^- * \varepsilon_1^+ - \frac{2\epsilon_F}{\pi} \exp(\pi\lambda). \tag{6.1.86}$$

The last equation has been solved in § 5.1.4. Using this solution and eqn. (6.1.85) we obtain the functions

$$\varepsilon_n^+\left[\lambda + \frac{1}{\pi}\ln\left(\frac{2\epsilon_F}{H}\left(\frac{2}{\pi e}\right)^{1/2}\right)\right] = -\frac{H}{2^{3/2}}\int_{-\infty}^{+\infty} d\omega$$
$$\times \exp(-i\omega\lambda - (n-1)|\omega|/2)\,\frac{G^{(-)}(\omega)}{(\omega - i0)(\omega - i\pi)} + (n-1)H. \tag{6.1.87}$$

The linear equations (6.1.85) and (6.1.86) are the first approximation of the perturbation-theory expansion in $T/H$ at $T \ll H$. This theory will be constructed in the next section.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

6.1.10. *Low-temperature expansion at* $\mu_B H \gg k_B T$

At $H \gg T$ all $\varepsilon_n > H$ except $\varepsilon_1$. Therefore, at $n > 1$

$$\ln(1+\exp(-\varepsilon_n/T) \sim O(\exp(-H/T))$$

and within the exponential accuracy we have, instead of eqns. (6.1.33),

$$\varepsilon_1(\lambda) = H/2 - \frac{2\epsilon_F}{\pi}\exp(\pi\lambda) + T\int_{-\infty}^{+\infty} R(\lambda-\lambda')\ln(1+\exp(\varepsilon_1(\lambda')/T))\,d\lambda', \tag{6.1.88}$$

$$\varepsilon_n = (n+1)H + a_{n-1} * T\ln(1+\exp(\varepsilon_1/T)). \tag{6.1.89}$$

$R$ and $a_{n-1}$ are defined by (5.1.21) and (6.1.17). These equations enable us to calculate the coefficients in the expansion of free energy in $T/H$ (Filyov *et al.* 1981):

$$\mathscr{F}_i(T,H) - \mathscr{F}_i(O,H) = T\sum_{n=0}^{\infty}\gamma_n\left(\frac{H}{T_K}\right)\left(\frac{T}{H}\right)^{2n+1} \tag{6.1.90}$$

We use the trick suggested by Takahashi (1973). Let us rewrite the integral in (6.1.88) as

$$TR * \ln(1+\exp(\varepsilon_1(\lambda)/T)) = TR * \ln(1+\exp(-|\varepsilon_1(\lambda)|/T)) + \int_{-\infty}^{-B} R(\lambda-\lambda')\varepsilon_1^+(\lambda')\,d\lambda'. \tag{6.1.91}$$

We shall show below that $-\partial\varepsilon_1/\partial\lambda|_{-B} \sim H$. Therefore, the first integral in the right-hand side of (6.1.91) may be calculated in the saddle-point approximation:

$$TR * \ln(1+\exp(-|\varepsilon_1(\lambda)|/T)) \simeq R(\lambda+B)\pi^2T^2/6\left|\frac{\partial\varepsilon_1}{\partial\lambda}(-B)\right| + O(T^4). \tag{6.1.92}$$

Here we must confine ourselves by $B$ and $(\partial\varepsilon_1/\partial\lambda)(-B)$ calculated at $T=0$:

$$B = \frac{1}{\pi}\ln\left[\frac{2\epsilon_F}{H}\left(\frac{2}{\pi e}\right)^{1/2}\right] - \frac{\partial\varepsilon_1}{\partial\lambda}(-B) = 2\epsilon_F\rho_h(-B) = \frac{H\pi}{\sqrt{2}}. \tag{6.1.93}$$

Let us set

$$\varepsilon_1(\lambda) = \varepsilon_1^{(0)}(\lambda) + \frac{\pi^2T^2}{6|(\partial\varepsilon_1/\partial\lambda)(-B)|}U(\lambda), \tag{6.1.94}$$

where $\varepsilon_1^{(0)}(\lambda)$ is the solution of (6.1.88) at $T=0$ determined by (6.1.87), $U(\lambda)$ satisfies the following equation:

$$U(\lambda) - \int_{-\infty}^{-B} R(\lambda-\lambda')U(\lambda')\,d\lambda' = R(\lambda+B). \tag{6.1.95}$$

The free energy of impurity is

$$\mathscr{F}_i(T,H) - \mathscr{F}_i(0,H) = -T\int \mathscr{S}_{2S}(\lambda+1/g)\ln(1+\exp(-|\varepsilon_1(\lambda)|/T))\,d\lambda + \int_{-\infty}^{-B}\mathscr{S}_{2S}(\lambda+1/g)(\varepsilon_1(\lambda)-\varepsilon_1^{(0)}(\lambda))\,d\lambda, \tag{6.1.96}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where

$$\mathscr{S}_{2S}(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \frac{\exp(-i\omega\lambda-|\omega|(S-1/2))}{2\cosh\omega/2}.$$

According to (6.1.94) and (6.1.96) we have

$$\mathscr{F}_{\mathrm{i}}(T,H)-\mathscr{F}_{\mathrm{i}}(0,H)=-\frac{\pi^2T^2}{6|(\partial\varepsilon_1/\partial\lambda)(-B)|}V(-B)+O(T^4), \tag{6.1.97}$$

where $V(\lambda)$ satisfies the following equation:

$$V(\lambda)-\int_{-\infty}^{-B} R(\lambda-\lambda')V(\lambda')\,d\lambda'=\mathscr{S}_{2S}(\lambda+1/g). \tag{6.1.98}$$

Comparing eqn. (6.1.98) with eqn. (5.1.20*b*) we see that

$$V(\lambda)=\tilde{\rho}_{\mathrm{i}}(\lambda).$$

Thus, according to (6.1.97) the impurity heat capacity at $T\ll H$ is (Filyov *et al.* 1981):

$$C_{\mathrm{i}}=T\pi^2/6\epsilon_{\mathrm{F}}\lim_{\lambda\to-B}\tilde{\rho}_{\mathrm{i}}(\lambda)/\tilde{\rho}_n(\lambda). \tag{6.1.99}$$

To calculate $\tilde{\rho}_h(-B)$ and $\tilde{\rho}_{\mathrm{i}}(-B)$ it is convenient to use the relation (see Appendix to § 5.1.3):

$$\tilde{\rho}(-B)=i\lim_{\omega\to\infty}\omega\rho^-(\omega). \tag{6.1.100}$$

Using this relation and (5.1.33) we have

$$\tilde{\rho}_h(-B)=H\pi/2\sqrt{2\epsilon_{\mathrm{F}}} \tag{6.1.101}$$

$$\tilde{\rho}_{\mathrm{i}}(-B)=\sqrt{2(\pi H\chi_{\mathrm{i}}(H/T_H))}$$

and, hence,

$$\frac{1}{T}C_{\mathrm{i}}(H/T_{\mathrm{K}})=\frac{2\pi^2}{3}\chi_{\mathrm{i}}(H/T_{\mathrm{K}}). \tag{6.1.102}$$

So the Wilson–Nozières formula proves to be valid for arbitrary magnetic fields. This has been noted earlier (Wiegmann and Finkelstein 1978). Besides that we see that the limits $H\to0$ and $T\to0$ commute, as must be the case for a Fermi liquid.

The above method may be applied for finding higher terms in the expansion (6.1.90). However, the appropriate calculations are too cumbersome.

### 6.1.11. *High-temperature expansion (perturbation theory)*

In § 6.1.7 we showed that $D_1(\omega)$ is analytic in the upper half-plane. The values of this function at $\omega=i\pi(n+1/2)$, $n=0,1,\ldots$, determine the coefficients in the expansion of the heat capacity of an impurity with $S=1/2$ in powers of $T/T_{\mathrm{K}}$. Except for $D_1(i\pi/2)$, there is little hope of finding these quantities analytically.

The situation is quite different for the expansion in inverse logarithms both at $T\gg T_{\mathrm{K}}$ and at $T\ll T_{\mathrm{K}}$ when $S\neq1/2$. Indeed, the coefficients of the leading powers of $z$ are determined by the behaviour of $D_{2S}(\omega)$ at small values of $\omega$ or by the behaviour of $\varphi_{2S}(\lambda)$ as $\lambda\to\pm\infty$ and can be found from eqns. (6.1.34) by an iterative method. Here

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

we shall construct the first iteration of eqns. (6.1.60) and show that (Filyov *et al.* 1981, Fateev and Wiegmann 1981 b):

$$\operatorname{Disc} D_{2S}(-i|\omega|, H/T\to 0)=\frac{2}{3}S(S+1)((H/T)^2-\omega^2)\left(1-\frac{\omega}{2\pi}\ln|\omega|\right). \tag{6.1.103}$$

This formula, according to § 6.1.6, leads to asymptotic expressions (2.2.24) known from perturbation theory.

It is convenient to rewrite eqns. (6.1.60) as

$$C_n(\lambda)=\ln\{1+\exp[-\delta_{n1}\exp(\pi\lambda)+s*(C_{n-1}(\lambda)+C_{n+1}(\lambda))]\},\qquad C_0=0. \tag{6.1.104}$$

The zeroth approximation to the $C_n$s are their asymptotics at $\lambda\to\pm\infty$:

$$C_n^{(0)}=\begin{cases}2\ln\Phi_n & \lambda<0\\ 2\ln\Phi_{n-1} & \lambda>0, n\neq 1\end{cases}$$

and

$$C_1^{(0)}(\lambda)=\ln(1+\Phi(1)\exp(-\exp(\pi\lambda)))\quad \text{at } \lambda\to+\infty.$$

Let us find the next approximation

$$d_n=C_n-C_n^{(0)}.$$

Linearizing eqns. (6.1.104) and going over to Fourier transforms, we have:

$$d_n^-\frac{\Phi^2(n)}{\Phi(n-1)\Phi(n+1)}+d_n^+\frac{\Phi^2(n-1)}{\Phi(n-2)\Phi(n)}=s*(d_{n+1}+d_{n-1}),\qquad n\geqslant 3, \tag{6.1.105}$$

$$d_2^-\frac{\Phi^2(2)}{\Phi(1)\Phi(3)}+d_2^+\frac{\Phi^2(1)}{\Phi(2)}=s*(d_3+d_1^-)+Y_+, \tag{6.1.106}$$

$$d_1^+\frac{\Phi^2(1)}{\Phi(2)}=s*d_2+Y_-, \tag{6.1.107}$$

where $Y_\pm\simeq\pm z'/(\omega\pm i0)$ and

$$d^+(\omega)=\int_0^\infty\exp(i\omega\lambda)d(\lambda)\,d\lambda,\qquad d^-(\omega)=\int_{-\infty}^0\exp(i\omega\lambda)d(\lambda)\,d\lambda.$$

We did not write the equation for $d_1^+$ because this quantity is not small. The solution of the boundary-value problem (6.1.105)–(6.1.107) as $\omega\to 0$ leads to (6.1.103), since

$$D_n(\omega)=d_n(\omega)+O(\omega^3). \tag{6.1.108}$$

Here we shall obtain only the principal order in $|\omega|$ in (6.1.103). To this end we neglect the influence of the regions $\lambda>0$ and $\lambda<0$ on each other. In other words in eqns. (6.1.105)–(6.1.107) we leave only terms with $d_n^+$ or terms with $d_n^-$. These equations then transform into equations for $d_n^+$, defined on the real axis:

$$\left.\begin{aligned} d_n^-\frac{\Phi^2(n)}{\Phi(n-1)\Phi(n+1)}&=s*(d_{n+1}^-+d_{n-1}^-),\\ d_1^-\frac{\Phi^2(1)}{\Phi(2)}&=s*d_2^-+Y_+\end{aligned}\right\} \tag{6.1.109}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

and

$$\left.\begin{aligned} d_n^+ \frac{\Phi^2(n-1)}{\Phi(n-2)\Phi(n)} &= s * (d_{n+1}^+ + d_{n-1}^+), \\ d_2^+ \frac{\Phi^2(1)}{\Phi(2)} &= s * d_3^+ + Y_-. \end{aligned}\right\} \tag{6.1.110}$$

Hence, we see that at least in this approximation $d_n^- = d_{n+1}^+$ and the duality of the coefficients of the expansion in $z$ at $T \gg T_K$ and $T \ll T_K$ described in § 6.1.7 occurs. It can be proved that this is true for all orders of perturbation theory. The recurrence equations (6.1.109) and (6.1.110) are encountered in studies of high-temperature expansion for the one-dimensional Haisenberg model (Takahashi 1971 a), Johnson and McCoy 1972). Their solution is

$$d_n^-(\omega) = -\frac{2\cosh\omega/2}{\Phi(1)\Phi(n)} \frac{i}{\omega - i0} [\Phi(n+1)\exp(-n|\omega|/2) - \Phi(n-1)\exp(-(n+2)|\omega|/2)]. \tag{6.1.111}$$

This implies that $d_n(\omega)$ and, hence, $D_n(\omega)$ both have a discontinuity that passes through point $\omega = 0$. Retaining, in (6.1.111), the leading terms as $\omega \to 0$, we arrive at (6.1.103).

Therefore, the impurity part of the free energy is

$$\mathscr{F}_i(T) = \begin{cases} -T\ln(2S+1) - T\dfrac{S(S+1)}{3} f(T/T_K), & T \gg T_K, \\ -T\ln 2S - T\dfrac{(S^2-1/4)}{3} f(T/T_K), & T \ll T_K, \end{cases} \tag{6.1.112}$$

where

$$f(x) = \frac{H^2}{2T^2}\left(1 - \frac{1}{\ln x}\right) - \frac{\pi^2}{\ln^3 x}.$$

In conclusion, we note that the accuracy of iterations grows with the growth of $n$ of the function $C_n$. Indeed, as $n$ increases, the difference between the asymptotics at $\lambda \to \pm\infty$ and at $H/T \to 0$ becomes smaller. Therefore, the parameter in the perturbation-theory approach is not only small $|\omega|$ but large $n$ as well. At $n \gg 1$ we can retain the entire dependence on $\ln T/T_K$. Therefore, at $S \gg 1$ we have†

$$\mathscr{F}_i = -T\ln 2S + \frac{T}{2\pi}\left[\tan^{-1}(\pi S/\ln T/T_K) - \frac{\pi \ln T/T_K}{\ln^2 T/T_K + (\pi S)^2}\right] - \frac{H^2}{6T} S^2 \left[1 - \frac{1}{2\pi S}\ln\left(\frac{\pi S}{\ln T/T_K}\right)\right] \tag{6.1.113}$$

This formula is equally suited for $T \gg T_K$ and $T \ll T_K$. The next iterations of eqns. (6.1.105)–(6.1.107) are more complicated.

† Equation (6.1.113) is similar to the 'exact solution' of the Suhl–Nagoaka equations (for a review see Müller-Hartmann and Zittartz (1971)).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

6.1.12. *Numerical solution of the non-linear integral equations*

We have shown in § 6.1.5 that the thermodynamic properties of the impurity are derived from the system of the dimensionless universal non-linear equations. The analytical properties of the solutions of eqns. (6.1.60) obtained in § 6.1.7 enable us to describe the impurity behaviour at low- and high-temperatures. The only way to obtain information about impurity thermodynamics which is beyond the perturbation theory and the Fermi-liquid approach frameworks, e.g. to study the crossover regime between weak- and strong-coupling limits, is by a numerical investigation.

Recently, three groups of authors have almost simultaneously numerically solved the thermodynamic non-linear integral equations (6.1.60) and derived the impurity thermodynamics† (Melnicov 1982‡, Desgranges and Schotte 1982, Rajan *et al.* 1982). Here we give a brief review of their results.

The right-hand side of eqns. (6.1.60), considered as an operator, is found to realize a shrinking transformation. It enabled all the above authors to solve system (6.1.60) iteratively. Since the number of equations in system (6.1.60) is infinite it is necessary to truncate the system in a certain way and to check the convergence of this procedure with the increase in the number of the equations. Different authors have used different ways of truncation as well as different procedures of numerical integration. Nevertheless, the overlapping final results obtained by different ways are identical.

Melnicov has computed the specific heat and magnetic susceptibility for $S=1/2$, 1, 3/2 impurity in zero magnetic field. Actually, he has solved eqns. (6.2.13) of the anisotropic model for anisotropy $(\cos I_{\parallel}/2)/(\cos I_{\perp}/2)=\cos \pi/\nu$, where $\nu$ increases from 3 to 10. In this case (see § 6.2.1) the number of equations is finite and equal to $\nu-1$.

To control the accuracy of calculation and the convergence of the interational procedure, the integral $C_1(i\pi/2, 0)$ was calculated by iterations to compare it with its exact value, which is equal to $\pi/6$ independent of $\nu$ (see 6.1.72). For $\nu=10$ after 120 iterations this integral converged to $\pi/6\times 0{\cdot}9997$.

It was sufficient to get, in the range $|\ln T/T_k| \lesssim 8$, the overall accuracy better than 1% for the specific heat and magnetic susceptibility. The simultaneous computation of these quantities by a Wang-2200-VP minicomputer took about 6 hours.

The convergence of the specific heat with $\nu$ was quite rapid. This is not surprising, since the difference of the Oliveira and Wilkins (1981) results (see § 3.1.1, fig. 3.1) from those at the Toulouse limit, corresponding to $\nu=2$, is minor at $T<T_K$.

In fact, the difference in the specific heat calculated at $\ln T/T_K \sim 5$ for $\nu=3$ and $\nu=10$ is about 10% and is much smaller at low temperatures (at $T<T_K$ the difference is smaller than 2%). Substantial differences should naturally occur at large $T \gg T_K$ due to the perturbative power-like asymptotics of $C_i(T)$. However, the numerical results testify that perturbation theory is valid only at very large $T$. The rapid convergence of $C_i(T)$ with $\nu$ makes one believe that the numerical results for $\nu=10$ in the region $\ln T/T_K \gg 1$ should be very close to the specific heat of the isotropic exchange model. In this case it is known (see eqn. (6.1.112)) that $C_i(T)=S(S+1)\pi^2(\ln T/T_K)^{-4}$ at $\ln T/T_K \gg 1$. At $S=1/2$ for example, the specific heat calculated at $\ln T/T_K \sim 8$ with the use of this expression is half as big as $C_i(T)$ computed for $\nu=10$ (see table 1).

† Similar equations describing the thermodynamics of the 1/2-spin Haisenberg ring were numerically solved earlier by Takahashi (1974 a).

‡ We are greatly indebted to V. I. Melnicov for permission to use his unpublished results.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Table 1. Values of the universal Kondo specific heat for $S=1/2, 1, 3/2$. The specific heat for 1/2-spin impurity is given for certain values of the anisotropy parameter $\nu$ (after Melnicov 1982 b, Desgranges and Schotte 1982).

| | | $C_{1/2}$ | | | | |
|---|---|---|---|---|---|---|
| $\ln T/T_K$ | $T/T_K$ | $\nu=3$ | $\nu=5$ | $\nu=11$ | $C_1$ | $C_{3/2}$ |
| −8·1 | 0·0003 | 0·00031 | 0·00031 | 0·00031 | 0·00131 | 0·00257 |
| −7·8 | 0·0004 | 0·00042 | 0·00042 | 0·00042 | 0·00156 | 0·00295 |
| −7·5 | 0·0005 | 0·00057 | 0·00057 | 0·00057 | 0·00187 | 0·00339 |
| −7·2 | 0·0007 | 0·00078 | 0·00078 | 0·00078 | 0·00224 | 0·00390 |
| −6·9 | 0·0010 | 0·00105 | 0·00105 | 0·00105 | 0·00272 | 0·00449 |
| −6·6 | 0·0013 | 0·00142 | 0·00142 | 0·00142 | 0·00332 | 0·00516 |
| −6·3 | 0·0018 | 0·00192 | 0·00192 | 0·00192 | 0·00408 | 0·00593 |
| −6·0 | 0·0024 | 0·00259 | 0·00259 | 0·00259 | 0·00504 | 0·00682 |
| −5·7 | 0·0033 | 0·00350 | 0·00350 | 0·00350 | 0·00624 | 0·00782 |
| −5·4 | 0·0045 | 0·00472 | 0·00472 | 0·00472 | 0·00773 | 0·00894 |
| −5·1 | 0·0060 | 0·00638 | 0·00637 | 0·00637 | 0·00953 | 0·01019 |
| −4·8 | 0·0082 | 0·00860 | 0·00860 | 0·00860 | 0·01168 | 0·01157 |
| −4·5 | 0·0111 | 0·01161 | 0·01161 | 0·01160 | 0·01420 | 0·01308 |
| −4·2 | 0·0149 | 0·01564 | 0·01564 | 0·01564 | 0·01715 | 0·01471 |
| −3·9 | 0·0202 | 0·02106 | 0·02106 | 0·02106 | 0·02005 | 0·01645 |
| −3·6 | 0·0273 | 0·02830 | 0·02830 | 0·02829 | 0·02442 | 0·01828 |
| −3·3 | 0·0368 | 0·03788 | 0·03788 | 0·03788 | 0·02876 | 0·02018 |
| −3·0 | 0·0497 | 0·05037 | 0·05036 | 0·05035 | 0·03351 | 0·02211 |
| −2·7 | 0·0672 | 0·06627 | 0·06624 | 0·06623 | 0·03856 | 0·02402 |
| −2·4 | 0·0907 | 0·08570 | 0·08564 | 0·08563 | 0·04375 | 0·02588 |
| −2·1 | 0·1224 | 0·10806 | 0·10794 | 0·10792 | 0·04884 | 0·02760 |
| −1·8 | 0·1652 | 0·13158 | 0·13135 | 0·13131 | 0·05357 | 0·02915 |
| −1·5 | 0·2231 | 0·15330 | 0·15290 | 0·15285 | 0·05762 | 0·03047 |
| −1·2 | 0·0311 | 0·16970 | 0·16905 | 0·16897 | 0·06073 | 0·03150 |
| −0·9 | 0·4065 | 0·17781 | 0·17688 | 0·17676 | 0·06268 | 0·03220 |
| −0·6 | 0·5488 | 0·17644 | 0·17520 | 0·17505 | 0·06334 | 0·03255 |
| −0·3 | 0·7408 | 0·16647 | 0·16496 | 0·16478 | 0·06270 | 0·03255 |
| 0·0 | 1·0000 | 0·15031 | 0·14861 | 0·14839 | 0·06085 | 0·03219 |
| 0·3 | 1·3498 | 0·13100 | 0·12921 | 0·12898 | 0·05799 | 0·03151 |
| 0·6 | 1·8221 | 0·11105 | 0·10927 | 0·10902 | 0·05435 | 0·03054 |
| 0·9 | 2·4596 | 0·09224 | 0·09056 | 0·09030 | 0·05021 | 0·02933 |
| 1·2 | 3·3201 | 0·07554 | 0·07403 | 0·07377 | 0·04582 | 0·02793 |
| 1·5 | 4·4816 | 0·06130 | 0·06002 | 0·05976 | 0·04139 | 0·02639 |
| 1·8 | 6·0496 | 0·04949 | 0·04846 | 0·04820 | 0·03708 | 0·02475 |
| 2·1 | 8·1661 | 0·03985 | 0·03909 | 0·03884 | 0·03300 | 0·02306 |
| 2·4 | 11·0231 | 0·03207 | 0·03157 | 0·03133 | 0·02922 | 0·02136 |
| 2·7 | 14·8797 | 0·02582 | 0·02557 | 0·02534 | 0·02574 | 0·01968 |
| 3·0 | 20·0855 | 0·02080 | 0·02078 | 0·02057 | 0·02255 | 0·01805 |
| 3·3 | 27·1126 | 0·01678 | 0·01696 | 0·01677 | 0·01977 | 0·01647 |
| 3·6 | 36·5982 | 0·01354 | 0·01390 | 0·01372 | 0·01709 | 0·01497 |
| 3·9 | 49·4024 | 0·01093 | 0·01144 | 0·01128 | 0·01479 | 0·01356 |
| 4·2 | 66·6863 | 0·00882 | 0·00945 | 0·00931 | 0·01278 | 0·01224 |
| 4·5 | 90·0171 | 0·00711 | 0·00783 | 0·00771 | 0·01104 | 0·01102 |
| 4·8 | 121·5104 | 0·00573 | 0·00652 | 0·00641 | 0·00954 | 0·00990 |
| 5·1 | 164·0219 | 0·00461 | 0·00544 | 0·00535 | 0·00825 | 0·00888 |
| 5·4 | 221·4064 | 0·00371 | 0·00456 | 0·00448 | 0·00714 | 0·00795 |
| 5·7 | 298·8674 | 0·00298 | 0·00383 | 0·00377 | 0·00620 | 0·00711 |
| 6·0 | 403·4287 | 0·00239 | 0·00322 | 0·00318 | 0·00539 | 0·00635 |

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

To calculate the magnetic susceptibility at zero magnetic field Melnicov linearized system (6.1.60) in $(H/T_K)^2$ by substitution

$$\ln(1+\exp(\varepsilon_n(\lambda)/T)) = C_n(\lambda) + H^2/T_K^2\Psi_n(\lambda) \tag{6.1.114}$$

and solved the doubled set of equations for the $C_n$s and $\Psi_n$s.

Desgranges and Schotte have calculated the specific heat and entropy for the 1/2-spin impurity. They truncated the system of eqns. (6.1.60) by approximating the function $\varepsilon_n$ in the last equation by the starting function of the iteration process. To obtain the percentage accuracy it was necessary to iterate 20 equations 26 times.

The most complete numerical solution was given by Rajan *et al.* (1982). They computed the specific heat and magnetic susceptibility for $S=1/2$, 1, 3/2 impurities in the presence of a magnetic field and compared their results with the experimental data. They also truncated the infinite system of eqns. (6.1.60) by a certain $v$, taking $T\ln(1+\exp(\varepsilon_n/T))$ at $n \geqslant v$ to be equal to $\varepsilon_n$. The error in this approximation is shown to be of the order of $1/v^2$. The free energy was calculated and the susceptibility and specific heat were obtained by numerical differentiation.

Now we turn to the results of the calculations. Figure (6.2) shows the functions $C_n = \ln(1+\exp(\varepsilon_n/T))$. This picture gives a good illustration of the analytical treatment described in §6.1.6. Figure 6.4 displays the temperature dependence of the specific heat in zero magnetic field for $S=1/2$, 1, 3/2 impurities. The points in this figure are a renormalization group of calculation results (Oliveira and Wilkins 1981).

One can see from fig. 6.4 that the impurity makes its largest contribution to the specific heat around $T=0{\cdot}5\,T_K$. As the spin of the impurity increases, its contribution decreases. In fact, the higher spin impurity acts more and more like a free classical rotator. The positions and values of maxima of the $C_n$s are given in table 2. The impurity contribution to the entropy is presented in fig. 6.5 (Desgranges and Schotte 1982).

Table 2. The positions and values maxima of the impurity specific heat for $S=1/2$, 1, 3/2 (after Melnicov 1982 a).

| $S$ | $T_M/T_K$ | $C(T_M)$ |
|---|---|---|
| 1/2 | 0·45 | 0·177 |
| 1 | 0·53 | 0·063 |
| 3/2 | 0·56 | 0·033 |

Melnicov has calculated directly the first analytically uncalculable terms in the temperature expansions of the specific heat and magnetic susceptibility for $S=1/2$:

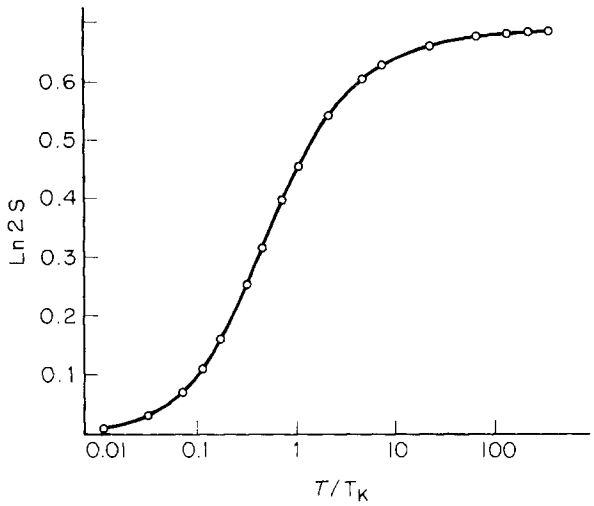
$$C_i(T) = \frac{\pi}{3}\frac{T}{T_K} - 15{\cdot}4(T/T_K)^3,$$

$$\chi_i(T) = 1/2\pi T_K - 0{\cdot}433(T/T_K)^2.$$

Figures 6.6 and 3.3 show 1/2-spin impurity specific heat and magnetic susceptibility on a linear temperature scale. The magnetic susceptibility curve $\chi_i^{(1/2)}(T)$ was first obtained by Wilson (1975) by the numerical renormalization group approach. In the temperature range $0{\cdot}3\,T_K < T < 10\,T_K$, where the interpolation

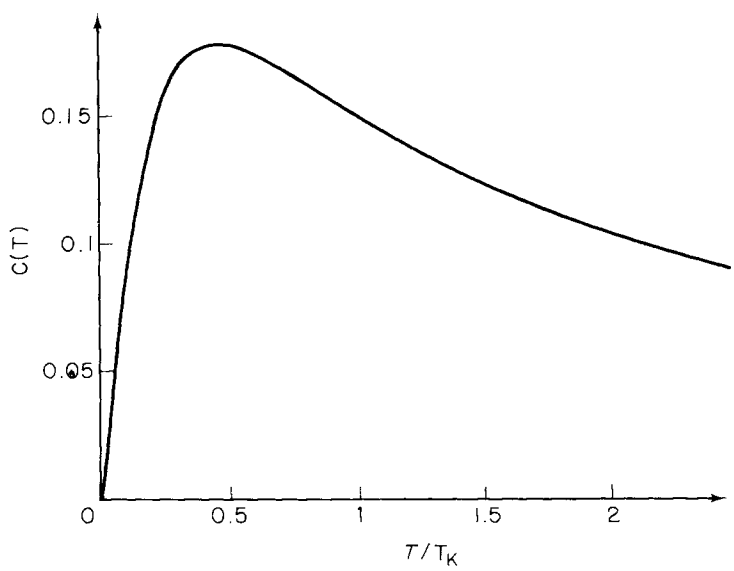
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 6.5




The 1/2-spin impurity contribution to the entropy (Desgranges and Schotte 1982).

Fig. 6.6




The universal Kondo specific heat for 1/2-spin impurity versus $T/T_K$ (after Melnicov 1982 a, Desgranges and Schotte 1982. The figure is taken from Melnicov 1982 a).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

(3.1.23) is valid, the new numerical results agree with (3.1.23) with good accuracy, $\sim 0{\cdot}5\%$.

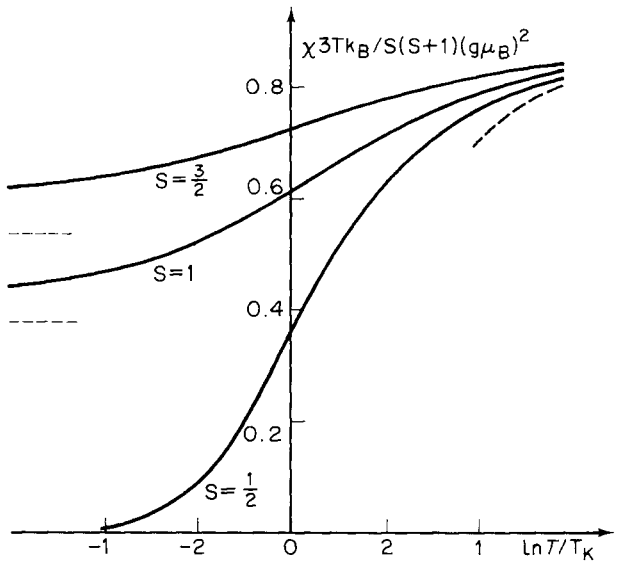
We believe it useful to give the results for the magnetic susceptibility at $T < 0{\cdot}5\,T_K$ both in table 3 and in fig. 3.3 (Melnicov 1982 b). The crosses in this figure correspond to the renormalization group results given in table V in Krishna-Murthy *et al.*

Table 3. Values of the universal Kondo susceptibility versus $T/T_K$ for figs. 3.3–3.5. For $T \gtrsim 13\,T_K$ $\chi_i(T)$ is accurately calculable using eqns. (3.1.20) and (3.1.22) (after Melnicov 1982 b).

| $\ln T/T_K$ | $T/T_K$ | $S=1/2$ | $S=1$ | $S=3/2$ |
|---|---|---|---|---|
| −6·6 | 0·0013 | 0·15886 | 213·02547 | 563·65320 |
| −6·3 | 0·0018 | 0·15886 | 158·47150 | 418·85551 |
| −6·0 | 0·0024 | 0·15886 | 117·95038 | 311·34671 |
| −5·7 | 0·0033 | 0·15886 | 87·84407 | 231·50623 |
| −5·4 | 0·0045 | 0·15885 | 65·46840 | 172·19893 |
| −5·1 | 0·0060 | 0·15885 | 48·83160 | 128·13215 |
| −4·8 | 0·0082 | 0·15883 | 36·45573 | 95·37983 |
| −4·5 | 0·0111 | 0·15881 | 27·24411 | 71·02924 |
| −4·2 | 0·0149 | 0· 15877 | 20·38286 | 52·91870 |
| −3·9 | 0·0202 | 0·15869 | 15·26821 | 39·44401 |
| −3·6 | 0·0273 | 0·15854 | 11·45817 | 29·41440 |
| −3·3 | 0·0368 | 0·15823 | 8·60222 | 21·94581 |
| −3·0 | 0·0497 | 0·15782 | 6·47145 | 16·38167 |
| −2·7 | 0·0672 | 0·15701 | 4·87638 | 12·23433 |
| −2·4 | 0·0907 | 0·15561 | 3·68064 | 9·14142 |
| −2·1 | 0·1224 | 0·15328 | 2·78280 | 6·83361 |
| −1·8 | 0·1652 | 0·14960 | 2·10739 | 5·11068 |
| −1·5 | 0·2231 | 0·14409 | 1·59830 | 3·82368 |
| −1·2 | 0·3011 | 0·13641 | 1·21377 | 2·86178 |
| −0·9 | 0·4065 | 0·12646 | 0·92269 | 2·14248 |
| −0·6 | 0·5488 | 0·11452 | 0·70189 | 1·60434 |
| −0·3 | 0·7408 | 0·10121 | 0·53409 | 1·20154 |
| 0·0 | 1·0000 | 0·08734 | 0·40637 | 0·89994 |
| 0·3 | 1·3498 | 0·07373 | 0·30906 | 0·67403 |
| 0·6 | 1·8221 | 0·06102 | 0·23488 | 0·50480 |
| 0·9 | 2·4596 | 0·04963 | 0·17833 | 0·37799 |
| 1·2 | 3·3201 | 0·03978 | 0·13523 | 0·28298 |
| 1·5 | 4·4816 | 0·03150 | 0·10242 | 0·21179 |
| 1·8 | 6·0496 | 0·02468 | 0·07746 | 0·15846 |
| 2·1 | 8·1661 | 0·01917 | 0·05850 | 0·11852 |
| 2·4 | 11·0231 | 0·01479 | 0·04412 | 0·08861 |
| 2·7 | 14·8797 | 0·01135 | 0·03323 | 0·06622 |
| 3·0 | 20·0855 | 0·00868 | 0·02500 | 0·04946 |
| 3·3 | 27·1126 | 0·00661 | 0·01878 | 0·03693 |
| 3·6 | 36·5982 | 0·00501 | 0·01409 | 0·02756 |
| 3·9 | 49·4024 | 0·00379 | 0·01056 | 0·02056 |
| 4·2 | 66·6863 | 0·00285 | 0·00791 | 0·01533 |
| 4·5 | 90·0171 | 0·00215 | 0·00592 | 0·01143 |
| 4·8 | 121·5104 | 0·00161 | 0·00442 | 0·00851 |
| 5·1 | 164·0219 | 0·00121 | 0·00330 | 0·00634 |
| 5·4 | 221·4064 | 0·00090 | 0·00246 | 0·00472 |
| 5·7 | 298·8674 | 0·00067 | 0·00184 | 0·00351 |
| 6·0 | 403·4287 | 0·00050 | 0·00137 | 0·00261 |
| 6·3 | 544·5719 | 0·00037 | 0·00102 | 0·00194 |
| 6·6 | 735·0951 | 0·00028 | 0·00070 | 0·00144 |

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 6.7




The $3k_B T\chi_s/S(S+1)(g\mu_B)^2$ versus $\ln T/T_K$ plot for $S=1/2$, 1, 3/2 impurities. The dashed line in the right-hand side of the figure is the high-temperature asymptotic behaviour: $3T\chi_s/S(S+1)\to 1-1/(\ln T/T_K)$. The dashed lines in the left-hand side are the low-temperature ones: $3T\chi_s\to S^2-1/4$ (after Melnicov 1982 a).

(1980 a). $3\chi/S(S+1)$ for zero magnetic field for $S=1/2$, 1, 3/2 as a function of $\ln T/T_K$ (Melnikov 1982 a, Rajan *et al.* 1982 are plotted in fig. 6.7. Rajan *et al.* (1982) also calculated the specific heat of the $S=1/2$ impurity and the impurity magnetization as a function of $H/T$ for various values of the magnetic field.

### 6.2. *The anisotropic s–d exchange model at finite temperatures*

The description of the anisotropic s–d exchange model at finite temperatures is more complicated and contains some new elements not encountered in the isotropic case. This is due to the complicated classification of the general solutions of eqns. (4.3.B):

$$\exp(ik_jL)=\prod_{\alpha=1}^{M}\frac{\sinh\mu(\lambda_\alpha+i/2)}{\sinh\mu(\lambda_\alpha-i/2)}, \tag{6.2.A}$$

$$\left[\frac{\sinh\mu(\lambda_\alpha+i/2)}{\sinh\mu(\lambda_\alpha-i/2)}\right]^N\frac{\sinh\mu(\lambda_\alpha+f/\mu+i/2)}{\sinh\mu(\lambda_\alpha+f/\mu+i/2)}=-\prod_{\beta=1}^{M}\frac{\sinh\mu(\lambda_\alpha-\lambda_\beta+i)}{\sinh\mu(\lambda_\alpha-\lambda_\beta-i)}. \tag{6.2.B}$$

This classification is defined in the leading order of $1/N$. We have already mentioned that eqns. (6.2.B), without the impurity term, coincides with the Bethe equations for an anisotropic Haisenberg chain ($XXZ$ model). The $XXZ$ model at finite temperatures was investigated in detail in the remarkable paper by Takahashi and Suzuki (1972). Their paper contains all the necessary mathematics. In this section we treat the thermodynamics of the anisotropic s–d model using our unpublished results and the paper by Hida *et al.* (1983). We shall consider the case $I_{\|}>I_{\perp}$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

6.2.1. *Classification of states and basic equations for $I_\perp < I_\parallel < \pi$*

In the thermodynamic limit $N, M_n, L \to \infty$, $N/L, M_n/L = \text{const.}$ the roots of (6.2.B) are grouped in various strings characterized by a common real abscissa $\lambda_\alpha^{(n,v)}$, order and purity $v = \pm 1$:

$$\lambda_\alpha^{(n,k,+)} = \lambda_\alpha^{(n,+)} + i\left(\frac{n+1}{2} - k\right) + O(\exp(-\delta N)) \qquad \left(\operatorname{mod} \frac{i\pi}{\mu}\right),$$

$$\lambda_\alpha^{(n,k,-)} = \lambda_\alpha^{(n,-)} + i\left(\frac{n+1}{2} - k\right) + \frac{i\pi}{2\mu} + O(\exp(-\delta N) \qquad \left(\operatorname{mod} \frac{i\pi}{\mu}\right), \quad (6.2.1)$$

where $\alpha = 1, \ldots, M_n$, $k = 1, 2, \ldots, n$, and $\lambda_\alpha^{(n,v)}$ is real. These states are the $n$th-order strings with + and − parities, respectively.

The parity $v$ and order $n$ of a bound state should satisfy the conditions (Takahashi and Suzuki 1972)

$$v \sin \mu k \sin \mu(n-k) > 0, \qquad k = 1, \ldots, n \quad (6.2.2)$$

which are proved in Appendix A to 6.2.1 and solved in Appendix B to 6.2.1.

The classification of numbers $(n, v)$, permitted by (6.2.2), which was done by Takahashi and Suzuki (1972) for an arbitrary $\mu$, is rather complex. For the sake of simplicity we consider the simplest case

$$\pi/\mu = \nu \geqslant 2 \quad (6.2.3)$$

($\nu$ is an integer). The fundamental equations for an arbitrary $\mu \leqslant \pi/2$ is written down in Appendix B to 6.2.1. For $\mu = \pi/\nu$ the classification of solutions is quite simple. Only $\nu$ pairs $(n, v)$ satisfy the condition (6.2.2):

$$v = +, \qquad n_j = j = 1, 2, \ldots, \nu - 1,$$
$$v = -, \qquad n_\nu = 1.$$

As in the isotropic case, the discrete equations for real $\lambda_\alpha^{(n,v)}$ have the form (6.1.8), but now we should define $p_n$ and $\Xi_{nm}$ as follows:

$$\left.\begin{aligned} p(\lambda; n, v) &= 2v \tan^{-1}[(\cot n\mu/2)^v \tanh \lambda\mu] \\ \Xi_{jk}(\lambda) &= p(\lambda, |n_j - n_k|, v_j v_k) + p(\lambda, n_j + n_k, v_j v_k) \\ &\quad + 2 \sum_{q=1}^{\min(n_j, n_k)-1} p(\lambda, |n_j - n_k| + 2q, v_j v_k). \end{aligned}\right\} \quad (6.2.4)$$

At $\mu = \pi/\nu$ the function $p(\lambda, n_j, v_j)$ monotonously increases for $j = 1, \ldots, \nu - 1$ and decreases for $j = \nu$. Therefore, the solutions $\lambda_\alpha^{(n,v)}$ monotonously increase with increasing $J_\alpha^{n,v}$ when $j = \nu, v_j = +1$ and monotonously decrease when $j = \nu$ and $v_\nu = -1$. Taking this into account let us write down the equations for distribution functions of particles and holes:

$$\left.\begin{aligned} a_j(\lambda) + \frac{1}{N} a_j(\lambda + f/\mu) &= \tilde{\rho}_j(\lambda) + A_{jk} * \rho_k(\lambda) + b_j * \rho_\nu(\lambda), \qquad j = 1, \ldots, \nu - 1, \\ a_\nu(\lambda) + \frac{1}{N} a_\nu(\lambda + f/\mu) &= -\tilde{\rho}_\nu(\lambda) - \rho_\nu(\lambda) + a_2 * \rho_\nu(\lambda) + b_j * \rho_j(\lambda), \end{aligned}\right\} \quad (6.2.5)$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where

$$\left.\begin{aligned}
a_j(\lambda) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \exp(-i\omega\lambda))\left[\frac{\sinh(v-j)\omega/2}{\sinh v\omega/2}\right]d\omega,\\
a_v(\lambda) &= -\frac{1}{2\pi}\int_{-\infty}^{+\infty} \exp(-i\omega\lambda)\left[\frac{\sinh\omega/2}{\sinh v\omega/2}\right]d\omega,\\
b_j(\lambda) &= \delta_{j,v-1}\delta(\lambda) - \frac{1}{\pi}\int_{-\infty}^{+\infty} \exp(-i\omega\lambda)\frac{\cosh\omega/2\sinh j\omega/2}{\sinh v\omega/2}d\omega,\\
A_{jk} &= a_{|j-k|} + a_{j+k} + 2\sum_{q=1}^{\min(j,k)-1} a_{|j-k|+2q} + \delta_{jk}\delta(\lambda).
\end{aligned}\right\} \tag{6.2.6}$$

The energy of the system is

$$E^{\mathrm{sp}} = -\sum_{j=1}^{v}\int d\lambda\rho_j(\lambda)(p(\lambda, n_j, v_j) + \pi\theta(v_j) - n_j\mu) + \frac{v-1}{v}HS^z. \tag{6.2.7}$$

As usual it is convenient to express all the quantities in terms of the hole distribution. Reversing the matrix $A$

$$(A^{-1})_{jk}(\lambda) = \delta_{jk}\delta(\lambda) - s(\lambda)(\delta_{j,k+1} + \delta_{j,k-1}) \tag{6.2.8}$$

and using the relations

$$(A^{-1})_{jk} * a_k(\lambda) = \delta_{j1}s(\lambda), \qquad (A^{-1})_{jk} * b_k(\lambda) = -\delta_{j,v-2}s(\lambda) \tag{6.2.9}$$

we obtain

$$\delta_{j1}\left(s(\lambda) + \frac{1}{N}s\left(\lambda + \frac{f}{\mu}\right)\right) = \rho_j(\lambda) + (A^{-1})_{jk} * \tilde{\rho}_k(\lambda) - s * \rho_v(\lambda)\delta_{j,v-2}, \tag{6.1.10 a}$$

$$\rho_v(\lambda) + \tilde{\rho}_v(\lambda) = s * \tilde{\rho}_{v-2}(\lambda), \tag{6.2.10 b}$$

$$\frac{1}{N}E = E^{(0)} + \frac{2\epsilon_{\mathrm{F}}}{\pi}\int \tan^{-1}\exp(\pi\lambda)\tilde{\rho}_1(\lambda)\,d\lambda, \tag{6.2.10 c}$$

$$\frac{1}{N}S^z = \frac{v}{2}\left(\int \tilde{\rho}_{v-1}(\lambda)\,d\lambda - \int \rho_v(\lambda)d\lambda\right). \tag{6.2.10 d}$$

Analogously, the equations for energies of elementary excitations take the form

$$\left.\begin{aligned}
\varepsilon_j(\lambda) &= Ts * \ln(1 + \exp(\varepsilon_{j-1}(\lambda)/T))(1 + \exp(\varepsilon_{j+1}(\lambda)/T)) + \delta_{j,v-2}\\
&\quad \times T\ln(1 + \exp(-\varepsilon_v(\lambda)/T))\\
&\quad -(2\epsilon_{\mathrm{F}}/\pi)\delta_{j1}\tan^{-1}\exp(\pi\lambda); \qquad j \leqslant v-2,\\
\varepsilon_{v-1}(\lambda) &= H(v-1)/2 + Ts * \ln(1 + \exp(\varepsilon_{v-2}(\lambda)/T)),\\
\varepsilon_v(\lambda) &= H(v-1)/2 - Ts * \ln(1 + \exp(\varepsilon_{v-2}(\lambda)/T)).
\end{aligned}\right\} \tag{6.2.11}$$

Thus, in the case $\mu = \pi/v$ we have a finite number of equations. The first $v-3$ equations coincide with those for the isotropic case.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The free energy has the following form:

$$\frac{1}{N}\mathscr{F}_{\mathrm{h}}^{\mathrm{sp}} = -T\int s(\lambda)\ln\left(1+\exp\left(1+\exp\frac{\varepsilon_1(\lambda)}{T}\right)\right)d\lambda$$

$$= \frac{T}{2\epsilon_{\mathrm{F}}}\sum_{n=1}^{\nu}\int_{\min\varepsilon_n}^{\max\varepsilon_n} d\varepsilon \ln n(-\varepsilon), \tag{6.2.12 a}$$

$$\mathscr{F}_{\mathrm{i}} = -T\int s(\lambda+f/\mu)\ln\left(1+\exp\left(\varepsilon_1(\lambda)/T\right)\right)d\lambda. \tag{6.2.12 b}$$

When $T \ll \epsilon_{\mathrm{F}}$, $\mu < \pi/2$ one should put $\tan^{-1}\exp(\pi\lambda) \simeq \exp(\pi\lambda)$ in the first equation of (6.2.11). Then eqns. (6.2.11) become universal equations for the dimensionless functions $\varphi_n$:

$$\varphi_n(\lambda) = \frac{1}{T}\varepsilon_n\left(\lambda+\frac{1}{\pi}\ln\frac{\pi T}{2\epsilon_{\mathrm{F}}}\right), \qquad n=1,\ldots,\nu-2,$$

$$\varphi_{\nu-1}(\lambda) = \frac{1}{T}\varepsilon_{\nu-1}\left(\lambda+\frac{1}{\pi}\ln\frac{T\pi}{2\epsilon_{\mathrm{F}}}\right) - \frac{H(\nu-1)}{2T}.$$

We have

$$\left.\begin{aligned}
&\varphi_n(\lambda) = s*\ln\left(1+\exp\left(\varphi_{n-1}(\lambda)\right)\right)\left(1+\exp\left(\varphi_{n+1}(\lambda)\right)\right) - \delta_{n1}\exp(\pi\lambda),\\
&\varphi_{\nu-2} = s*\ln\left(1+\exp\left(\varphi_{\nu-3}\right)\left(1+2\cosh\frac{H(\nu-1)}{2T}\right.\right.\\
&\qquad\qquad\left.\left.\times\exp\left(\varphi_{\nu-1}\right)+\exp\left(2\varphi_{\nu-1}\right)\right)\right),\\
&\varphi_{\nu-1} = s*\ln\left(1+\exp\left(\varphi_{\nu-2}\right)\right),
\end{aligned}\right\} \tag{6.2.13 a}$$

$$\mathscr{F}_{\mathrm{i}} = -T\int s\left(\lambda+\frac{1}{\pi}\ln\frac{T}{T_{\mathrm{K}}}\right)\ln\left(1+\exp\left(\varphi_1(\lambda)\right)\right)d\lambda. \tag{6.2.13 b}$$

For $\nu=2$ (Toulouse limit) eqns. (6.2.13 *a*) turn into

$$\varphi_1(\lambda) = -\exp(\pi\lambda) + H/2T. \tag{6.2.14}$$

Using this relation and eqn. (6.2.13 *b*) we obtain the expression

$$\mathscr{F}_{\mathrm{i}}\left(\mu=\frac{\pi}{2}\right) = -\frac{T}{\pi}\int_0^\infty \frac{T_{\mathrm{K}}\,dk}{k^2+T_{\mathrm{K}}^2}\ln\left(1+\exp\frac{H/2-k}{T}\right), \tag{6.2.15}$$

which corresponds to the Toulouse hamiltonian (see § 3.1.1).

The next simple case is that of $\nu=3$. There are only two equations:

$$\left.\begin{aligned}
&\varphi_1(\lambda) = -\exp(\pi\lambda) + s*\ln\left(1+2\cosh H/T\exp\left(\varphi_2(\lambda)\right)+\exp\left(2\varphi_2(\lambda)\right)\right),\\
&\varphi_2(\lambda) = s*\ln\left(1+\exp\left(\varphi_1(\lambda)\right)\right),\\
&\mathscr{F}_{\mathrm{i}} = -T\varphi_2\left(-\frac{1}{\pi}\ln\frac{T}{T_{\mathrm{K}}}\right).
\end{aligned}\right\} \tag{6.2.16}$$

The eqns. (6.2.13) for $\nu=2,3,\ldots$ have been chosen as consecutive approximations to the infinite system (6.1.60) for a numerical analysis (Melnicov 1982) (see also § 6.1.11). Such a procedure proved to be rapidly convergent.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

6.2.2. *Impurity thermodynamics at $I_\perp < I_\parallel < \pi$*

We present below a detailed realization of the program discussed in § 6.1.

The function $\varphi_\nu$ monotonously increases and $\varphi_j\, j \neq \nu$, monotonously decreases. Let us define the function $f_j(\lambda)$:

$$f_j^2(\lambda) = (1 + \exp(\varphi_j(\lambda))).$$

When $\lambda \to -\infty$, satisfy the following system of equations for $\bar{f}_j = \lim_{\lambda \to -\infty} f_j(\lambda)$:

$$\bar{f}_j^2 - 1 = \bar{f}_{j+1}\, \bar{f}_{j-1}(1 + \delta_{j,\nu-2}\, \bar{f}_{\nu-2} \exp(-H(\nu-1)/2T)), \tag{6.2.17}$$

$$\varphi_\nu(-\infty) = -\ln \bar{f}_{\nu-2}, \qquad \varphi_{\nu-1}(-\infty) = \ln \bar{f}_{\nu-2}, \tag{6.2.18}$$

with boundary condition $\bar{f}_0 = 1$.

The solution is

$$\bar{f}_j = \sinh\left[\frac{H(\nu-1)}{2T\nu}(j+1)\right] \Big/ \sinh\frac{H(\nu-1)}{2T\nu} \tag{6.2.19}$$

when $\lambda \to +\infty$, the limiting functions $\tilde{f}_j = \lim_{\lambda \to +\infty} f_j(\lambda)$ satisfy the same eqns. (6.2.17)–(6.2.18) with another boundary condition:

$$\tilde{f}_1 = 1.$$

In that case one obtains

$$\tilde{f}_j = \frac{\sinh H_j/2T}{\sinh H/2T}. \tag{6.2.20}$$

In such a manner we see that all the $\varepsilon_j$s are positive except the function $\varepsilon_1(\lambda)$ which changes a sign when $\lambda$ approaches $-B$. The qualitative behaviour of the $\varepsilon_j$s is illustrated in fig. 6.8 (*a*).

Therefore, for zero temperature there remains only one equation for $\varepsilon_1(\lambda)$:

$$\varepsilon_1(\lambda) + \int_{-B}^{\infty} a_2(\lambda - \lambda')\varepsilon_1(\lambda')\, d\lambda' = 2H\frac{(\nu-1)}{\nu} - \frac{\epsilon_F}{\pi}\left(p_1(\lambda) + \pi\left(1 - \frac{1}{\nu}\right)\right). \tag{6.2.21}$$

One may be convinced that eqns. (6.2.11) and (6.2.12 *a*) describe the thermodynamics of a free gas. According to (6.2.10 *d*) and the relation between $\rho_j$ and $\varepsilon_j$ we have the correct magnetic moment:

$$S^z = \frac{T\nu}{4\epsilon_F}\ln\left(\frac{1 + \exp(\varepsilon_{\nu-1}(\lambda)/T)}{1 + \exp(-\varepsilon_\nu(\lambda)/T)}\right)\Bigg|_{+\infty}^{-\infty} = \frac{H}{4\epsilon_F} \tag{6.2.22}$$

The spin part of the entropy has the following form:

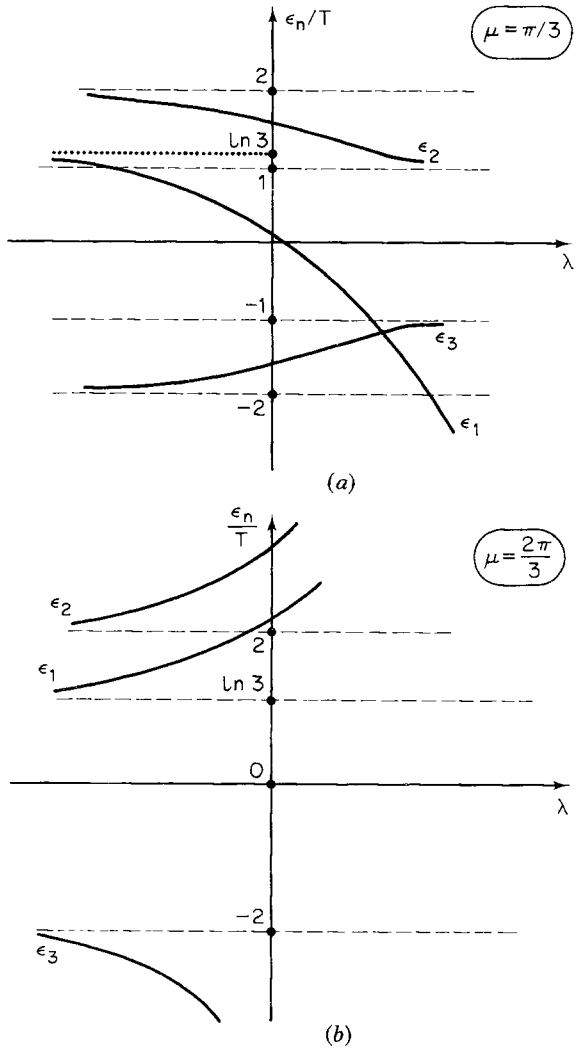
$$S^{sp} = -\frac{T}{2\epsilon_F}\sum_{n=1}^{\nu}\int_{\min\varepsilon_n}^{\max\varepsilon_n} d\varepsilon(n(\varepsilon)\ln n(\varepsilon) + (1 - n(\varepsilon))\ln(-n(\varepsilon))). \tag{6.2.23}$$

In the Appendix to 6.2.2 we prove that this complex expression does lead to the correct value—half of the entropy of the free Fermi gas

$$S^{sp} = \frac{\pi^2}{6}T/\epsilon_F. \tag{6.2.24}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 6.8




Schematic sketch of the excitation spectrum of the anisotropic s–d model ($T\neq 0$) (*a*) $\mu=\pi/\nu$ ($\nu=3,4,\ldots$); (*b*) $\mu=\pi(1-1/\nu)$ ($\nu=3,4,\ldots$).

As in the isotropic case one obtains the ratio $C_i/T\chi_i$

$$C_i/T\chi_i=2\pi^2/3.$$

This ratio appears to be independent of the anisotropy (Wiegmann and Finkelstein 1978).

The analysis of eqns. (6.2.13) is quite analogous to that of the isotropic case. One may show that the function

$$C(\omega, H/T)=\int_{-\infty}^{+\infty}\exp(-i\omega\lambda)\ln(1+\exp(\varphi_1(\lambda)))\,d\lambda$$

has no singularities in the lower half-plane except $-i\infty$ and it has a set of poles

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$\omega = i\mu n$ and zeros $\omega = i\pi n$ in the upper half-plane. This property leads to the law of integer powers at $T \ll T_K$:

$$\mathscr{F}_i = -\frac{\pi}{6}\frac{T^2}{T_K} + T\sum_{n=1}^{\infty} a_n\left(\frac{T}{T_K}\right)^{2n+1}$$

and to the scaling expansion for $T \gg T_K$:

$$\mathscr{F}_i = -T\ln 2 + \sum_{n=1}^{\infty} b_n (T_K/T)^{2\mu n/\pi}.$$

6.2.3. *Impurity thermodynamics at* $\pi < I_{\|} < 2\pi$

We restrict our consideration below by $\mu = \pi(1-1/\nu)(\nu = 2, 3, \ldots)$. Generally speaking, in this case the classification of the complex solutions of eqns. (4.3.B) differs from that used above. However, instead of deriving all thermodynamics anew one may use all the results of § 6.2.2 by employing the following trick. In eqns. (6.2.A) and (6.2.B) make the following change of variables:

$$(1-1/\nu)\lambda = \lambda'/\nu + i/2.$$

Then from eqns. (4.3.A.) and (4.3.B) we obtain

$$\left.\begin{aligned} \exp(ik_jL) &= \prod_{\alpha=1}^{M} \frac{\sinh(\pi/\nu)(\lambda_\alpha - i/2)}{\sinh(\pi/\nu)(\lambda_\alpha + i/2)}, \\ \left[\frac{\sinh(\pi/\nu)(\lambda_\alpha + i/2)}{\sinh(\pi/\nu)(\lambda_\alpha - i/2)}\right]^N & \frac{\sinh[(\pi/\nu)(\lambda_\alpha + i/2) + f]}{\sinh[(\pi/\nu)(\lambda_\alpha - i/2) + f]} \\ &= -\prod_{\beta=1}^{M} \frac{\sinh(\pi/\nu)(\lambda_\alpha - \lambda_\beta + i)}{\sinh(\pi/\nu)(\lambda_\alpha - \lambda_\beta - i)} \end{aligned}\right\} \quad (6.2.25)$$

Thus eqns. (6.2.25) bring us back to the case of $\mu = \pi/\nu < \pi/2$. The only difference is that the sign of the spin part of energy changes:

$$E^{sp} = \sum_{j=1}^{\nu}\sum_{\alpha=1}^{M_{n_j}}\left[p(\lambda_\alpha, n_j, v_j) + \pi\theta(v_j) - \frac{\pi}{\nu}n_j\right]$$

(compare with (6.2.7)). Therefore, we may use eqns. (6.2.11) changing sign at $\tan^{-1}\exp(\pi\lambda)$ in them. This innocuous change of sign alters the structure of the ground state cardinaly. The general behaviour of the $\varepsilon_j$'s change: all $\varepsilon_j$ $(j \neq \nu)$ are monotonously increasing and $\varepsilon_\nu$ is monotonously decreasing. However, the limiting values of these functions at $-\infty$ are not influenced by the free term and are still equal to those given by (6.2.19). On the contrary, the limiting values of the $\varepsilon_j$'s at $+\infty$ change and are now of the order of $\varepsilon_F$.

It is convenient to use again the matrix $A$ and rewrite eqns. (6.2.11) in such a way:

$$\left.\begin{aligned} &\varepsilon_\nu + TK * \ln(1+\exp(\varepsilon_\nu/T)) - Q_j * T\ln(1+\exp(-\varepsilon_j/T)) = \varepsilon_\nu^{(0)} + H/2, \\ &\varepsilon_j + TB_{jk} * \ln(1+\exp(-\varepsilon_k/T)) - Q_j * T\ln(1+\exp(\varepsilon_\nu/T)) \\ &\qquad\qquad = \varepsilon_j^{(0)} + H/2\delta_{j,\nu-1}, \end{aligned}\right\} (6.2.26)$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where the Fourier transforms of the kernels are

$$\left.\begin{aligned}
K(\lambda)&=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega\exp(-i\omega\lambda)\frac{\sinh(\nu-2)\omega/2}{2\sinh\omega/2\cosh(\nu-1)\omega/2},\\
Q_j(\lambda)&=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega\exp(-i\omega\lambda)\left[\frac{\coth\omega/2\sinh j\omega/2}{\cosh(\nu-1)\omega/2}\right.\\
&\qquad\left.-\delta_{jm\nu-1}\frac{\sinh\nu\omega/2}{2\cosh(\nu-1)\omega/2\sinh\omega/2}\right],\\
B_{jk}&=A_{jk}+b_j\frac{1}{1-a_2}b_k
\end{aligned}\right\}\tag{6.2.27}$$

and the right-hand sides are

$$\left.\begin{aligned}
\varepsilon_\nu^{(0)}&=-\varepsilon_{\nu-1}^{(0)}(\lambda)=-\frac{2\epsilon_F}{\pi}\tan^{-1}\exp(\pi\lambda/(\nu-1)),\\
\varepsilon_j^{(0)}(\lambda)&=\frac{4\epsilon_F}{\pi}\left[\pi/2+\tan^{-1}\left(\frac{\sinh\pi\lambda/(\nu-1)}{\sin\pi j/2(\nu-1)}\right)\right],\qquad j=1,\ldots,\nu-1.
\end{aligned}\right\}\tag{6.2.28}$$

The region of $\varepsilon_j\sim T$ gives the main contribution to all integrals in eqns. (6.2.26). In leading order in $T/\epsilon_F$ one may use asymptotics of

$$\begin{aligned}
\varepsilon_j^{(0)}(\lambda)&=C_j\exp(\pi\lambda/\nu-1),\qquad j=1,\ldots,\nu;\\
C_j&=\frac{4\epsilon_F}{\pi}\sin(\pi j/2(\nu-1));\qquad (j=1,\ldots,\nu-2);\\
C_\nu&=-C_{\nu-1}=-2\epsilon_F/\pi;
\end{aligned}$$

and define a dimensionless function

$$\varphi_j(\lambda)=\frac{1}{T}\varepsilon_j\left(\lambda+\frac{(\nu-1)}{\pi}\ln\frac{\pi T}{2\epsilon_F}\right).$$

The function $\varphi_j$ satisfies the following universal equations:

$$\left.\begin{aligned}
&\varphi_\nu+K*\ln(1+\exp(\varphi_\nu))+\sum_{j=1}^{\nu-1}Q_j*\ln(1+\exp(-\varphi_j))\\
&\quad=H/2T-\exp(\pi\lambda/\nu-1),\\
&\varphi_j+B_{jk}*\ln(1+\exp(-\varphi_k))+Q_j*\ln(1+\exp(\varphi_\nu))\\
&\quad=H/2T\delta_{j,\nu-1}+(2\sin\pi j/2(2\nu-1)-\delta_{j,\nu-1})\exp(\pi\lambda/\nu-1).
\end{aligned}\right\}\tag{6.2.29}$$

The free energy is

$$\mathscr{F}_{\mathrm{i}}=-T\sum_{j=1}^{\nu}\int\rho_j\left(\lambda+\frac{\nu-1}{\pi}\ln\frac{T}{T_K}\right)\ln(1+\exp(-\varphi_j(\lambda)(-1)^{\theta(\nu-j-1)})),\tag{6.2.30 a}$$

$$\mathscr{F}_{\mathrm{h}}^{\mathrm{sp}}=N\mathscr{F}_{\mathrm{i}}(T_K=2\epsilon_F/\pi),\tag{6.2.30 b}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where

$$\rho_j(\lambda)=\frac{1}{2\epsilon_F}(-1)^{\theta(\nu-j-1)}\frac{\partial\varepsilon_j^{(0)}(\lambda)}{\partial\lambda}.$$

The functions $\ln(1+\exp(\varphi\nu)$, $\ln(1+\exp(-\varphi_j))$ decrease as $\exp(-\exp(\pi\lambda/\nu-1))$ when $\lambda$ tends to plus infinity ($\lambda\to+\infty$) and all integrals in eqns. (6.2.29) and (6.2.30) are rapidly convergent.

We have already seen that only $\varepsilon_\nu$ changes its sign, all the $\varepsilon_j$s ($j\neq 0$) being positive. Therefore, eqns. (6.2.26) turn, for $T\to 0$, into a linear integral equation:

$$\varepsilon_\nu(\lambda)+\int_{-\infty}^{+\infty}K(\lambda-\lambda')\varepsilon_\nu(\lambda')\,d\lambda'=\frac{H}{2}-\frac{2\epsilon_F}{\pi}\exp\frac{\pi\lambda}{\nu-1}. \tag{6.2.31}$$

Equation (6.1.43) makes it obvious that eqn. (6.2.31) coincides with eqn. (5.2.10 *a*), already studied for $T=0$.

Note that in the region $\mu>\pi/2$ we have for $j\neq\nu$, $T=0$

$$\varphi_j(\lambda)=(2\sin\pi j/2(\nu-1)-\delta_{j,\nu-1})\exp(\pi\lambda/\nu-1)+O(H/\epsilon_F).$$

Contrary to the case $\mu<\pi/2$ the functions $\varphi_j$ do not vanish even at $H$, $T=0$.

It is shown in the Appendix to 6.2.2 that the formulae (6.2.29) and (5.2.30 *b*) describe a free non-interacting gas. The behaviour of the functions $\varphi_j(\lambda)$ is presented in fig. 6.8 (*b*).

*Appendix A to §6.2.1. The Proof of the 'string' hypothesis*

The 'string' hypothesis has a long history going back 50 years to Bethe's (1931) treatment of the one-dimensional Haisenberg spin chain. According to Bethe the accuracy of string solutions is of the order of $\exp(-\text{const}\,N)$. This does occur for strings forming a ground state (such kinds of strings appear, for instance, in the Haisenberg ring with high spin $S>1/2$(4.1.15), the Hubbard model (4.1.22) and in the Anderson model (§ 8 and Appendix to 8.2.1)). The strings, which are excitations, become a good approximation only when the density of other excitations keep finite when one passes to the thermodynamic limit

$$N\to\infty;\qquad L\to\infty;\qquad \frac{N}{L}=\text{const};\qquad n/L=\text{const}. \tag{A 1}$$

The accuracy of the strings is (Destri and Lowenstein 1982, Woynarovich 1982, Babelon *et al.* 1982):

$$O(\exp(-\text{const}\,n)). \tag{A 2}$$

At low temperature and magnetic field the average number of the gapless excitations $n\sim L\max(T,H)$. The conception of the thermodynamic limit determines the order of the limits $N,L\to\infty$ and $T,H\to 0$ which do not formally commute:

$$\lim_{H,T\to 0}\lim_{N\to\infty}O\left(\exp\left(-\frac{\max(T,H)}{\epsilon_F}N\right)\right)=0. \tag{A 3}$$

It means that the string hypothesis is valid in the thermodynamic limit. Here we prove the string hypothesis for the s–d exchange model. We confine our consideration to the case of the anisotropic model with $\mu<\pi/2$. One can extend this proof to the isotropic case passing in the end to the $\mu=0$ limit.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Let us consider eqns. (4.3.B). At first we drop the impurity term which does not change the classification of the strings. Then we have

$$\left(\frac{\sinh\mu(\lambda_\alpha+i/2)}{\sinh\mu(\lambda_\alpha-i/2)}\right)^N=-\prod_{\beta=1}^{M}\frac{\sinh\mu(\lambda_\alpha-\lambda_\beta+i)}{\sinh\mu(\lambda_\alpha-\lambda_\beta-i)}. \tag{A 4}$$

According to conjecture (6.2.1) the arrangement of zeros and poles of the $S$ matrix of bare particles (the right-hand side of (A 4)) establishes the form of the string. In our case this conjecture is

$$\lambda_\alpha^{(n,v,k)}=\lambda_\alpha^{(n,v)}+\left(\frac{n+1-2k}{2}\right)i+\frac{\pi}{4\mu}(1-v)i+\gamma_k^{(n,v)}\qquad\left(\mathrm{mod}\left(\frac{\pi}{\mu}i\right)\right), \tag{A 5}$$

$$k=1,\ldots,n;\quad v=\pm1,$$

where the $n$'s are some selected integers. Let us find the accuracy $\gamma_k^{(n,v)}$ of the conjecture (A 5)†. Let us consider the state with $M_n^v$ strings of order $n$. Inserting (A 5) into (A 4) we obtain

$$\left.\begin{aligned}&\left[\frac{\sinh\mu(\lambda+i(n/2+1-k))}{\sinh\mu(\lambda+i(n/2-k))}\right]^N\\&=\prod_{\substack{m\neq n\\m=1}}^{\infty}\prod_{l=1}^{m}\prod_{\beta=1}^{M_m^{(+)}}\frac{\sinh\mu(\lambda-\lambda_\beta^{(m,+)}+i(n-m/2+1-k-l))}{\sinh\mu(\lambda-\lambda_\beta^{(m,+)}+i((n-m)/2-1-k+l))},\\&\quad\times\prod_{l=1}^{n}\frac{\sin\mu(l+1-k+i\gamma^{(l)}-i\gamma^{(k)})}{\sin\mu(l-1-k+i\gamma^{(l)}-i\gamma^{(k)})}\\&\quad\times\prod_{m=1}^{\infty}\prod_{l=1}^{m}\prod_{\beta=1}^{M_m^{(-)}}\frac{\sinh\mu(\lambda-\lambda_\beta^{(m,-)}+i((n-m)/2+1-k+l))}{\sinh\mu(\lambda-\lambda_\beta^{(m,-)}+i((n-m)/2-1-k+l))}\end{aligned}\right\} \tag{A 6}$$

and for $v=-1$

$$\left.\begin{aligned}&\left[\frac{\cosh\mu(\lambda+i(n/2+1-k))}{\cosh\mu(\lambda+i(n/2-k)}\right]^N\\&=\prod_{\substack{m=n\\m=1}}^{\infty}\prod_{l=1}^{m}\prod_{\beta=1}^{M_m^{(-)}}\frac{\sinh\mu(\lambda-\lambda_\beta^{(m,-)}+i((n-m)/2+1-k+l))}{\sinh\mu(\lambda-\lambda_\beta^{(m,-)}+i((n-m)/2)-1-k+l))},\\&\quad\times\prod_{l=1}^{n}\frac{\sin\mu(l+1-k-i\gamma^{(l)}+i\gamma^{(k)})}{\sin\mu(l-1-k-i\gamma^{(l)}+i\gamma^{(k)})}\\&\quad\times\prod_{m=1}^{\infty}\prod_{l=1}^{m}\prod_{\beta=1}^{M_m^{(+)}}\frac{\cosh\mu(\lambda-\lambda_\beta^{(m,+)}+i((n-m)/2+1-k+l))}{\cosh\mu(\lambda-\lambda_\beta^{(m,+)}+i((n-m)/2-1-k+l))};\end{aligned}\right\} \tag{A 7}$$

we omit the subscripts $(n, v)$.

The symmetry of eqn. (A 4) enables us to confine our consideration to the $2k<n$ case:

$$|\gamma_{k+1}-\gamma_k|=|\gamma_{n-k+1}-\gamma_{n-k}|. \tag{A 8}$$

† The proof of the string hypothesis without the assumption (A 5) was made by Babelon *et al.* (1982).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

At first we derive the necessary condition which selects the orders of the strings. For this purpose it is sufficient to consider the case of particular $\{M_n\}$, namely,

$$M_{(n,v)}=\begin{cases}1, & (n,v)=(n_0,v_0)\\ 0, & (n,v)\neq(n_0,v_0).\end{cases}$$

It means that only the string with $(n_0, v_0)$ exists. In this case eqns. (A 6) and (A 7) give us

$$|\gamma_{k+1}-\gamma_k|=\text{const}\left[\left|\frac{\sinh\mu(\lambda+i(n/2-k))}{\sinh\mu(\lambda+in/2)}\right|\right]^N \qquad (v=+1), \tag{A 9}$$

$$|\gamma_{k+1}-\gamma_k|=\text{const}\left|\frac{\cosh\mu(\lambda+i(n/2-k))}{\cosh\mu(\lambda+in/2)}\right|^N \qquad (v=-1), \tag{A 10}$$

$$k=1,\ldots,[n/2].$$

The quantity $|\gamma_{k+1}-\gamma_k|$ is exponentially small only if

$$-\sin^2\mu(n/2-k)+\sin^2\mu n/2>0 \qquad (v=1) \tag{A 11}$$

or

$$-\cos^2\mu(n/2-k)+\cos^2\mu n/2>0 \qquad (v=-1). \tag{A 12}$$

One can rewrite (A 11) and (A 12) as

$$v\sin\mu k\sin\mu(n-k)>0; \qquad k=1,\ldots,<n/2 \tag{A 13}$$

(Takahashi and Suzuki 1972, Korepin 1979, Fowler and Zotos 1981, Hida 1981). The solution of this unequality is given in Appendix 6.2.9.

Let us return to eqns. (A 6) and (A 7) assuming that all the $n$'s satisfy conditions (A 13). Set, for simplicity, $\mu=\pi/v$ where $v$ is an integer. According to § 6.2.1 the continuous limit gives us

$$\left|\frac{\gamma_{k+1}-\gamma_k}{(\gamma_k-\gamma_{k-1})}1-\delta_{k1}\right|\sim\exp\left\{N\left(G_{n-2k+1,m}*\rho_m(\lambda)\right.\right.$$
$$\left.\left.-\operatorname{Re}\ln\left|\frac{\sinh\mu(\lambda+i(n/2+1-k))}{\sinh\mu(\lambda+i(n/2-k))}\right|-t_{n-2k+1}*\rho_v(\lambda)\right)\right\}, \tag{A 14}$$

where Fourier transforms of the kernels $G_{nm}$ and $t_n$ are

$$G_{nm}(\omega)=\frac{2\pi}{\omega}\frac{1}{\sinh v\omega/2}\left[\cosh\frac{(v-n-m-1)\omega}{2}+\cosh\frac{(v-n-m+1)\omega}{2}\right.$$
$$\left.-\cosh\frac{(v-|n-m-1|)\omega}{2}-\cosh\frac{(v-|n-m+1|)\omega}{2}\right]$$
$$(m=1,\ldots,v-1),$$
$$t_n(\omega)=\frac{2\sinh\omega}{\sinh v\omega/2}\sinh n\omega/2.$$

It is convenient to use the 'hole' distributions $\tilde{\rho}_n$ instead of $\rho_n$. According to (6.2.10) one has

$$\rho_n=-(A^{-1})_{nm}*\tilde{\rho}_m+\delta_{n,v-2}s*\rho_v+s\delta_{n1}.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Using the identity

$$(A^{-1})_{nm}G_{ml}=\frac{2\pi}{\omega}\tanh\frac{\omega}{2}(\delta_{n,l+1}+\delta_{n,l-1}) \tag{A 15}$$

we find

$$\left|\frac{\gamma_{k+1}-\gamma_k}{(\gamma_k-\gamma_{k-1})}1-\delta_{k1}\right|\sim\exp\left\{-\frac{N}{2}\int_{-\infty}^{+\infty}d\lambda'\ln|\coth\pi(\lambda-\lambda')|\right.$$
$$\left.\times(\tilde{\rho}_{n-2k}(\lambda')+\tilde{\rho}_{n-2k+2}(\lambda'))\right\}. \tag{A 16}$$

Finally from (A 16) one obtains the following estimate:

$$|\gamma_{k+1}-\gamma_k|\sim\exp\left\{-\frac{N}{2}\int_{-\infty}^{+\infty}d\lambda'\ln|\coth\pi(\lambda-\lambda')|\sum_{q=1}^{k}(\tilde{\rho}_{n-2q}(\lambda')\right.$$
$$\left.+\tilde{\rho}_{n-2q+2}(\lambda'))\right\}. \tag{A 17}$$

From (A 17) it follows that for any $k$

$$|\gamma_{k+1}-\gamma_k|\leqslant|\gamma_2-\gamma_1|\sim\exp\left\{-\frac{N}{2}\int_{-\infty}^{+\infty}d\lambda'\ln|\coth\pi(\lambda-\lambda')|\right.$$
$$\left.\times(\tilde{\rho}_{n-2}(\lambda')+\tilde{\rho}_n(\lambda'))\right\} \tag{A 18}$$

or

$$|\gamma_{p+1}|\leqslant\sum_{k=1}^{p}(\text{r.h.s of (A.18)}).$$

The quantity $\gamma_1$ may be included in the definition of the string's centre $\lambda_\alpha^{(n,m)}$. Estimate (A 18) is valid for $\nu\geqslant4$, both for $\mu=\pi/\nu$ and $\mu=\pi(1-1/\nu)$ (in particular for $\nu\to\infty$, i.e. for the isotropic case). Thus, if condition (A 13) is satisfied formula (A 5) is valid with exponential accuracy for any $\{M_n\}$ for which

$$N\int d\lambda'\ln|\coth\pi(\lambda-\lambda')|(\tilde{\rho}_{n-2}(\lambda')+\tilde{\rho}_n(\lambda'))\gg1.$$

For an equilibrium state at temperature $T$ the estimate (A 18) acquires the form

$$|\gamma_2^{(n,+)}-\gamma_1^{(n,+)}|=\text{const}\exp\left\{-LT\int_{-\infty}^{+\infty}\frac{d\lambda'}{\sinh\pi(\lambda-\lambda')}\right.$$
$$\left.\times\ln\left(1+\exp\frac{\varepsilon_{n-2}(\lambda')}{T}\right)\left(1+\exp\frac{\varepsilon_n(\lambda')}{T}\right)\right\}.$$

We note the difference between the $\mu<\pi/2$ and $\mu>\pi/2$ cases. According to §§ 6.2.2. and 6.2.3

$$T\ln(1+\exp(\varepsilon_n/T))\sim\begin{cases}\max(T,H), & \mu<\pi/2\\ \epsilon_F, & \mu>\pi/2.\end{cases} \tag{A 19}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Therefore,

$$|\gamma^{(n)}| \sim \begin{cases} \exp(-\text{const}\, L \max(T, H)) & \mu < \pi/2 \\ \exp(-\text{const}\, N) & \mu > \pi/2 \end{cases} \tag{A 20}$$

In both cases the string hypothesis is valid in the thermodynamic limit.

*Appendix B to §6.2.1. Thermodynamics equations for the arbitrary exchange anisotropy*

Takahashi and Suzuki (1972) obtained solutions of the constraint (6.2.2) in the following form. Let

$$p_0 = \begin{cases} \pi/\mu & 0 < \mu < \pi/2 \\ \dfrac{\pi}{\pi - \mu} & \pi/2 < \mu < \pi. \end{cases}$$

Let us represent the quantity $p_0^{-1}$ by the continued fraction:

$$\frac{1}{p_0} = \cfrac{1}{v_1 + \cfrac{1}{v_2 + \cfrac{1}{v_3 + \dots}}},$$

where $v_i$ are integers $v_1 \geqslant 2$. Let us define a series of integers $v_i, m_i, y_i$ and a series of real numbers $p_i$ as follows:

$$p_1 = 1, \qquad v_i = [p_{i-1}/p_i], \qquad p_i = p_{i=2} - p_{i-1} v_{i-1}$$

$$m_0 = 0, \qquad m_i = \sum_{k=1}^{i} v_k$$

$$y_{-1} = 0, \qquad y_0 = 1, \qquad y_1 = v_1, \qquad y_2 = v, v_2 + 1$$

and

$$y_i = y_{i-1} + v_i y_{i-1}, \qquad i = 1, 2, \dots .$$

Then the order and parity of all bound states are given by

$$n_j = y_{i-1} + (j - m_i) y_i \quad \text{for} \quad m_i \leqslant j < m_{i+1}, \quad j = 1, 2, \dots$$

$$v_1 = +1, \qquad v_{m_1} = -1 \quad \text{and} \quad v_j = (-1)^{[(n_j - 1)/p_0]},$$

where $[x]$ is the integer part of $x$ (Gauss' symbol).

In these notations the non-linear integral equations have the form:

$$T \ln(1 + \exp(\varepsilon_0(\lambda)/T)) = 2\epsilon_F \theta(\lambda) \operatorname{sign}(\mu - \pi/2),$$

$$\varepsilon_j = T(1 - 2\delta_{m_{i-1}, j}) s_i * \ln(1 + \exp(\varepsilon_{j-1}/T)) + T s_i * \ln(1 + \exp(\varepsilon_{j+1}/T)) \quad \text{for } m_{i-1} \leqslant j \leqslant m_i - 2,$$

$$\varepsilon_j = T(1 - 2\delta_{m_{i-1}, j}) s_i * \ln(1 + \exp(\varepsilon_{j-1}/T)) + T d_i * \ln(1 + \exp(\varepsilon_j/T)) + T s_{i+1} * \ln(1 + \exp(\varepsilon_{j+1}/T)) \quad \text{for } j = m_i - 1,$$

$$\lim_{j \to \infty} \varepsilon_j / n_j = H(1 - \mu/\pi).$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Here

$$s_i(\lambda)=\frac{1}{2p_i}\operatorname{sech}(\pi\lambda/p_i),$$

$$d_i(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega\exp(-i\omega\lambda)\frac{\cosh((p_i-p_{i+1})\omega/2)}{2\cosh p_i\omega/2\cosh p_{i+1}\omega/2},$$

$$\mathscr{F}_i=-T\int s_1\left(\lambda+\frac{fp_0}{\pi}\right)\ln(1+\exp(\varepsilon_1(\lambda)/T))d\lambda.$$

*Appendix to §6.2.2. The proof of the identity (6.2.24)*

Let us prove that the spin part of the host entropy is equal to

$$\frac{1}{N}S^{\mathrm{sp}}=\frac{\pi^2}{6}\frac{T}{\epsilon_{\mathrm{F}}}.$$

Let

$$\gamma(a,b)=-\int_a^b dx\left[\frac{\ln x}{1-x}+\frac{\ln(1-x)}{x}\right].$$

Then

$$\frac{2\epsilon_{\mathrm{F}}}{TN}S^{\mathrm{sp}}=\sum_{j=1}^{\nu}\gamma\left(\frac{\max\varepsilon_j(\lambda)}{T},\min\frac{\varepsilon_j(\lambda)}{T}\right).$$

When $\mu<\pi/2$ according to (6.2.19) and (6.2.20) we have

$$\frac{2\epsilon_{\mathrm{F}}}{TN}S^{\mathrm{sp}}=\gamma\left(1,\frac{1}{(\nu-1)^2}\right)+2\gamma\left(\frac{1}{\nu-1},\frac{1}{\nu}\right)\equiv\Delta_1(\nu).$$

Let us prove that this quantity does not depend on $\nu$. Differentiating with respect to $y=(\nu-1)^{-1}$ one obtains:

$$\frac{d}{dy}\Delta_1(y)=0.$$

Therefore,

$$\frac{1}{N}S^{\mathrm{sp}}=\frac{T}{2\epsilon_{\mathrm{F}}}\Delta_1(\nu=2)=\frac{\pi^2T}{6\epsilon_{\mathrm{F}}}.$$

When $\mu>\pi/2$, $\varepsilon_j(+\infty)\sim\epsilon_{\mathrm{F}}$ $(j\neq\nu)$, $\varepsilon_\nu(+\infty)\sim-\epsilon_{\mathrm{F}}$, the $(\varepsilon_j(-\infty)$'s being the same. Then

$$\frac{2\epsilon_{\mathrm{F}}}{TN}S^{\mathrm{sp}}=2\gamma\left(\frac{1}{\nu},0\right)+\sum_{j=1}^{\nu-2}\gamma\left(\frac{1}{(j+1)^2},0\right)\equiv\Delta_2(\nu).$$

As above, we prove that $\Delta_2(\nu)$ does not depend on $\nu$ and in particular $\Delta_2(\nu)=\Delta_1(\nu)$.

$$\Delta_2(\nu+1)-\Delta_2(\nu)=-2\gamma\left(\frac{1}{\nu},\frac{1}{\nu+1}\right)+\gamma\left(\frac{1}{\nu^2},0\right)=0.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

## §7. Introduction to thermodynamics of the degenerate exchange model

It has been argued in §2 that dilute magnetic alloys of Ce and Yb may be described by the exchange hamiltonian (4.4.1). The Bethe Ansatz for the degenerate exchange model has been constructed in §4.4. Now using the previous results we shall study the thermodynamics of this model.

This section is written for a reader who has already studied the previous sections. Therefore, we change the traditional scheme and start our consideration from finite temperatures. The integral equations describing the system at $T\neq 0$ are cumbersome. Even for $T=0$ we succeeded in finding the analytical expression for $\chi_i(H)$ only for $n=3$ $(J=1)$. If $n=3$ the system of Wiener–Hopf equations with arbitrary $N_j$ seems to be unsolvable in an analytical form. Thus, most mathematical problems formulated in this section should be solved numerically.

At low energies the reliable Fermi-liquid approach, which is not related to the possibility of an analytical solution, becomes adequate.

The results of the present section were obtained by Tsvelick and Wiegmann 1981, 1982 a) and Rasul (1982).

### 7.1. *Basic equations*

1. The spectrum of the hamiltonian (4.4.1) is described by the Bethe-Ansatz hierarchy (4.4.A)–(4.4.C). The solutions $\lambda_\alpha^{(j)}$ of eqns. (4.4.B) lie in a complex plane. In the thermodynamic limit they are grouped in strings (Takahashi 1974 b)

$$\lambda_{p,k;\alpha}^{(j)}=\lambda_{p;\alpha}^{(j)}+i(p+1-2k)/2; \qquad k=1,\ldots,p. \tag{7.1.1}$$

2. From (4.4.A)–(4.4.B) and (7.1.1) we obtain the integral equations for the distribution functions $\rho_p^{(j)}$ and $\tilde{\rho}_p^{(j)}$ of particles and holes in strings for the thermodynamic limit as follows:

$$\tilde{\rho}_p^{(j)}(\lambda)+A_{pr}*C^{jk}*\rho_r^{(k)}(\lambda)=A_{1p}\delta_{j1}\left(s(\lambda)+\frac{1}{N}s(\lambda+1/g)\right), \tag{7.1.2}$$

$$p,r=1,2,\ldots; \qquad j,k=1,\ldots,n \qquad (n=2J+1).$$

The matrix $\mathbf{A}$ coincides with (6.1.24) and $C^{jk}$ is given by the formula

$$C^{jk}(\lambda)=\delta^{jk}\delta(\lambda)-s(\lambda)(\delta^{j,k+1}+\delta^{j,k-1}). \tag{7.1.3}$$

It is interesting that elements of the matrices $\mathbf{A}^{-1}$ and $\mathbf{C}$ are proportional to each other. The energy of the system and the length of a column in the Young tableau are, respectively, equal to

$$\frac{1}{N}E=E^{(0)}-\frac{2\epsilon_F}{\pi}\sum_{p=1}^{\infty}\int d\lambda\rho_p^{(1)}(\lambda)\left(\frac{\pi}{2}+\tan^{-1}\frac{2\lambda}{p}\right), \tag{7.1.4}$$

$$\frac{N_j}{N}=\sum_{p=1}^{\infty}p\int(\rho_p^{(j)}(\lambda)-\rho_p^{(j-1)}(\lambda))d\lambda, \tag{7.1.5}$$

where $E^{(0)}$ is the ground state energy.

3. The entropy is given by

$$\frac{S}{N}=\sum_{j,p}\int[(\rho_p^{(j)}+\tilde{\rho}_p^{(j)})\ln(\rho_p^{(j)}+\tilde{\rho}_p^{(j)})-\rho_p^{(j)}\ln\rho_p^{(j)}-\tilde{\rho}_p^{(j)}\ln\tilde{\rho}_p^{(j)}]\,d\lambda. \tag{7.1.6}$$

Minimizing the free energy

$$\mathscr{F} = E - TS - \sum_j h^{(j)} N_j$$

with respect to $\rho_p^{(j)}$ we obtain the following non-linear equations for $\varepsilon_p^{(j)} = T \ln \tilde{\rho}_p^{(j)} / \rho_p^{(j)}$:

$$T \ln n(-\varepsilon_p^{(j)}(\lambda)) - A^{jk} * C_{pr} * T \ln n(\varepsilon_r^{(k)}(\lambda)) - \delta_{p1} \frac{2\epsilon_F}{\pi} \tan^{-1}\left[\frac{\sin \pi j/n}{\exp(-2\pi\lambda/n) - \cos \pi j/n}\right] = 0, \quad (7.1.7)$$

where

$$A^{jk}(\lambda) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \exp(-i\omega\lambda) \frac{2 \coth \omega/2}{\sinh n\omega/2} \sinh\left[\frac{\omega}{2}(n\text{-}\max(j,k))\right] \times \sinh\left[\frac{\omega}{2} \min(j,k)\right].$$

The impurity part of free energy and the free energy of the host metal are given by

$$\mathscr{F}_i = T \sum_{j=1}^{n-1} \int d\lambda \rho_0^{(j)}(\lambda + 1/g) \ln n(\varepsilon_1^{(j)}(\lambda)), \quad (7.1.8)$$

$$\mathscr{F}_h = -\frac{T^2\pi^2}{12\epsilon_F} + T \sum_{j=1}^{n-1} \int d\lambda \rho_0^{(j)}(\lambda) \ln n(\varepsilon_1^{(j)}(\lambda)), \quad (7.1.9)$$

where

$$\rho_0^{(j)}(\lambda) = \frac{1}{n} \frac{\sin(\pi j/n)}{\cosh(2\pi\lambda/n) - \cos(\pi j/n)}. \quad (7.1.10)$$

The first term in (7.1.9) is the contribution of charge excitations.

4. Universality. If $T \ll \epsilon_F$, the main contribution to all integrals in eqns. (7.1.7)–(7.1.9) comes from the region $\lambda \ll -(n/2\pi) \ln \epsilon_F / T$. Therefore, one should keep only the asymptotics of the free term in (7.1.7): $\tan^{-1}[\ldots] \simeq \sin(\pi j/n) \exp(2\pi\lambda/n)$. Introducing the dimensionless functions

$$\varphi_p^{(j)}(\lambda) = \frac{1}{T} \varepsilon_p^{(j)}\left(\lambda - \frac{n}{2\pi} \ln \frac{2\epsilon_F}{\pi T}\right) \quad (7.1.11)$$

we obtain the following universal integral equations:

$$A^{jk} * C_{pr} * \ln(1 + \exp(\varphi_r^{(k)}(\lambda))) - \ln(1 - \exp(-\varphi_p^{(j)}(\lambda))) = \delta_{p1} \sin(\pi j/n) \exp(2\pi\lambda/n); \quad \lim_{p \to \infty} \varphi_p^{(j)}/p = h^{(j)}/T, \quad (7.1.12)$$

$$\mathscr{F}_i = -T \sum_{j=1}^{n-1} \int d\lambda \rho_0^{(j)}(\lambda + n/2\pi \ln T/T_K) \ln(1 + \exp(\varphi_1^{(j)}(\lambda))), \quad (7.1.13)$$

where

$$T_K = \frac{2\epsilon_F}{\pi} \exp\left(-\frac{2\pi}{ng}\right) \quad (7.1.14)$$

is the Kondo temperature.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Equations (7.1.12)–(7.1.14) completely describe the thermodynamics of the $n$-fold degenerate exchange model for arbitrary $h^{(j)}$.

### 7.2. *Low-temperature thermodynamics*

It follows from (7.1.12) that

$$\lim_{\lambda\to+\infty} \varphi_1^{(j)}(\lambda)\exp(-2\pi\lambda/n) < \infty$$

and, therefore, all integrals

$$\int_{-\infty}^{+\infty} \exp(2\pi\lambda k/n)\ln(1+\exp(\varphi_1^{(j)}(\lambda)))\,d\lambda$$

converge. Thus if $T, h^{(j)} \ll T_K$ the impurity part of free energy is expanded in power series in $T/T_K$:

$$\mathscr{F}_i = -T\left(\frac{\gamma}{2}\frac{T}{T_K} + \sum_{n=1}^{\infty} b_n\left(\frac{T}{T_K}\right)^{2n+1}\right), \tag{7.2.1}$$

at zero temperature the entropy being zero. The impurity ground state is a singlet.

Using the Fermi-liquid speculations it is easy to find the impurity part of the specific heat and magnetic susceptibility $\chi^j = \partial N_j/\partial h^{(j)}$ at $T=0$, $h_j=0$. According to (7.1.9) and (7.9.11) we have, at $T\to 0$,

$$\frac{1}{N}\mathscr{F}_h = -\frac{\pi^2T^2}{12\epsilon_F} + \frac{\pi T^2}{\epsilon_F}\sum_{j=1}^{n-1}\sin(\pi j/n)\int_{-\infty}^{+\infty}\exp(-2\pi\lambda/n)\ln n(\varphi_1^{(j)}(\lambda))\,d\lambda.$$

Comparing it with (7.1.13) one finds at $T\to 0$

$$\mathscr{F}_i = \frac{2\epsilon_F}{\pi T_K}\left(N^{-1}\mathscr{F}_h + \frac{\pi^2T^2}{12\epsilon_F}\right). \tag{7.2.2}$$

We already know the left-hand side of eqn. (7.2.2). (We may prove it using the relation

$$\rho_p^{(j)}(\lambda) = -\frac{1}{2\epsilon_F}\frac{\partial\varepsilon_p^{(j)}(\lambda)}{\partial\lambda}n(\varepsilon_p^{(j)}(\lambda)) \tag{7.2.3}$$

as has been done for the s–d exchange model (see §6.1.4)),

$$\frac{1}{N}\mathscr{F}_h = -n\frac{\pi^2T^2}{12\epsilon_F} - \frac{1}{16\epsilon_F}\sum_{j=1}^{n} h_j^2. \tag{7.2.4}$$

Therefore, the specific heat and partial susceptibility are

$$\left.\begin{aligned} C_i/C_h &= \frac{(n-1)}{n}\frac{2\epsilon_F}{T_K\pi}, \\ \chi_i^j/\chi_h^j &= \frac{2\epsilon_F}{\pi T_K} \end{aligned}\right\} \tag{7.2.5}$$

and

$$C_i = \frac{\pi}{3}(n-1)\frac{T}{T_K}, \tag{7.2.6 a}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\chi_{\mathrm{i}}^{(j)}=\frac{1}{2\pi T_{\mathrm{K}}}. \tag{7.2.6 b}$$

### 7.3. *Magnetic susceptibility*

It follows from eqn. (7.2.3) that $\varepsilon_p^{(j)}(\lambda)$ monotonously decreases. Equation (7.1.7) states that all the $\varepsilon_p^{(j)}$'s except the $\varepsilon_1^{(j)}$'s are positive. The functions $\varepsilon_1^{(j)}$ change sign at some $-B_j$'s:

$$\varepsilon_1^{(j)}(-B_j)=0. \tag{7.3.1}$$

In other words, the ground state is formed only by real solutions of eqns. (4.4.B). For $T\to 0$ one has the following system of linear integral equations:

$$\varepsilon_1^{(j)}(\lambda)-\int_{-\infty}^{-B_k} R_{jk}(\lambda-\lambda')\varepsilon_1^{(k)}(\lambda')d\lambda'=-\frac{2\epsilon_{\mathrm{F}}}{\pi}\sin\left(\frac{\pi j}{n}\right)\exp(2\pi\lambda/n)$$
$$+\frac{1}{2n}\left[j\sum_{k=j+1}^{n}h^{(k)}-(n-j)\sum_{k=1}^{j}h^{(k)}\right], \tag{7.3.2}$$

where

$$R_{jk}(\lambda)=\int\frac{d\omega}{2\pi}\exp(-i\omega\lambda)(A^{jk}(\omega)-\delta^{jk})/(1+\exp(-|\omega|)). \tag{7.3.3}$$

A length of column in the Young tableau is

$$N_j=m_{j-1}-m_j,$$
$$N_j=-\frac{\partial}{\partial h(j)}\sum_{k=1}^{n-1}\int_{-\infty}^{-B_k}\rho_0^{(k)}(\lambda+1/g)\varepsilon_1^{(k)}(\lambda)\,d\lambda. \tag{7.3.4}$$

The Wiener–Hopf system (7.3.2) with arbitrary values of the $B_j$'s ($h^{(j)}$'s) can hardly be solved analytically. However, we shall show below that for

$$h^{(j)}=H\sin\pi j/n \tag{7.3.5}$$

all the $B_j$'s are equal to each other and the system (7.3.2) may be easily solved.

The 'magnetic susceptibility' $\chi(H)=-\partial^2E_{\mathrm{i}}/\partial H^2$ has the following form

$$\left.\begin{aligned}\chi(H)&=\frac{n^2}{2\pi H}\sin\frac{\pi}{2n}\int_{-\infty}^{+\infty}d\omega\left(\frac{i\omega+0}{e}\right)^{i\omega}\Gamma\left(\frac{1}{2n}-\frac{i\omega}{2}\right)\\&\quad\times\Gamma\left(1-\frac{1}{2n}-\frac{i\omega}{2}\right)\exp\left(i\omega n\ln\frac{H}{T_H}\right),\\\frac{T_H}{T_{\mathrm{K}}}&=4\pi\cos\frac{\pi}{2n}\frac{(ne)^{-1/2}}{n\Gamma(1/n)}.\end{aligned}\right\} \tag{7.3.6}$$

The analytical properties of this expression are analogous to those of (5.1.33) for $n=2$. It is easy to check that expression (7.3.6) for $n=2$ coincides with the expression for the magnetic susceptibility of the s–d exchange model with $S=1/2$.

If $H\gg T_H$ we obtain, from (7.3.6), a power-series expansion in $z(H)$, the invariant charge $z(H)$ being defined as follows:

$$\frac{1}{z(H)}-\frac{1}{n}\ln z(H)=\ln\frac{H}{T_H}. \tag{7.3.7}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The first term of that expansion is

$$\chi(H \gg T_K) = \frac{z^2(H)}{H}. \tag{7.3.8}$$

If $H < T_H$ the function $\chi(H)$ is analytical with respect to $H$:

$$\chi(H) = \frac{n}{4\pi T_K} + \sum_{n=1}^{\infty} a_n \left(\frac{H}{T_K}\right)^{2n+1}. \tag{7.3.9}$$

When $H \to 0$ the susceptibility remains finite and a *complete screening* of an impurity magnetic moment takes place.

Let us assume that the crystal field splitting is negligible compared with $T_K$. Then, generally speaking, one should write the Zeeman term as follows

$$-\mu_B(g_i \mathbf{J}_i^z + g_e(2\mathbf{S}^z + \mathbf{L}^z))\mathfrak{h}, \tag{7.3.10}$$

where $\mathbf{J}_i^z$ is a projection of total impurity momentum, and $\mathbf{S}^z$, $\mathbf{L}^z$ are spin and orbital momentum operators of the conduction electrons. This term does not commute with the hamiltonian (4.4.1) and breaks the integrability. However, we can neglect the remagnetization of an impurity caused by the conduction electrons and rewrite the Zeeman terms as

$$-\mu_B g_i \mathfrak{h} \mathbf{J}^z \equiv -\mu_B \mathbf{g}_i \mathfrak{h} \sum_{j=1}^{n} (m_{j-1} - m_j)\left(\frac{n+1}{2} - j\right), \tag{7.3.11}$$

where $\mathbf{J}^z$ represents the total momentum of the whole system. Indeed, any electron term in (7.3.10) gives small corrections of the order of $g$ compared with the impurity term.

Term (7.3.11) commutes with the hamiltonian. Expressing the quantities $h^{(j)}$ in terms of $\mathfrak{h}$ we find:

$$h^{(j)} = \mu_B g_i \mathfrak{h}\left(\frac{n+1}{2} - j\right). \tag{7.3.12}$$

Conditions (7.3.12) and 7.3.5) coincide only for $J = 1/2$ ($\mu_B g_i \mathfrak{h} = H$) and $J = 1$ ($g_i \mu_B \mathfrak{h} = \sqrt{3}H$).

If $J = 1/2$ or $J = 1$ formula (7.3.6) determines the impurity magnetic susceptibility as a function of the magnetic field, the crystal-field splitting being small compared to $\mu_B g_i \mathfrak{h}$. Substituting (7.3.12) into (7.2.6 *b*) we obtain

$$\chi_i(0) = \sum_{j=-J}^{J} j^2 \chi_i^{(j)}(0) = \frac{J(J+1)(2J+1)}{3\pi T_K}(\mu_B g_i)^2. \tag{7.3.13}$$

Comparing (7.2.6 *a*) and (7.3.13) we have the expression generalizing the Wilson formula:

$$\lim_{T \to 0} (\mu_B g_i)^2 C_i / T\chi_i = \frac{2\pi^2}{n^2 - 1}. \tag{7.3.14}$$

This result was obtained by Nozières and Blandin (1980) from the phenomenological theory, discussed in § 3.1.3.

As for $n = 2$ the first terms of the perturbation theory expansion for $H$, $T \gg T_K$ and arbitrary $n$ may be derived from eqn. (7.1.12) by iterations, but the corresponding calculations are too complicated.

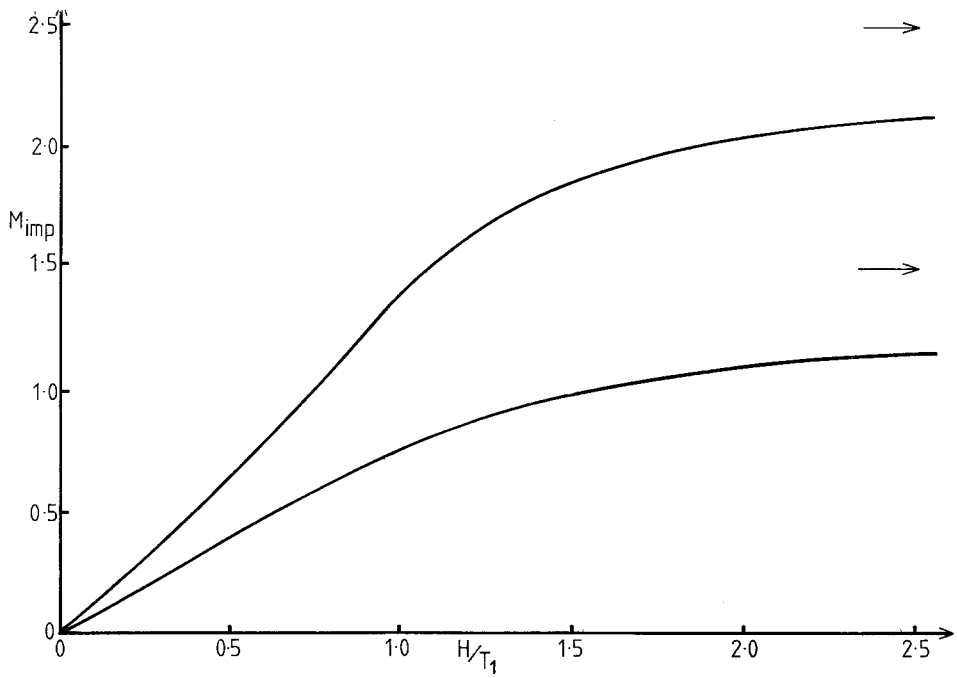
Downloaded by [University of Chicago Library] at 18:11 18 August 2015

### 7.4. *Discussion*

A numerical investigation of eqns. (7.1.12) may be used for interpretation of experimental data. The relation (7.3.14) is very simply verified. However, the necessary condition for the validity of the present theory is that the Kondo temperature exceeds the magnitude of the crystal field. The authors do not know of any experiments with rare-earth alloys for which this condition is satisfied.

Recently, Hewson *et al.* (1982) numerically calculated the impurity magnetization as a function of the magnetic field for the $n=4$, 6 case. The results are displayed in fig. 7.1. The correction to the linear term for $H \ll T_K$ is positive both for $n=4$ and $n=6$. This contrasts with the $n=2$ case, where this correction is negative. One can expect the maximum on the magnetic susceptibility curve at $H \sim T_K$ at large $n$.

Fig. 7.1




The impurity magnetization in the $n=4$ and $n=6$ degenerate exchange model. The arrows denote their respective saturation values. The scale $T_1$ is defined by $T_1 = H \exp(2\pi B_1)$ (after Hewson *et al.* 1983).

## §8. Exact solution of the Anderson model

### 8.1. *Introduction*

In this section we present in detail the exact results found for the non-degenerate Anderson model. The most interesting phenomena, such as local moment formation, the Kondo effect, the mixed-valence phenomenon, can be described by the Anderson model, the mathematical description of which is the subject of the present section. These are observed in the strong-coupling region and, therefore, cannot be

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

studied in the framework of perturbation theory with respect either to $U$ or to $\Gamma$. The results of perturbation theory lead either to singularities in each term of the perturbation theory expansion or to diverging series†. This points to the fact that the ground state of the impurity is essentially non-perturbative. The most reliable results in the Anderson model obtained by phenomenology, numerical and scaling approaches have been discussed in § 3.2.

In § 4.5 we demonstrated that the Anderson hamiltonian (4.5.1) and (4.5.2) is completely integrable, and diagonalized it assuming the Fermi energy to be the largest of the energy scales. The relevant spectrum of the Anderson hamiltonian is described by the Bethe-Ansatz equations (4.5.A)–(4.5.C). In this section we employ these equations for a detailed discussion of the Anderson model. The mathematical procedure and technical details relevant to the Bethe-Ansatz equations have been borrowed from the preceding sections on the exchange models. The results to be presented below were obtained in a series of papers by Kawakami and Okiji (Kawakami and Okiji 1982 a–c, Okiji and Kawakami 1982 a, b) and by Filyov, Tsvelick and Wiegmann (Wiegmann *et al.* 1982,, Wiegmann and Tsvelick 1982, 1983, Tsvelick and Wiegmann 1982 b, 1983, Filyov *et al.* 1982). Our presentation follows that of Tsvelick and Wiegmann (1983) and Wiegmann and Tsvelick (1983).

## 8.2. *Physical properties at zero temperature*

### 8.2.1. *The Bethe-Ansatz equations for a large number of particles*

In § 4.5 we have shown that all eigenstates of the Anderson hamiltonian (4.5.1) and (4.5.2) are described by the set of charge $\{k_j\}$ and spin $\{\lambda_\alpha\}$ rapidities, which are restricted by the periodic boundary condition (the Bethe-Ansatz equations):

$$\exp(ik_jL+i\delta(k_j))=\sum_{\alpha=1}^{M}\frac{g(k_j)-\lambda_\alpha+i/2}{g(k_j)-\lambda_\alpha-i/2}, \tag{8.2.A}$$

$$\prod_{j=1}^{N}\frac{\lambda_\alpha-g(k_j)+i/2}{\lambda_\alpha-g(k_j)-i/2}=-\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta+i}{\lambda_\alpha-\lambda_\beta-i}, \tag{8.2.B}$$

where $N$ is the total number of particles and $M$ is the total number of the spin-up particles:

$$S^z-N/2-M. \tag{8.2.C}$$

The eigenvalues of the hamiltonian (4.5.1) are given as follows

$$E=\sum_{j=1}^{N}k_j. \tag{8.2.D}$$

Here $g(k)$ and $\delta(k)$ are defined by eqns. (4.5.16), (4.5.13) and (4.5.25). We shall obtain below a continuous form of eqns. (8.2.A)–(8.2.D) for the ground state of a system with given spin and number of particles $N$. We take that $N, L, S^z\to\infty$, then $N/L=\epsilon_F/\pi$, $S^z/L$ being fixed.

† In the light of recent work this statement and a similar one by Okiji and Kawakami (1982 b), should be modified. In the symmetric model it has been shown by Zlatić and Horvatić (1983), for the susceptibilities, and by Ueda and Apel (1983), for the ground-state energy, that there are no singularities in these quantities and a perturbative approach around $U/2\Delta=0$ is justified.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

As before let us be convinced that eqns. (8.2.A)–(8.2.B), with the accuracy $1/L$, describe the free Fermi gas with the constant density of states $\rho_\sigma(k)=1/2\pi$. The factor $\exp(i\delta)$ in eqn. (8.2.A) corresponds to the impurity. Neglecting this term and multiplying eqns. (8.2.A) and (8.2.B) by each other, we get

$$\exp(iEL)=1. \tag{8.2.1}$$

Equations (8.2.A) and (8.2.B) without the impurity factor in (8.2.A) describe free particles fairly specifically. The description of free particles with spin in terms of charge and spin variables is more complicated than the conventional description in terms of particles with up and down spins but, yet, is natural and adequate for the problem with a magnetic impurity (for a discussion see, § 4.6).

It is clear that the energy of free particles with a constant density of states is unbounded from below. This factor has been taken into consideration when the model of (4.5.1) has been formulated. Momenta of spin excitations $p(\lambda)=(2/L)\sum_{j=1}^{N}\tan^{-1}(2\lambda-2g(k_j))$ and the energy associated with them, as follows from (8.2.A) and (8.2.B), are bounded: $|p(\lambda)|\lesssim\epsilon_F$. The fact that the total energy is unbounded from below is related to the fact that the charge excitation momenta are unbounded. Therefore, one should cut all $k_j$ by the conduction bandwidth $D$, i.e. to add to (8.2.A) and (8.2.B) the condition

$$k_j\geqslant -D. \tag{8.2.2}$$

Solutions of eqns. (8.2.A) and (8.2.B) as usual lie in the complex plane of the rapidities $k_j$ and $\lambda_\alpha$. They are grouped into series called 'spin' and 'charge' complexes. The classification of these equations at large $N$ and $S^z$ is of the form:

(i) $n$ spin rapidities $\lambda_\alpha$ may form a spin complex with an equidistant imaginary part

$$\lambda_\alpha^{(n,j)}=\lambda_\alpha^n+i\left(\frac{n+1}{2}-j\right); \qquad j=1,\ldots,n. \tag{8.2.3}$$

Here $\lambda_\alpha^n$ is a real rapidity of the complex centre, $n$ is the order of the complex, an arbitrary positive integer ($n\ll N$).

(ii) With each spin complex a charge complex consisting of bounded rapidities $k_\alpha^{(+)}$ and $k_\alpha^{(-)}$ may be related:

$$\left.\begin{aligned} g(k_\alpha^{(+,n,p)})&=\lambda_\alpha^n+i\left(\frac{n}{2}+1-p\right), \qquad (p=1,\ldots,n).\\ g(k_\alpha^{(-,n,p)})&=\lambda_\alpha^n+i\left(\frac{n}{2}-p\right)\end{aligned}\right\} \tag{8.2.4}$$

Except the complex with $k^{\pm}=\epsilon_d\mp i\Gamma$.

The simplest bound state of charge excitations corresponds to the real spin rapidity

$$g(k_\alpha^{(\pm)})=\lambda_\alpha\pm i/2. \tag{8.2.5}$$

(iii) Finally, there are real (unbounded) rapidities $k_j$. The above classification is valid with the exponential accuracy in the continuous limit. Its proof is given in the Appendix to 8.2.1. The wavefunctions of (4.5.21) with the parameters $k$ and $\lambda$ defined according to the above classification form a complete set.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The character of the ground state with a given projection of spin $S^z$ depends on the sign of $U$. Only the case when $U>0$ is physically interesting. Then it is shown by Kawakami and Okiji (1982 a) that the ground state is formed by real $\lambda_\alpha$ and the bound charge states associated with them (8.2.5). Yet at $U<0$, the ground state is simpler: all $k$ and $\lambda$ are real. Both assertions will be proved in what follows.

We shall deal below only with the repulsive case $U<0$. Yet, besides the direct calculation at $U<0$ there is another technically different and sometimes simpler method based on the following symmetry. Let $E(A, S^z/L, U, \epsilon_d)$ be the energy of the system with a given projection of spin $S^z$ and the number of particles $N$. Here $A=\pi N/L-D$ is a difference of the chemical potential from the bandwidth. Then,

$$E(A, S^z/L, U, \epsilon_d)=E(S^z/L, A, -U, \epsilon_d+U)+N\epsilon_F+\epsilon_d. \tag{8.2.6}$$

This relation results from a replacement of particles with up-spin by holes:

$$C^+_{k\uparrow}\to C_{k\uparrow}, \qquad d^+_\uparrow\to d_\uparrow, \qquad \sum_k C^+_{k\uparrow}C_{k\uparrow}\to N\epsilon_F-\sum_k C^+_{k\uparrow}C_{k\uparrow}, \qquad n_\uparrow\to 1-n_\uparrow.$$

Therefore, if we wish to study the case $U>0$, we can study the case $U<0$ in eqns. (8.2.A) and (8.2.B), subsequently replacing $S^z/L$ by $A$ and $\epsilon_d$ by $\epsilon_d+U$. This method is convenient to compare direct calculations for $U>0$. Therefore, we shall consider both approaches below.

### 8.2.2. *The continuous limit*

As has been said above, in the ground state all $\lambda_\alpha$ are real and $k_j$ for $j=N-2M+1,\ldots,N$ form bound states

$$g(k_\alpha^{(\pm)})=g(x(\lambda_\alpha)\mp iy(\lambda_\alpha))+\gamma_\alpha^{(\pm)}, \qquad \alpha=1,\ldots,M, \tag{8.2.7}$$

where $\gamma_\alpha^{(\pm)}=O(\exp(\text{const}\,L))$. Then according to (8.2.5) we have

$$\begin{aligned} x(\lambda)&=\epsilon_d+U/2-(U\Gamma)^{1/2}(\lambda+(\lambda^2+1/4)^{1/2})^{1/2},\\ y(\lambda)&=(U\Gamma)^{1/2}(-\lambda+(\lambda^2+1/4)^{1/2})^{1/2}. \end{aligned} \tag{8.2.8}$$

The remaining unbounded $k_1,\ldots,k_{N-2M}$ are real. Inserting (8.2.5) and (8.2.7) into (8.2.A) for $j=N-2M+1,\ldots,N$ we get

$$\left.\begin{aligned} \exp(ik_\alpha^{(+)}L+i\delta(k_\alpha^{(+)}))&=\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta+i}{\lambda_\alpha-\lambda_\beta+\gamma_\alpha^{(+)}},\\ \exp(ik_\alpha^{(-)}L+i\delta(k_\alpha^{(-)}))&=\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta+\gamma_\alpha^{(-)}}{\lambda_\alpha-\lambda_\beta-i} \end{aligned}\right\} \tag{8.2.9}$$

and eqn. (8.2.B) thus takes the form

$$\prod_{j=1}^{N-2M}\frac{\lambda_\alpha-g(k_j)+i/2}{\lambda_\alpha-g(k_j)-i/2}=-\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta-\gamma_\beta^{(-)}}{\lambda_\alpha-\lambda_\beta-\gamma_\beta^{(+)}}. \tag{8.2.10}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

To exclude from the quantities $\gamma^{(\pm)}$ from (8.2.8)–(8.2.10) we shall multiply eqns. (8.2.9) by each other. Then, employing (8.2.10), we have

$$\exp\left[2ix(\lambda_\alpha)L+2i\,\mathrm{Re}\,\delta(k^{(+)}(\lambda_\alpha))\right] = \prod_{j=1}^{N-2M}\frac{\lambda_\alpha-g(k_j)+i/2}{\lambda_\alpha-g(k_j)-i/2}\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta+i}{\lambda_\alpha-\lambda_\beta-i}. \tag{8.2.11}$$

Equation (8.2.11) with eqn. (8.2.A), for $j=1,\ldots,N-2M$, forms a complete system of equations for the rapidities $\lambda_\alpha$ and $k_j$. Logarithmization yields (Kawakami and Okiji 1982 a)

$$k_jL+\delta(k_j)=2\pi N_j-\sum_{\beta=1}^{M}\theta_1(g(k_j)-\lambda_\beta), \tag{8.2.12}$$

$$2\pi J_\alpha+\sum_{\beta=1}^{M}\theta_2(\lambda_\alpha-\lambda_\beta)+\sum_{j=1}^{N-2M}\theta_1(\lambda_\alpha-g(k_j)) = -2x(\lambda_\alpha)L-2\,\mathrm{Re}\,\delta(x(\lambda_\alpha)-iy(\lambda_\alpha)), \tag{8.2.13}$$

where $\theta_n(x)=2\tan^{-1}2x/n$ and $N_j, J_\alpha$ are integers—quantum numbers of the system.eThe energy of the system is

$$E=\sum_{j=1}^{N-2M}k_j+2\sum_{\alpha=1}^{M}x(\lambda_\alpha). \tag{8.2.14}$$

As has been said in § 5.1.1 the quantities $\lambda_\alpha$, $k_j$ and, consequently, $N_j$, $J_\alpha$, cannot be identical— in this case the wavefunction (4.5.21) is zero.

Function $x(\lambda)$ and quantities $J_\alpha$ are not bounded from below and may generally acquire any value. Therefore, one should manually restrict the energy by the bandwidth, assuming that $\lambda<Q_1$ so that $x(Q_1)=-D$ and $J(Q_1)>J_\alpha$. At $D+\epsilon_d+U/2\gg(U\Gamma)^{1/2}$

$$Q_1\simeq(D+\epsilon_d+U/2)^2/2U\Gamma.$$

By virtue of the monotonic dependence of the energy on $\lambda$ the quantities $J_\alpha$ subsequently occupy the interval from $J(Q_1)-M$ up to $J(Q_1)$, and the rapidities $\lambda$ occupy the interval from $Q$ to $Q_1$ (where $Q$ is a so far unknown quantity). They are described by the distribution

$$\delta(\lambda)=\lim_{M\to\infty}\frac{1}{L(\lambda_{\alpha+1}-\lambda_\alpha)}.$$

If $M=0$ and all the spins are up-spins, the energy is determined by the first term of (8.2.14). In this case the energy is determined by a large negative $k_j$. They also should be restricted by the bandwidth (8.2.2). By virtue of the monotonical dependence of the energy on $k$ and the dependence of $k$ on $N_j$ the integers $N_j$ subsequently occupy the interval from $-DL/2\pi$ to $-DL/2\pi+N-2M$ and $k_j$ are densely distributed in the interval $(-D,B)$ with the density $\rho(k)$.

Differentiating eqns. (8.2.12) and (8.2.13) in the standard way we pass over to the integral equations for the distributions $\rho(k)$ and $\sigma(\lambda)$:

$$\rho(k)=\frac{1}{2\pi}+\frac{1}{L}\Delta(\varepsilon,k)+g'(k)\int_Q^\infty a_1(g(k)-\lambda)\sigma(\lambda)\,d\lambda, \tag{8.2.15}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\sigma(\lambda)+\int_{Q}^{\infty} a_2(\lambda-\lambda')\delta(\lambda')=-\frac{1}{\pi}x'(\lambda)+\frac{1}{L}\tilde{\Delta}(\lambda)-\int_{-\infty}^{B} a_1(\lambda-g(k))\rho(k)\,dk. \quad (8.2.16)$$

Here

$$a_n(x)=\frac{2n}{\pi}(n^2+4x^2)^{-1}; \qquad \tilde{\Delta}(\lambda)=-\frac{1}{\pi}\frac{\partial}{\partial\lambda}\operatorname{Re}\delta(x(\lambda)-iy(\lambda)).$$

The limits $B$ and $Q$ are determined by the conditions

$$S^z/L=\frac{1}{2}\int_{-D}^{B}\rho(k)\,dk, \quad (8.2.17)$$

$$N/L=2\int_{Q}^{Q_1}\sigma(\lambda)\,d\lambda+\int_{-B}^{B}\rho(k)\,dk \quad (8.2.18)$$

and the energy by

$$\frac{E}{L}=\int_{-D}^{B}k\rho(k)\,dk+2\int_{Q}^{Q_1}x(\lambda)\sigma(\lambda)\,d\lambda. \quad (8.2.19)$$

In eqns. (8.2.15)–(8.2.17) we have deliberately replaced the limits $D$ and $Q_1$ by infinity, retaining them in (8.2.18) and (8.2.19). Since $\sigma(\lambda\to\infty)\sim\lambda^{-1/2}$ all the integrals of $\lambda$ in (8.2.15) and (8.2.16) converge. Finite limits of $Q_1$ yield small corrections of the order of $(U\Gamma)^{1/2}/D$. This is the accuracy to which we have studied only the states in the vicinity of the Fermi surface and regard the spectrum as linear. In the symmetric case the applicability condition of the basic eqns. (8.2.A) and (8.2.B) is

$$(U\Gamma)^{1/2}\ll D \qquad (U\sim-2\epsilon_d) \quad (8.2.20)$$

and in the asymmetric case

$$U\ll D \qquad (U\ll|\epsilon_d|,\Gamma). \quad (8.2.21)$$

On the other hand, in (8.2.18) all the integrals are determined by a region of large momenta and thus one cannot set $Q_1=\infty$. Furthermore, it is not difficult to prove that $\rho(k)\sim\exp(\pi k^2/2U\Gamma)$ at $k\to-\infty$. Therefore, to retain the limit $-D$ everywhere in (8.2.15)–(8.2.19) as finite, would lead only to exponentially small corrections at $D\gg(U\Gamma)^{1/2}$. This is associated with the fact that $\rho(k)$ describes excitations above the ground state $S^z=0$ and is not related to divergencies on the bandwidth.

### 8.2.3. *The particle–hole symmetry*

Let us now study the ground state of the system at $U<0$ and then employ the symmetry (8.2.6) to resume the case we are interested in, i.e. $U>0$.

In this approach, as we have already mentioned, all solutions of eqn. (8.2.B) are real. Logarithmizing eqns. (8.2.A) and (8.2.B) we get

$$k_jL=2\pi N_j-\sum_{\alpha=1}^{M}\theta_1(g(k_j)-\lambda_\alpha)-\delta(k), \quad (8.2.22)$$

$$\sum_{j=1}^{N}\theta_1(\lambda_\alpha-g(k_j))=2\pi J_\alpha+\sum_{\beta=1}^{M}\theta_2(\lambda_\alpha-\lambda_\beta). \quad (8.2.23)$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

It is convenient to replace the variables in eqns. (8.2.22) and (8.2.23) by changing the signs of $k_j - \epsilon_d$ and $N_j$, $\lambda_\alpha$. Then $U$ can be regarded as positive everywhere. The result of this replacement is

$$E = -\sum_{j=1}^{N} k_j. \tag{8.2.24}$$

Then the energy is not bounded from below since the numbers are not limited.

Therefore, all $k_j$ are sensitive to the bandwidth and must change in the interval $(B, D)$. The energy is still a monotonic but restricted function of $\lambda$ so that $\lambda \epsilon (Q, \infty)$.

Introducing distributions $\rho_1(k)$ and $\sigma_1(\lambda)$ (we differentiate them from $\rho(k)$ and $\sigma(\lambda)$ in (8.2.5) by the subscript (1)) instead of (8.2.22) and (8.2.23) we have

$$\rho_1(k) + \tilde{\rho}_1(k) = \frac{1}{2\pi} + \frac{1}{L}\Delta(k) + g'(k) \int a_1(g(k) - \lambda)\sigma_1(\lambda)\, d\lambda, \tag{8.2.25}$$

$$\sigma_1(\lambda) + \tilde{\sigma}_1(\lambda) + \int a_2(\lambda - \lambda')\sigma_1(\lambda') d\lambda = \int a_1(\lambda - g(k))\rho_1(k)\, dk, \tag{8.2.26}$$

where

$$\Delta(k) = \frac{1}{2\pi}\frac{\partial}{\partial k}\delta(k).$$

We have written down the equations so that they are defined over the whole real axis and not only in the intervals $(Q, \infty)$ and $(B, D)$. For this purpose we assert that outside these intervals $\rho_1 = \sigma_1 = 0$ but the 'hole' distribution functions $\tilde{\rho}_1$ and $\tilde{\sigma}_1$, determining the right-hand sides of (8.2.25) and (8.2.26), are defined (for details see § 5.1.1).

Similarly the right-hand sides of eqns. (8.2.15) and (8.2.16) determine the functions $\tilde{\rho}$ and $\tilde{\sigma}$ in the intervals $(B, \infty)$, $(-\infty, Q)$. For instance, eqn. (8.2.15) is of the form

$$\rho(k) + \tilde{\rho}(k) = \frac{1}{2\pi} + \frac{1}{L}\Delta(k) + g'(k) \int a_1(g(k) - \lambda)\sigma(\lambda)\, d\lambda.$$

Further, the symmetry (8.2.6) brings us back to the appropriate sign of the interaction $U > 0$

$$2S^z \leftrightarrow N - \frac{DL}{\pi},$$

therefore, we have

$$\delta(\lambda) = \sigma_1(\lambda), \qquad \tilde{\sigma}(\lambda) = \tilde{\sigma}_1(\lambda)$$

$$\rho(k) = \tilde{\rho}_1(k), \qquad \tilde{\rho}(k) = \rho_1(k).$$

It is easy to make sure that

$$\frac{S^z}{L} = \frac{N}{2L} - \int \sigma_1(\lambda)\, d\lambda = \frac{1}{2}\int \rho_1(k)\, dk - \int \sigma_1(\lambda)\, d\lambda.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

For this purpose let us express $\rho_1$ in eqns. (8.2.25) and (8.2.26) in terms of $\tilde{\rho}_1$. Applying (8.2.26) we have

$$\sigma_1(\lambda)+\tilde{\sigma}_1(\lambda)+\int a_2(\lambda-\lambda')\sigma_1(\lambda')\,d\lambda'=-\int a_1(\lambda-g(k))\tilde{\rho}_1(k)\,dk$$
$$+\int_{-\infty}^{+\infty} a_1(\lambda-g(k))\left(\frac{1}{2\pi}+\frac{1}{L}\Delta(k)\right)dk \qquad (8.2.27)$$

and

$$\frac{S^z}{L}=\frac{1}{2}\int\tilde{\rho}_1(k)\,dk; \qquad \frac{N}{L}=2\int\sigma_1(\lambda)\,d\lambda+\int\tilde{\rho}_1(k)\,dk.$$

(Here we have used the fact that

$$\int_{-\infty}^{+\infty} f(g(k))g'(k)\,dk=0.$$

Therefore, comparing (8.2.25) and (8.2.27) with (8.2.15) and (8.2.16) we see that this correspondence is established if the following relations hold

$$-\frac{dx(\lambda)}{d\lambda}=\frac{1}{2}\int_{-\infty}^{+\infty} a_1(\lambda-g(k))\,dk, \qquad (8.2.28)$$

$$-\frac{1}{\pi}\frac{d}{d\lambda}\operatorname{Re}\delta(x(\lambda)-iy(\lambda))=\int_{-\infty}^{+\infty} a_1(\lambda-g(k))\Delta(k)\,dk, \qquad (8.2.29)$$

$$\Delta(k)=\frac{1}{\pi}\frac{\Gamma}{(k-\epsilon_d)^2+\Gamma^2}.$$

Relations (8.2.28) and (8.2.29) are actually valid and play an important role later on.

### 8.2.4. *Ground state of the symmetric Anderson model*

Equations (8.2.18) and (8.2.19) can be written in a more convenient form involving no integrals over $\lambda$ diverging at the bandwidth. Then it is necessary to pass over to the equation for the 'hole' distribution function $\tilde{\sigma}(\lambda)$. Integrating (8.2.16) over $\lambda$ in the range $-\infty$ to $Q_1$, instead of (8.2.18) and (8.2.19), we have the condition

$$\int_{-\infty}^{Q}\tilde{\sigma}(\lambda)d\lambda=\frac{1}{2\pi}(\epsilon_d+U/2-A). \qquad (8.2.30)$$

The energy of the ground state is

$$E_t^{(0)}=E_h^{(0)}+E_i^{(0)}+\int_{-\infty}^{Q} s(\lambda)\tilde{\sigma}(\lambda)\,d\lambda, \qquad (8.2.31)$$

where

$$E_i^{(0)}=\frac{(2U\Gamma)^{1/2}}{16\pi^{1/2}}\int_{-\infty}^{+\infty}\frac{d\omega}{i\omega+0}\frac{(\cosh\omega/2)^{-2}}{(i\omega-0)^{1/2}}\int_{-\infty}^{+\infty}\exp(i\omega g(k))\Delta(k)\,dk. \qquad (8.2.32)$$

It follows from (8.2.17) that at $S^z=0$ the limit $B=-\infty$ and at $\epsilon_d+U/2=0$ the limit $Q=-\infty$. Therefore, in particular, the quantity $E_h^{(0)}$ is the energy of the ground state of the free Fermi gas with the density of states $1/2\pi$ and $E_i^{(0)}$ is the impurity part of the

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

ground-state energy of the symmetric Anderson model at $S^z=0$ (Kawakami and Okiji 1982 a). The numerical calculation of $E_i^{(0)}$ together with the perturbation calculation up to $(U/\Gamma)^4$ by Yamada (1975) are shown in fig. 3.7.

8.2.5. *Basic equations*

It is convenient to pass over the functions $\rho$ and $\tilde{\sigma}$ in eqns. (8.2.15) and (8.2.16). Then, performing a Fourier transformation of eqn. (8.2.16) let us express the function $\sigma$ by $\tilde{\sigma}$ and insert it into (8.2.15). Together with conditions (8.2.17) and (8.2.30) we then obtain the basic set of equations:

$$\rho(k)+g'(k)\int_{-\infty}^{+\infty} R(g(k)-g(p))\rho(p)\,dp = \rho_h^{(0)}(k)+\frac{1}{L}\rho_i^{(0)}(k)-g'(k)\int_{-\infty}^{Q} s(g(k)-\lambda)\tilde{\sigma}(\lambda)\,d\lambda, \tag{8.2.33}$$

$$\tilde{\sigma}(\lambda)-\int_{-\infty}^{Q} R(\lambda-\lambda')\tilde{\sigma}(\lambda')\,d\lambda' = \int_{-\infty}^{+\infty} s(\lambda-g(\lambda))\left(\frac{1}{2\pi}+\frac{\Delta(k)}{L}\right)dk-\int_{-\infty}^{B} s(\lambda-g(k))\rho(k)\,dk, \tag{8.2.34}$$

where

$$R(x)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp(-i\omega x)(1+\exp(|\omega|))^{-1}d\omega, \qquad s(x)=(2\cosh\pi x)^{-1}, \tag{8.2.35}$$

$$\rho_h^{(0)}=\frac{1}{2\pi}\left(1+g'(k)\int_{-\infty}^{+\infty} R(g(k)-g(p))\,dp\right), \tag{8.2.36}$$

$$\rho_i^{(0)}(k)=\Delta(k)+g'(k)\int_{-\infty}^{+\infty} R(g(k)-g(p))\Delta(p)\,dp. \tag{8.2.37}$$

The limits $B$ and $Q$ are determined by the conditions:

$$\frac{H}{2\pi}=\int_{-\infty}^{B}\rho(k)\,dk, \qquad \frac{1}{2\pi}(\epsilon_d+U/2)=\int_{-\infty}^{Q}\tilde{\sigma}(\lambda)\,d\lambda \tag{8.2.38}$$

and the energy is

$$E(H,\epsilon_d+U/2)-E(0,0)=\int_{-\infty}^{B}\varepsilon^{(0)}(k)\rho(k)\,dk, \tag{8.2.39}$$

where

$$\varepsilon^{(0)}(k)=k-\epsilon_d-U/2+\int_{-\infty}^{+\infty} R(g(k)-g(p))pg'(p)\,dp. \tag{8.2.40}$$

Equations (8.2.33)–(8.2.40) completely determine properties of the Anderson model at $T=0$ (Kawakami and Okiji 1982 a, b, Wiegmann *et al.* 1982).

8.2.6. *Valency of an impurity ion*

In the following we shall use the trick described in § 5.1.2. In the right-hand sides of (8.2.33) and (8.2.34) it is convenient to distinguish between the terms of the order

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

of unity and of the order of $1/L$. By virtue of the linearity of the equations, solutions will also involve two terms

$$\rho=\rho_{\mathrm{h}}+\frac{1}{L}\rho_{\mathrm{i}}; \qquad \tilde{\sigma}=\tilde{\sigma}_{\mathrm{h}}+\frac{1}{L}\tilde{\sigma}_{\mathrm{i}} \tag{8.2.41}$$

corresponding to the host metal and the impurity, respectively. As we have already mentioned in § 8.2.1 the functions $\rho_{\mathrm{h}}$ and $\tilde{\sigma}_{\mathrm{h}}$ with the conditions (8.2.36) and (8.2.37) describe a free Fermi gas. The functions $\rho_{\mathrm{i}}$ and $\tilde{\sigma}_{\mathrm{i}}$ together with (8.2.40) determine the impurity part of the energy. Thus, the limits $B$ and $Q$ can be found only if solutions of (8.2.33) and (8.2.34) are applied in the leading order with respect to $1/L$ and the impurity part of the energy can be found if solutions of these equations are used in the next order with respect to $1/L$. The values of $B$ and $Q$ should not be calculated with a great accuracy since this leads to corrections to the energy of the order of $1/L^2$.

The impurity parts of the magnetic moment $M_{\mathrm{i}}$ and the number of particles (valency $n_d$) can be easily calculated without minimizing the thermodynamic potential $E-HS^z-AN$ by directly calculating contributions of the functions $\rho_{\mathrm{i}}$ and $\tilde{\sigma}_{\mathrm{i}}$ into the total spin and the number of particles

$$M_{\mathrm{i}}=\frac{1}{2}\int_{-\infty}^{B}\rho_{\mathrm{i}}(k)\,dk, \tag{8.2.42}$$

$$n_d=-\int_{-\infty}^{Q}\tilde{\sigma}_{\mathrm{i}}(\lambda)\,d\lambda. \tag{8.2.43}$$

The simplest problem associated with the investigation of eqns. (8.2.33) and (8.2.34) is a problem of calculating the valence at $H=0$. In this case $S^z=0$, therefore $B=-\infty$ and $\rho=0$. There is only one equation left for $\sigma$:

$$\tilde{\sigma}(\lambda)-\int_{-\infty}^{Q}R(\lambda-\lambda')\tilde{\sigma}(\lambda')\,d\lambda'=\int_{-\infty}^{+\infty}s(\lambda-g(k)\left(\frac{1}{2\pi}+\frac{\Delta(k)}{L}\right)dk, \tag{8.2.44}$$

solved explicitly by the Wiener–Hopf method (see the Appendix to 5.1.3). Let

$$G^{(\pm)}(\omega)=\frac{\sqrt{(2\pi)}((\mp i\omega+0)/2\pi)^{\pm i\omega/2\pi}}{\Gamma\left(\frac{1}{2}\mp i\omega/2\pi\right)}$$

be familiar analytical functions having no zeros in the upper (lower) half-plane factorizing the function

$$(1-R(\omega))^{-1}=G^{(+)}(\omega)G^{(-)}(\omega), \tag{8.2.45}$$

where $R(\omega)$ are the Fourier transforms of the function (8.2.35). The Fourier transform of the right-hand side of (8.2.44) has the form:

$$\left(2\cosh\frac{\omega}{2}\right)^{-1}\int_{-\infty}^{+\infty}\exp\left(i\omega g(k)\right)\left(\frac{1}{2\pi}+\frac{1}{L}\Delta(k)\right)dk.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

According to eqn. (6) from Appendix 5.1.3 the solution of (8.2.44) is

$$\left.\begin{aligned}\tilde{\sigma}(\lambda)&=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp\left(-i\omega(\lambda-Q)\right)\sigma^{(-)}(\omega)\,d\omega;\\ \sigma^{(-)}(\omega)&=-\frac{i}{2\pi}G^{(-)}(\omega)\int_{-\infty}^{+\infty}\frac{d\omega'}{\omega-\omega'-i0}\,\frac{\exp\left(-i\omega'Q-|\omega'|/2\right)}{G^{(-)}(\omega')}\\ &\quad\times\left[\left(\frac{U\Gamma}{-2\pi i\omega'+0}\right)^{1/2}+\frac{1}{L}\int_{-\infty}^{+\infty}\exp\left(i\omega' g(k)\right)\Delta(k)\,dk\right]\end{aligned}\right\}\quad(8.2.46)$$

Inserting $\tilde{\sigma}_{\mathrm{h}}(\lambda)$ into (8.2.36) we get a condition for $Q$

$$\frac{U/2+\epsilon_d}{(2U\Gamma)^{1/2}}=\frac{i}{(2\pi)^{1/2}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i0}\,\frac{\exp\left(-|\omega|/2-i\omega Q\right)}{G^{(-)}(\omega)}\,\frac{1}{(-i\omega+0)^{1/2}},\quad(8.2.47)$$

and $\eta_d$ according to (8.2.43) is

$$n_d=1-\frac{i}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i0}\,\frac{\exp\left(-|\omega|/2\right)}{G^{(-)}(\omega)}\int_{-\infty}^{+\infty}\exp\left(i\omega(g(k)-Q)\Delta(k)\,dk.\right.\quad(8.2.48)$$

Formulae (8.2.47) and (8.2.48) parametrically set $n_d$ as a function of $\Gamma$, $\epsilon_d$, $U$ (Wiegmann *et al.* 1982). In the symmetric case $n_d=1$. Let us now study the two limits $(U/2+\epsilon_d)\ll(U\Gamma)^{1/2}$ and $(U/2+\epsilon_d)\gg(U\Gamma)^{1/2}$.

(*a*) *The symmetric limit* $(U+2\epsilon_d)\ll(U\Gamma)^{1/2}$. In this case $Q<0$ and closing the integration path into the upper half-plane we have

$$\frac{U/2+\epsilon_d}{(U\Gamma)^{1/2}}=\frac{2}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^{3/2}}G^{(+)}(i\pi(1+2n))\exp\left(\pi Q(1+2n)\right).\quad(8.2.49)$$

The valence is also exponential with respect to $Q$

$$n_d=1-\frac{\sqrt{2}}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}G^{(+)}(i\pi(2n+1)\int_{-\infty}^{+\infty}\exp\left(-\pi(1+2n)(g(k)-Q)\right)\Delta(k)\,dk,\quad(8.2.50)$$

i.e. is expanded in powers of $(U+2\epsilon_d)/(U\Gamma)^{1/2}$:

$$n_d=1-\sum_{n=0}^{\infty}f_n\left(\frac{U}{\Gamma}\right)\left(\frac{\epsilon_d+U/2}{(U\Gamma)^{1/2}}\right)^{2n+1}\quad(8.2.51)$$

The charge susceptibility in this case equals (Kawakami and Okiji 1982 c)

$$\chi_{\mathrm{ch}}\left(\epsilon_d=-\frac{U}{2}\right)\equiv\left.\frac{\partial n_d}{\partial\epsilon_d}\right|_{\epsilon_d=-U/2}=\frac{1}{(2U\Gamma)^{1/2}}\int_{-\infty}^{+\infty}\exp\left(\frac{-\pi k^2}{2U\Gamma}\right)\Delta(k)\,dk.\quad(8.2.52)$$

At $U\gg\Gamma$

$$\chi_{\mathrm{ch}}\left(\epsilon_d=-\frac{U}{2}\right)\simeq\frac{4\Gamma}{\pi U^2}\left(1+O\left(\frac{\Gamma^2}{U^2}\right)\right).$$

At $\epsilon_d+U/2\sim(U\Gamma)^{1/2}$ but $U\gg\Gamma$

$$1-n_d\sim(\Gamma/U)^{3/2}.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

(*b*) The most interesting is the *asymmetric limit* $U+2\epsilon_d \gg (U\Gamma)^{1/2}$. In this case $Q>0$ and moreover $Q\gg 1$. Closing the integration path into the lower half-plane and integrating around the cut, we get, from (8.2.47),

$$\frac{\epsilon_d+U/2}{(2U\Gamma)^{1/2}}=q_*^{1/2}+\sum_{n=1}^{\infty} C_n q_*^{-n-1/2}, \tag{8.2.53}$$

where $q_*$ is related to $Q$ as

$$Q=q_*+\frac{1}{2\pi}\ln(2\pi e q_*). \tag{8.2.54}$$

In the interesting case $U\gg\Gamma$ (8.2.48) is significantly simplified. Actually,

$$\int_{-\infty}^{+\infty}\exp(i\omega g(k))\Delta(k)\,dk \simeq \exp(-|\omega|/2+iU/8\Gamma\omega). \tag{8.2.55}$$

Therefore†,

$$n_d=1-\frac{i}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i0}\,\frac{\exp(-|\omega|+i\omega/I^*)}{G^{(-)}(\omega)} \tag{8.2.56}$$

(Wiegmann and Tsvelick 1982), where

$$\frac{1}{I^*}=\frac{U}{8\Gamma}-Q=-\frac{\epsilon_d(\epsilon_d+U)}{2U\Gamma}-\frac{1}{2\pi}\ln(2\pi e q_*)+O\left(\frac{U\Gamma}{(\epsilon_d+U/2)^2}\right). \tag{8.2.57}$$

In (8.2.56) and (8.2.57) the quantities $\epsilon_d$ and $U$ can be of the same order. A certain simplification is observed in the intermediate valence region $|\epsilon_d|\ll U$. Then the quantity $\epsilon_d^*=-2\Gamma/I^*$ can be regarded as renormalization of the level $\epsilon_d$. According to (8.2.53) and (8.2.54) we have

$$\epsilon_d^*=\epsilon_d+\frac{\Gamma}{\pi}\ln\left(\frac{\pi e U}{4\Gamma}\right). \tag{8.2.58}$$

Formula (8.2.58) is well known. It has been derived in the framework of the perturbation theory, with respect to $\Gamma$, and the scaling approach used by many authors (Barabanov *et al.* 1974, Varma and Yafet 1976, Haldane (1978 a, b) and has been discussed in § 3.2.4.

We repeat the discussion of § 3.2.4 in more detail below. The sign of $I^*$ substantially affects analytical properties of the integral (8.2.56). The point $I^*=\infty$ may be regarded as the boundary between regions with a localized moment and the intermediate valence region.

At $I^*<0$ the integration path in (8.2.56) can be closed into the lower half-plane. Integrating around the cut of function $\exp(-|\omega|)$, we get

$$n_d=\frac{1}{\pi^{3/2}}\int_0^{\infty}dt\,\frac{\sin 2\pi t}{t}\exp\left(\frac{2\pi t}{I^*}\right)\Gamma(1/2+t)\left(\frac{t}{e}\right)^{-t} \tag{8.2.59}$$

† Note that (8.2.56) coincides with the magnetic susceptibility for the Kondo model with the impurity spin $S=1$ with the replacement of $\ln H/T_H$ by $\pi/I^*$ (see § 5.1.3). The reader may probably find in this coincidence a deeper physical analogy.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

At $I*>0$ the integration path can be closed into the cut of the integrand in the upper half-plane. Then with exponential accuracy we get

$$n_d = 1 - \frac{1}{\pi^{1/2}} \int_0^\infty dt \frac{\tan \pi t}{t} \exp\left(\frac{-2\pi t}{I^*}\right) \frac{(t/e)^t}{\Gamma(1/2+t)} + O\left(\exp\left(\frac{-\pi}{I^*}\right)\right). \tag{8.2.60}$$

The formulae (8.2.59) and (8.2.60) are both expanded in powers of the 'invariant charge' $I^{**}$ determined by the equation (compare with (2.4.22)):

$$I_{**}^{-1} + \ln(|I^{**}|/e) = 2\pi I^{*-1}. \tag{8.2.61}$$

At $|\epsilon_d^*| \ll U$ condition (8.2.61) determines the 'effective level' (Barabanov *et al.* 1974, Haldane 1978 a, b):

$$\left.\begin{aligned} \epsilon_d^{**} &= -\frac{\Gamma}{\pi} I_{**}^{-1}, \\ \epsilon_d^{**} - \frac{\Gamma}{\pi} \ln \frac{U}{4|\epsilon_d^{**}|} &= \epsilon_d, \end{aligned}\right\} \tag{8.2.62}$$

in inverse integer powers of which the physical quantities are expanded.

At $|I^*| \ll 1$ from (8.2.59) and (8.2.60) follow the known asymptotics,

$$\left.\begin{aligned} n_d &= -2I_{**} + \ldots \qquad (I^*<0), \\ n_d &= 1 - I_{**} + \ldots \qquad (I^*>0), \end{aligned}\right\} \tag{8.2.63}$$

obtained previously in accordance with the perturbation theory (Tsvelick and Barabanov 1978, Haldane 1978 a, b). They have already been discussed in § 3.2.4.

It is interesting to note that it is possible to calculate the physical quantities on the boundary of the regions of the intermediate valence and localized moment ($\epsilon_d^* = 0$, $I^* = \infty$) and to construct the expansion over $I^{*-1}$,

$$n_d = 2 - \sqrt{2} + \frac{\pi}{3\sqrt{2}} I^{*-1} + O(I^{*-2}). \tag{8.2.64}$$

The calculations are given in the Appendix to § 8.2.6. Note that at $\epsilon_d = 0$ the valence $n_d \simeq 0{\cdot}58$ not 2/3 as usually expected. Expansion (8.2.64) can be obtained only from the exact solution. A numerical calculation of function $n_d(1/I^*)$ is presented in fig. 3.11 (Melnikov 1982 b).

### 8.2.7. *Magnetic susceptibility of the symmetric Anderson model in an arbitrary magnetic field*

It follows from (8.2.38) that in the symmetric limit $U = -2\epsilon_d$, $Q = -\infty$ and $\tilde{\sigma} = 0$. In this simple case instead of two coupled equations, (8.2.33) and (8.2.34), there is only one linear equation

$$\begin{aligned} \rho(k) + \frac{k}{U\Gamma} \int_{-\infty}^{B} R\left(\frac{k^2-p^2}{2U\Gamma}\right) \rho(p)\, dp + \tilde{\rho}(k) \\ = \frac{1}{2\pi} + \frac{\Delta(k)}{L} + \frac{k}{U\Gamma} \int_{-\infty}^{+\infty} R\left(\frac{k^2-p^2}{2U\Gamma}\right)\left(\frac{1}{2\pi} + \frac{\Delta(p)}{L}\right) dp. \end{aligned} \tag{8.2.65}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

According to the method described in §8.2.6, let us single out from (8.2.65) parts corresponding to the host metal and the impurity: $\rho=\rho_h+(1/L)\rho_i$. From (8.2.36) in the leading order with respect to $1/L$, i.e. employing function $\rho_h$, we shall find the relation of $B$ with the total spin of the system $S^z$, which for free particles equals $S^z/L=H/4\pi$ (set $\mu_B g_i=1$). Therefore,

$$H/2\pi=\int_{-\infty}^{B}\rho_h(k)\,dk. \tag{8.2.66}$$

The impurity magnetic moment, according to (8.2.36), is

$$M_i=\frac{1}{2}\int_{-\infty}^{B}\rho_i(k)\,dk. \tag{8.2.67}$$

Equation (8.2.65) is reduced to an equation with a difference kernel and is solved by the Wiener–Hopf method. However, it is necessary to distinguish between the two cases: $B<0$ and $B>0$. We understand that $B(H)$ is a monotonically increasing function of $H$. Therefore, the point $B(H_0)=0$ separates the region of low fields $H<H_0$ from the region of high fields $H>H_0$. In eqn. (8.2.65), where the impurity parts involving the factor $1/L$ are omitted, there is only one parameter of the dimension of the energy, i.e. $(U\Gamma)^{1/2}$. Therefore, $H_0\sim(U\Gamma)^{1/2}$. If the magnitude of the magnetic field exceeds this value, the intermediate regime occurs. At very high fields we can neglect either the mixing $\Gamma$, if $\Gamma\ll H\ll U$, or the Coulomb repulsion, if $U\ll H\ll\Gamma$, or both, if $H\gg\max(U,\Gamma)$ (see fig. 3.5). The same takes place for the temperature. Let us stress that the intermediate regime takes place at $H\sim(U\Gamma)^{1/2}$ and not at $H\sim\max(\Gamma, U)$ as is usually thought. We shall see below that when $T$ and $H$ cross $T_0$ and $H_0$ analytical properties of the thermodynamic functions change. The transition displays itself in the fact that at $\operatorname{Re}T=T_0$ and $\operatorname{Re}H=H_0$ in the complex plane of $T$ and $H$ there are complex singularities of the physical quantities. Yet, on the real axis, all physical quantities are infinitely differentiable at any $T$ and $H$ as should be the case in low-dimensional systems.

We shall study below two individual cases: $H\leqslant H_0$ and $H>H_0$.

(a) *Low magnetic fields* $H\leqslant H_0=const\,(U\Gamma)^{1/2}$

At $B<0$ in the interval $(-\infty,B)$ the function $g(k)=k^2/2U\Gamma$ is monotonous. Equation (8.2.65) becomes an equation with the difference kernel at the replacement of the variables:

$$\left.\begin{aligned} z&=g(k);\\ p_{h,i}(z)&=-\rho_{h,i}(k)/g'(k)|_{k=-(2U\Gamma z)^{1/2}},\\ p_{h,i}^{(0)}(z)&=-\rho_{h,i}^{(0)}(k)/g'(k)|_{k=-(2U\Gamma z)^{1/2}}.\end{aligned}\right\} \tag{8.2.68}$$

We have:

$$p_h(z)-\int_b^{\infty}R(z-z')p_h(z')\,dz'=p_h^{(0)}(z), \tag{8.2.69}$$

$$p_i(z)-\int_b^{\infty}R(z-z')p_i(z')\,dz'=p_i^{(0)}(z), \tag{8.2.70}$$

where $b=B^2/2U\Gamma$. The Wiener–Hopf method enables us to find solutions to both equations. It is then convenient to take advantage of the following integral

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

representations of the right-hand sides of (8.2.65), (8.2.66), (8.2.69) and (8.2.70). In view of the great importance of this representation we give the proof of it in Appendix A to 8.2.7.

$$p_{\mathrm{h}}^{(0)}(z)=\frac{i}{8\pi^{3/2}}\int_{-\infty}^{+\infty}d\omega\exp(-iz\omega)\tanh\frac{\omega}{2}\left(\frac{2U\Gamma}{i\omega+0}\right)^{1/2}\qquad(z>0).\tag{8.2.71}$$

$$p_{\mathrm{i}}^{(0)}(z)=(2\cosh\pi(z-1/I))^{-1}+\frac{i}{4\pi}\int_{-\infty}^{+\infty}d\omega\,\exp(-i\omega z)\tanh\frac{\omega}{2}$$
$$\times\int_{-\infty}^{+\infty}dk\Delta(ik)\exp(-i\omega g(k))\qquad(z>0).\tag{8.2.72}$$

Using (8.2.69), (8.2.71) and (8.2.72) we get

$$p_{\mathrm{h,i}}(z)=\frac{i}{4\pi^2}\int_{-\infty}^{+\infty}d\omega G^{(+)}(\omega)\exp(-i\omega(z-b))\int_{-\infty}^{+\infty}d\omega'\exp(-i\omega' b)$$
$$\times\frac{G^{(-)}(\omega')}{\omega-\omega'+i0}p_{\mathrm{h,i}}^{(0)}(\omega'),\tag{8.2.73}$$

where $G^{(\pm)}(\omega)$ are defined in (8.2.45).

Inserting (8.2.73) into (8.2.66) and (8.2.67) we have the formula determining the dependence of $b$ on $H$:

$$\frac{H}{(\Gamma U)^{1/2}}=\frac{2}{\pi}\sum_{n=0}^{\infty}\frac{G^{(+)}(i\pi(2n+1))}{(2n+1)^{3/2}}\exp(-\pi b(2n+1));\tag{8.2.74}$$

and the formula for the impurity part of the magnetic moment

$$M_{\mathrm{i}}=M_{\mathrm{Kondo}}+m.\tag{8.2.75}$$

Here

$$M_{\mathrm{Kondo}}(b)=-\frac{i}{2\sqrt{2}\,\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega-i0}\frac{G^{(-)}(\omega)}{2\cosh\omega/2}\exp\left(-i\omega\left(b-\frac{1}{I}\right)\right),\tag{8.2.76}$$

where $1/I=(U^2-4\Gamma^2)/8U\Gamma$ is the Schrieffer–Wolf exchange constant

$$m(b)=\frac{1}{\sqrt{2}\,\pi}\sum_{n=0}^{\infty}\frac{G^{(+)}(i\pi(1+2n))}{2n+1}\exp(-\pi b(2n+1))$$
$$\times\int_{-\infty}^{+\infty}dp\exp\left(\frac{-\pi(2n+1)p^2}{2U\Gamma}\right)\Delta(ip).\tag{8.2.77}$$

Formulae (8.2.74)–(8.2.77) parametrically determine the dependence of the impurity magnetization on the magnetic field at $H<H_0$ and arbitrary $U,\Gamma$ and $\epsilon_d=-U/2$. The value of $H_0$ is determined by the series (8.2.74) at $b=0$

$$\frac{H_0}{(U\Gamma)^{1/2}}=\frac{i}{2\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega-i0}\frac{G^{(-)}(\omega)}{(i\omega+0)^{1/2}}\tanh\frac{\omega}{2}.\tag{8.2.78}$$

It follows from (8.2.74)–(8.2.77) that, independently of the relation between $\Gamma$ and $U$, the magnetic paramagnetism at $H\to 0$ vanishes. Actually, at $H\ll H_0$ the value $b\gg 1$ and we can confine ourselves to only the first terms of the series (8.2.74) and (8.2.77)

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

and the integral (8.2.76) to take into account only the pole in the lower half-plane adjacent to zero. Therefore,

$$b = -\frac{1}{\pi}\ln\left(\frac{H}{2}\left(\frac{\pi e}{U\Gamma}\right)^{1/2}\right), \tag{8.2.79}$$

$$M_{\text{Kondo}}(H) = \frac{H}{2(2U\Gamma)^{1/2}}\exp\left(\frac{\pi}{I}\right) + O(H^3), \tag{8.2.80}$$

$$m(H) = \frac{H}{2(2U\Gamma)^{1/2}}\int_{-\infty}^{+\infty} dp\Delta(ip)\exp\left(\frac{-\pi p^2}{2U\Gamma}\right) + O(H^3). \tag{8.2.81}$$

Combining (8.2.80) and (8.2.81) we get $M_i(0)=0$ and the magnetic susceptibility is-

$$\chi_{\text{sp}} = \frac{1}{2(2U\Gamma)^{1/2}}\left(\exp(\pi/I) + \int_{-\infty}^{+\infty} dk\Delta(ik)\exp\left(-\frac{\pi k^2}{2U\Gamma}\right)\right) \tag{8.2.82}$$

(Wiegmann *et al.* 1982, Kawakami and Okiji 1982 c). At $U \ll \Gamma$ the first term in (8.2.82) is exponentially small. The magnetic susceptibility is determined by the resonance level width $\chi_{\text{sp}} \sim 1/\Gamma$. This regime is usually called non-magnetic (see fig. 3.5). The susceptibility is expanded in series over $U/\Gamma$

$$\chi_{\text{sp}} = \frac{1}{2\pi\Gamma}\sum_{n=0}^{\infty} C_n\left(\frac{U}{2\Gamma}\right)^n,$$

where

$$\left.\begin{aligned} C_{2n} &= \sum_{m=0}^{n} C_{2n}^{2m}(-1)^{n+m}2^m(2m-1)!!, \\ C_{2n+1} &= \sum_{m=1}^{n+1} C_{2n+1}^{2m}2^m(-1)^{n+m+1}(2m-1)!!. \end{aligned}\right\} \tag{8.2.83}$$

The first four terms of this expansion have been calculated in Yamada (1975) according to the perturbation theory. Note that the exponential term in (8.2.82), as indicated in the footnote on p. 647, is cancelled by higher-order terms and a particular approach still holds for the susceptibility.

At $U=2\Gamma$ we can observe a sharp change in magnetic properties. The magnetic susceptibility becomes exponentially large, then the main role is played by the term originating from $M_{\text{Kondo}}$. The point $U=2\Gamma$ does not coincide with the boundary of the non-magnetic region in the Hartree–Fock approximation (Anderson 1961).

(b) *The strong-coupling limit* $\Gamma \gg U, H \ll H_0$

In fig. 3.5 this region is divided into two parts by the curve $H=T_{\text{K}}$, where $T_{\text{K}}$ is the Kondo temperature. As above we shall stick to the definition of the Kondo temperature given in § 5.1.2:

$$T_{\text{K}} = (2\pi\chi_{\text{sp}}(0))^{-1}. \tag{8.2.84}$$

According to (8.2.82) at $U \gg \Gamma$ we have:

$$\chi_{\text{sp}}(0) = (2\sqrt{(2U\Gamma)})^{-1}\exp\left(\frac{\pi U}{8\Gamma}\right), \tag{8.2.85}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$T_{\mathrm{K}}=\frac{(2U\Gamma)^{1/2}}{\pi}\exp\left(\frac{-\pi U}{8\Gamma}\right). \tag{8.2.86}$$

At $H<T_{\mathrm{K}}$ the susceptibility is exponentially large in comparison with the value at $U\sim\Gamma$. This region is called the *strong coupling region* in fig. 3.5. In this limit in the frame of the Hartree–Fock approximation (Anderson 1961) there should be formed a magnetic moment. Yet, thanks to a strong correlation between conduction electrons and impurity spin (Kondo effect), the localized moment vanishes at the decrease of the magnetic field. The fields $H>T_{\mathrm{K}}$ already break this correlation. In the region $T_{\mathrm{K}}\ll H\ll H_0$ we can speak of the localized moment.

The first term in (8.2.75) is marked by the subscript 'Kondo' because at $U\gg\Gamma$, $H\ll H_0$, where the Anderson model is equivalent to the s–d exchange model, the impurity magnetization is determined by the term $M_{\mathrm{Kondo}}$ (8.2.76) only. In this region all physical quantities, in particular the magnetization, must be universal functions of $H/T_{\mathrm{K}}$ and $T/T_{\mathrm{K}}$. In the strong-coupling region we have (8.2.79) and employing the definition (8.2.86) we get the familiar universal function (see § 5.1.3):

$$M_{\mathrm{Kondo}}(H)=-\frac{i}{4\sqrt{2\pi}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega-i0}\frac{G^{(-)}(\omega)}{\cosh\omega/2}\exp\left(i\frac{\omega}{\pi}\ln\frac{H}{T_H}\right),$$

$$T_H=\left(\frac{2\pi}{e}\right)^{1/2}T_H. \tag{8.2.87}$$

We then observe that in the region $\Gamma\ll U$, $H\ll H_0$ universal properties of the symmetric Anderson model and the s–d exchange model are identical.

We have already considered the function (8.2.87) in § 5.1.3. We repeat that at $H\ll T_{\mathrm{K}}$ the integral (8.2.87) is expanded in series in integer powers of $H/T_H$ and at $H\gg T_k$ the inverse $\ln H/T_H$ (see (5.1.36) and (5.1.74)). Thus, at $H\ll H_0$, $\Gamma\ll U$ eqns. (5.1.36) and (5.1.74)). Thus, at $H\ll H_0$, $\Gamma\ll U$ eqns. (8.2.69)·and (8.2.70) should describe the s–d exchange model. This fact is easily verified without solving eqns. (8.2.69) and (8.2.70). Indeed, according to the representations (8.2.71) and (8.2.72) the right-hand sides of eqns. (8.2.69) and (8.2.70) at $1\ll z\sim I^{-1}$ have the asymptotic form

$$p_{\mathrm{h}}^{(0)}(z)=\frac{(2U\Gamma)^{1/2}}{2\pi}\exp(-\pi z)+\ldots \qquad (z\gg 1),$$

$$p_{\mathrm{i}}^{(0)}(z)=\left(2\cosh\pi\left(z-\frac{1}{I}\right)\right)^{-1}+\ldots \qquad (1\ll z\sim I^{-1}).$$

Due to these relations eqns. (8.2.71) and (8.2.72) coincide with (5.1.20) at $b\gg 1$, $0<I\ll 1$.

(c) *High magnetic fields* $H>H_0=const\,(U\Gamma)^{1/2}$

At $B>0$ it is convenient to rewrite (8.2.65) using the distribution function of the 'holes' whose rapidities change in the interval $(B,\epsilon_{\mathrm{F}})$. In this interval $g'(k)$ does not change its sign and the replacement $z=g(k)$, $\tilde{p}(z)=\tilde{\rho}(k)/g'(k)$ makes the kernel difference.

Let us insert into the integral $\int R((k^2-p^2)/2U\Gamma)\rho(p)dp$ the quantity

$$\rho(k)=-\tilde{\rho}(k)-g'(k)\int_{-\infty}^{B}R\left(\frac{k^2-p^2}{2U\Gamma}\right)\rho(p)dp+(\text{r.h.s. of eqn. (8.2.65)})$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Then bearing in mind that

$$\int_{-\infty}^{+\infty} f(k^2)k\,dk = 0$$

we obtain the equation

$$\rho(k) + \tilde{\rho}(k) - \frac{k}{U\Gamma}\int_B^{\infty} R\left(\frac{k^2-p^2}{2U\Gamma}\right)\tilde{\rho}(p)\,dp = \frac{1}{2\pi} + \frac{\Delta(k)}{L} \tag{8.2.88}$$

which, after the above-mentioned replacement, becomes the kernel difference

$$\tilde{\rho}(z) - \int_b^{\infty} R(z-z')\tilde{\rho}(z')\,dz' = \left(\frac{U\Gamma}{2z}\right)^{1/2}\left(\frac{1}{2\pi} + \frac{1}{L}\Delta(\sqrt{(2U\Gamma z)})\right) \qquad (z>0). \tag{8.2.89}$$

The impurity spin and magnetic field are expressed by the following:

$$\left.\begin{aligned} M_{\mathrm{i}} &= \frac{1}{2} - \frac{1}{2}\int_b^{\infty} \tilde{\rho}_{\mathrm{i}}(z)\,dz, \\ \frac{H}{2\pi} &= \frac{N}{L} - \int_b^{D'} \tilde{\rho}_{\mathrm{h}}(z)\,dz, \qquad D' = \frac{\epsilon_{\mathrm{F}}^2}{2U\Gamma}. \end{aligned}\right\} \tag{8.2.90}$$

The solution of eqns. (8.2.89) is given in Appendix B to 8.2.7 and leads to the following expressions for $H$ and $M_{\mathrm{i}}$:

$$\frac{H-H_0}{(2U\Gamma)^{1/2}} = (2\pi)^{-1/2}\int_0^{\infty} \frac{dt}{t^{3/2}}(1-\exp(-2\pi bt))\frac{(t/e)^t}{\Gamma(\frac{1}{2}+t)}, \tag{8.2.91}$$

$$\frac{1}{2} - M_{\mathrm{i}} = \frac{1}{2\pi}\int_0^{\infty} \frac{dt}{t^{3/2}}\exp(-2\pi bt)\frac{(t/e)^t}{\Gamma(\frac{1}{2}+t)} \times \int_{-\infty}^{+\infty} dk\exp(-\pi k^2/U\Gamma)\Delta\left(\frac{ik}{t^{1/2}}\right). \tag{8.2.92}$$

Formulae (8.2.91) and (8.2.92) at $b \gg 1$ allow for an expansion in half-integer inverse powers of the parameter $z$ defined as

$$z - \frac{1}{2\pi}\ln(2\pi ez) = b. \tag{8.2.93}$$

Differentiating (8.2.91) in $b$ and employing (8.2.93) we get

$$\begin{aligned} \frac{\partial H}{\partial z} &= (4U\Gamma\pi)^{1/2}z^{-1/2}(1-(2\pi z)^{-1})\int_0^{\infty} \frac{dt}{t^{1/2}}\exp(-2\pi t)\frac{t^{t/z}}{\Gamma(1/2+t/z)} \\ &= (2U\Gamma)^{1/2}\sum_{n=0}^{\infty} \alpha_n z^{-1/2-n}, \qquad \alpha_0 = 1, \alpha_1 = 0, \end{aligned}$$

i.e.

$$\frac{H-H_0}{(2U\Gamma)^{1/2}} = -2\sum_{n=0}^{\infty} \frac{\alpha_n}{2n-1} z^{-n+1/2}. \tag{8.2.94}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Similarly for $M_i$:

$$\frac{1}{2}-M_i=\sum_{n=0}^{\infty}\beta_n\frac{2^{n+1}}{(2n+1)!!}(2\pi)^{n-1/2}z^{-n-1/2}$$
$$\times\int_0^{\infty}t^{n-1/2+t/z}\exp(-2\pi t)\frac{dt}{\Gamma(1/2+t/z)},\qquad(8.2.95)$$

where $\beta_n$ are the expansion coefficients

$$\beta_n=\frac{\operatorname{Im}\left(\frac{U}{2}+i\Gamma\right)^{2n+1}}{(2U\Gamma)^{n+1/2}}.\qquad(8.2.96)$$

At higher fields

$$H\simeq 2(U\Gamma z)^{1/2},$$

therefore, the expansion in (8.2.96) is performed in powers of the quantity $[(\max(U,\Gamma))/H]^2$. At $\Gamma, H\gg U$ it follows from (8.2.94) and (8.2.95) that

$$\chi_{sp}(H)=\Delta(H/2)+\Delta(-H/2)\qquad(8.2.97)$$

as it should be for the non-interacting resonance level.

Combining the results of the preceding sections let us describe the behaviour of the impurity magnetic moment in the entire region of the parameters $H$, $\Gamma$, $U$. Despite the fact that the function $M_i(H)$ is smooth at any $\Gamma, U, H$ it has a different character in various regions of fig. 3.6.

The simplest behaviour is discovered at $U\ll\Gamma$. At $H\ll H_0$ there is a *non-magnetic regime*: $M_i(H)\sim H/\Gamma$. At the increase of the field there is a smooth transition to the *free-orbital regime*; at the increase of $U$ the system transfers into the *strong-coupling regime*. The magnetic moment is expanded in powers of $H/T_K$ and $H/(U\Gamma)^{1/2}$, then at $\Gamma\sim U$ the quantities $T_K$ and $(2U\Gamma)^{1/2}$ are of the same order. At low fields (temperatures) the impurity is described by the Fermi-liquid theory (Yosida & Yamada 1970, 1975, Yamada 1975).

The increase of the magnetic field leads to the regime of *localized moment*: $(U\Gamma)^{1/2}\gg H\gg T_K$. In this region the magnetic moment differs from 1/2 by logarithmical corrections. A further increase of the field breaks the localized moment. All four states with $n_d=0,1,2$ make an almost identical contribution and again the free orbital regime arises. A qualitative picture of the magnetic moment variation is presented in fig. 8.1.

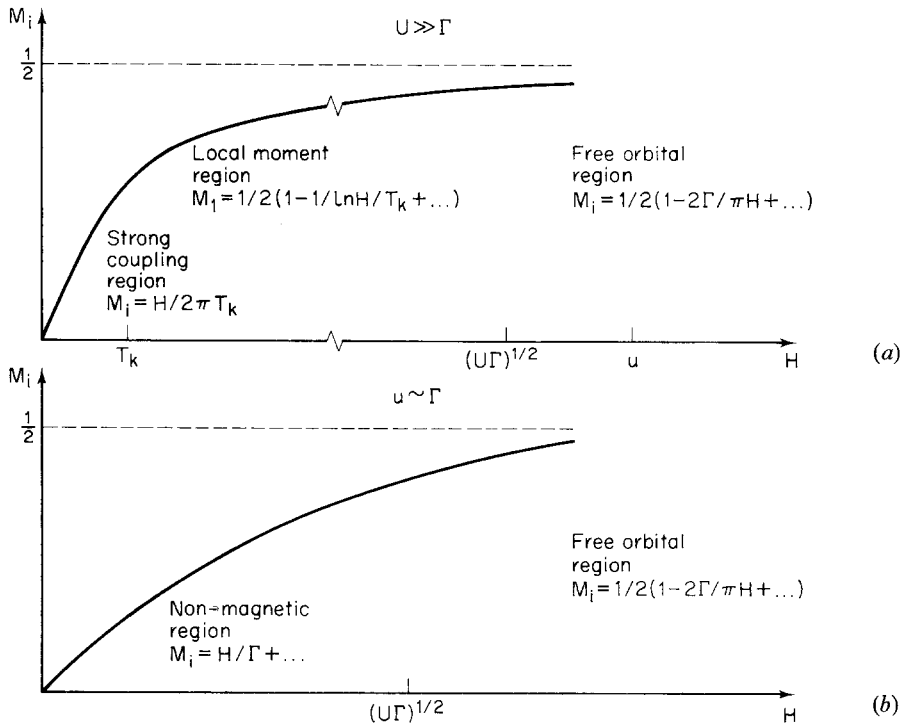
In conclusion to this subsection let us discuss the limit $U\to 0, H, \Gamma=\text{const}$. This limit is the zeroth approximation of the perturbation theory over $U$. As we see, perturbation theory corresponds to the 'high fields' region. The entire region $H\ll(U\Gamma)^{1/2}$, together with the Kondo effect, is outside the application of the perturbation theory. In the limit of high fields (or small $U$) from (8.2.88) we get a linear relation between the Fermi point and the magnetic field corresponding to the constant density of states. In other words at $U\to 0$ eqn. (8.2.88) brings us back to the conventional description of free particles, in terms of spin and charge variables.

At $U\to 0$ the function

$$\frac{k}{U\Gamma}R\left(\frac{k^2-p^2}{2U\Gamma}\right)\to\frac{1}{2}\delta(k^2-p^2).$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 8.1




Schematic sketch of the impurity magnetization $M_i$ versus $H$ for the symmetric Anderson model for (*a*) $U \gg \Gamma$ and (*b*) $U \sim \Gamma$. The dashed curves correspond to the universal Kondo magnetization. For $U \gg \Gamma$ there is a well-developed local-moment regime, whereas for $U \sim \Gamma$ there is direct transition from the non-magnetic regime to the free-orbital regime.

Therefore, eqn. (8.2.88) becomes

$$\tilde{\rho}(k) + \rho(k) + \frac{1}{2}(\tilde{\rho}(k) + \tilde{\rho}(-k)) = \frac{1}{2\pi} + \frac{1}{L}\Delta(k) \qquad \text{at } k > 0.$$

Hence we have

$$\rho(k) = \theta\left(\frac{H}{2} - |k|\right)\left(\frac{1}{2\pi} + \frac{1}{L}\Delta(k)\right) = \sum_{\sigma = \pm 1/2} \rho_\sigma(k),$$

where $\rho_\sigma(k) = \theta(\sigma H - k)(1/2\pi + \Delta(k)/L)$ is the density of particles with spin $\sigma = \pm 1/2$. So, for instance, the impurity magnetic susceptibility is given by (8.2.97) as it should be at $U = 0$.

### 8.2.8. *Magnetic susceptibility at $H = 0$ and arbitrary $\epsilon_d + U/2$*

At a finite magnetic field $H$ and an arbitrary value of $\epsilon_d + U/2$ the problem of investigation of eqns. (8.2.33) and (8.2.34) becomes complicated. In any case the system (8.2.33) and (8.2.34) could hardly be solved analytically at arbitrary $B$ and $Q$. We can construct an iteration scheme enabling us to determine the terms of the series

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

over $\exp(-\pi b)$ at $b\to\infty$ and fixed $Q$, i.e. series in powers of the magnetic field. In other words, magnetization of the impurity and the magnetic field, like the functions $b$ and $Q$, are expanded in powers of $\exp(-\pi b)$ and $\exp(-\pi(b-Q))$:

$$H=\sum_{n,m}\alpha_{nm}(Q)\exp(-\pi nb-\pi m(b-Q)). \tag{8.2.98}$$

The coefficients $\alpha_{nm}$ can be determined by iterations. Perturbation in the iteration scheme is the integral with $\rho$ in eqns. (8.2.34). At a low magnetic field $H\ll H_1=\min((U\Gamma)^{1/2},\Gamma U/(U+2\epsilon_d))$ the function $g(k)$ at $k<\epsilon_d+U/2$ is monotonical and we can perform the familiar replacement of the variables

$$z=g(k),\qquad p_{\mathrm{h,i}}(z)=-p_{\mathrm{h,i}}(k)/g'(k)|_{k=-\epsilon_d-U/2+(2U\Gamma z)^{1/2}}.$$

Let us rewrite eqn. (8.2.33) as

$$p_{\mathrm{h,i}}(z)-\int_b^\infty R(z-z')p_{\mathrm{h,i}}(z')\,dz'=r_{\mathrm{h,i}}(z)+\int_{-\infty}^Q s(z-\lambda)(\tilde\sigma_{\mathrm{h,i}}(\lambda)-\tilde\sigma^{(0)}_{\mathrm{h,i}}(\lambda))\,d\lambda, \tag{8.2.99}$$

where

$$r_{\mathrm{h,i}}(z)=p^{(0)}_{\mathrm{h,i}}(z)+\int_{-\infty}^Q s(z-\lambda)\tilde\sigma^{(0)}_{\mathrm{h,i}}(\lambda)\,d\lambda \tag{8.2.100}$$

and the functions $\tilde\sigma^{(0)}_{\mathrm{h,i}}$ are the 'hole' distributions in $\lambda$ at $H=0$ (see (8.2.46)). Equations (8.2.34) make it possible to express $\tilde\sigma$ by $\rho$. We have

$$\tilde\sigma(\lambda)-\tilde\sigma^{(0)}(\lambda)=\frac{i}{4\pi^2}\int_{-\infty}^{+\infty}d\omega\exp(-i\omega(\lambda-Q))G^{(-)}(\omega)$$
$$\times\int_{-\infty}^{+\infty}d\omega'\exp(-i\omega'(Q-b))\frac{\rho^{(+)}(\omega')}{\omega-\omega'-i0}\frac{G^{(+)}(\omega')}{2\cosh\omega'/2}, \tag{8.2.101}$$

where

$$\rho^{(+)}(\omega)=\int_0^\infty\exp(i\omega z)p(z+b)\,dz.$$

The right-hand side of (8.2.100) is expanded in series in powers of $\exp(-\pi z)$ at $z\to\infty$. With it the solution of (8.2.99) $p_{\mathrm{h,i}}(z)$ is also expanded in powers of $\exp(-\pi z)$ and it means, in its turn, that the functions $H(b)$ and $M_{\mathrm{i}}(b)$ are expanded in powers of $\exp(-\pi b)$. The principal term of this series is obtained if the second term in the right-hand side of (8.2.100) is neglected. According to (8.2.101), $\tilde\sigma(\lambda)-\tilde\sigma^{(0)}(\lambda)$, has an additional small quantity with respect to $\exp(-\pi b)$ since $p(z)\sim\exp(-\pi z)$ at $z\gg1$ and $\rho^{(+)}(\omega)$ is the analytical function in the upper half-plane. Therefore

$$\int\exp(\pi\lambda)(\tilde\sigma(\lambda)-\tilde\sigma^{(0)}(\lambda))d\lambda\sim\rho^{(+)}(i\pi)\exp(-\pi(b-Q)).$$

The subsequent terms of the expansion are obtained by iteration of eqns. (8.2.99) and (8.2.101).

We shall calculate the magnetic susceptibility at $H=0$. For this purpose let us neglect $\tilde\sigma-\tilde\sigma^{(0)}$ in (8.2.99) and with the same accuracy replace $r(z)$ in (8.2.100) by its asymptotics at $z\to\infty$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\left.\begin{aligned} p_{\mathrm{h}}(z)-\int_b^{\infty} R(z-z')p_{\mathrm{h}}(z')\,dz' &= A\exp(-\pi z),\\ p_{\mathrm{i}}(z)-\int_b^{\infty} R(z-z')p_{\mathrm{i}}(z')\,dz' &= a\exp(-\pi z). \end{aligned}\right\} \tag{8.2.102}$$

The quantities $A$ and $a$ according to (8.2.71) and (8.2.72) are

$$A=\frac{(2U\Gamma)^{1/2}}{2\pi}+\exp(\pi Q)\tilde{\sigma}_{\mathrm{h}}(-i\pi), \tag{8.2.103}$$

$$a=\exp(\pi/I)+\frac{\Gamma}{\pi}\int_{-\infty}^{+\infty} dk\frac{\exp(-\pi k^2/2U\Gamma)}{(ik+U/2)^2+\Gamma^2}+\exp(\pi Q)\tilde{\sigma}_{\mathrm{i}}(-i\pi), \tag{8.2.104}$$

where $\tilde{\sigma}_{\mathrm{h}}, \tilde{\sigma}$ are given by eqn. (8.2.46). Below, we use the Fermi-liquid approach considered in §5.1.3 for the s–d exchange model. It follows from (8.2.102) that $M^{\mathrm{i}}/S^z=a/A$. Therefore, according to (8.2.35) and (8.2.41)

$$M_{\mathrm{i}}=\frac{H}{4\pi}\frac{a}{A}$$

and the magnetic susceptibility at $H=T=0$ is

$$\chi_{\mathrm{sp}}\left(\frac{2\epsilon_d+U}{\Gamma},\frac{U}{\Gamma}\right)=\left\{\exp\left[\pi\frac{(U^2-4\Gamma^2)}{8U\Gamma}\right]+\exp(\pi Q)\tilde{\sigma}_{\mathrm{i}}(-i\pi)\right.$$
$$\left.+\frac{\Gamma}{\pi}\int_{-\infty}^{+\infty}\frac{\exp(-\pi k^2/2U\Gamma)}{(ik+U/2)^2+\Gamma^2}\right\}\{2(2U\Gamma)^{1/2}+4\pi\exp(\pi Q)\tilde{\sigma}_{\mathrm{h}}(-i\pi)\}^{-1}. \tag{8.2.105}$$

Formula (8.2.105) is easily simplified in the limits of the symmetric and asymmetric models.

### 8.2.9. *Magnetic susceptibility of the asymmetric Anderson model*

In the vicinity of the symmetry case the coefficients of the series (8.2.97) are expanded in powers of $\exp(\pi Q)$. This gives rise to the fact that the magnetic susceptibility (8.2.105) is expanded in series in powers of $(\epsilon_d+U/2)/(U\Gamma)^{1/2}$. This expansion can easily be derived from (8.2.105) and (8.2.49). In the limit $\epsilon_d+U/2=0$, i.e. at $Q=-\infty$ formula (8.2.105) coincides with (8.2.82).

A different picture is observed in the asymmetric case $\epsilon_d+U/2\gg(U\Gamma)^{1/2}$. Now the coefficients $\alpha_{nm}$ in (8.2.98) are slow functions of $Q$ (in comparison with $\exp(-\pi Q)$). We shall see below that at $Q\to+\infty$, for instance, $\alpha_{0m}(Q)\sim q_*^{-1/2}+O(q_*^{-3/2})$. Therefore, in the asymmetric case with the exponential accuracy one should retain in (8.2.98) only the terms with $n=0$. This will become evident by the fact that in (8.2.100) and (8.2.103) we should neglect the second term in comparison with the first term. In the asymmetric limit

$$A=\frac{1}{2\pi}\left(\frac{U\Gamma}{\pi eq^*}\right)^{1/2}\exp(\pi Q),$$

$$a=\exp\left(\frac{\pi U}{8\Gamma}\right)+\exp(\pi Q)\tilde{\sigma}_{\mathrm{i}}(-i\pi).$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The criterion of this approximation is the condition $Q \gg 1$ or, according to (8.2.53), $\epsilon_d + U/2 \gg (U\Gamma)^{1/2}$. The following simplification occurs at $U \gg \Gamma$. Then, according to (8.2.55),

$$\chi_{sp} = \frac{(2\pi e)^{1/2}}{8\Gamma}\left(\frac{2\epsilon_d + U}{U}\right)\left[\exp\left(\frac{\pi}{I^*}\right) + \frac{i}{2\sqrt{(\pi e)}}\int_{-\infty}^{+\infty}\frac{d\omega}{i\pi+\omega}\,\frac{\exp(-|\omega| + i\omega/I^*)}{G^{(-)}(\omega)}\right]. \tag{8.2.106}$$

This formula describes the universal dependence of the magnetic susceptibility on the coupling constant $I^*$ (8.2.57). The second term in (8.2.106) is a slow function of $I^*$ resembling the function $n_d(I^*)$ from (8.2.56). Yet, the first term in (8.2.106) points to an essential difference of the phenomena observed in spin and charge channels. In the region of the formation of the localized moment $0 < I^* \ll 1$ the first term is exponentially large and the Kondo effect is observed

$$\chi_{sp} = (2\pi T_k)^{-1},$$

where the Kondo temperature in the asymmetric limit is

$$T_K = \frac{(2U\Gamma)^{1/2}}{\pi}\exp\left[\frac{\pi\epsilon_d(\epsilon_d + U)}{2U\Gamma}\right] = \frac{2}{\pi}\left(\frac{2}{\pi e}\right)^{1/2}\frac{\Gamma U}{U + 2\epsilon_d} \times \exp(-\pi/I^*). \tag{8.2.107}$$

The second term in (8.2.106) is of the order of $\Gamma/\epsilon_d^{**2}$ at $|I^*| \ll 1$ and in the Kondo-effect region is negligibly small in comparison with $T_K^{-1}$. If $|I^*| \sim 1$ then the localized moment gradually vanishes and both the terms are of the same order. At a further increase of $I^*$ the first term in (8.2.106) is exponentially small.

On the boundary of the intermediate-valence region $0 < -I^* \ll 1$, the magnetic susceptibility has previously been studied within the framework of perturbation theory with respect to $\Gamma/\epsilon_d^{**}$. Formula (8.2.106) makes it possible to calculate the terms of this series. For this purpose the integration contour can be closed into the cut of the integrand in the lower half-plane of $\omega$ in (8.2.106):

$$\chi_{sp} = \frac{1}{8\sqrt{\pi}\Gamma}\int_0^{\infty}\frac{dt}{1/2 - t}\exp\left(\frac{2\pi t}{I^*}\right)\sin 2\pi t\left(\frac{t}{e}\right)^{-t}\Gamma\left(\frac{1}{2} + t\right). \tag{8.2.108}$$

At $I^* \to 0$ the integral (8.2.108) is expanded in series in powers of $I_{**}$ (see (8.2.61)). The first term of the expansion

$$\chi_{sp} = I_{**}^2/8\pi\Gamma + \ldots$$

has been calculated in (Haldane 1978 a).

Like the valence, the magnetic susceptibility can be expanded in powers of $I^{*-1}$ inside the region of the mixed valence. Applying the results obtained in the Appendix to 8.2.6 we have

$$\chi_{sp} = \frac{\pi}{4\sqrt{2}\Gamma} + O\left(\frac{1}{\Gamma I^*}\right). \tag{8.2.109}$$

The numerical calculation of $\chi_{sp}(I^*)$ of (8.2.106) is presented in fig. 3.12 (Melnikov 1982 b).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

8.2.10. *Localized-moment regime*

Formula (8.2.106) determines the first term of the expansion of the magnetic susceptibility in powers of the magnetic field $H$. In the asymmetric case there are two parameters of this expansion. The first term is associated with the expansion (8.2.97). Its estimate can be obtained from (8.2.53) and (8.2.104). Actually, at $Q \gg 1$ the expansion parameter in (8.2.97) is $\exp(-\pi(b-a))$. From (8.2.104), (8.2.53) and (8.2.54) it follows that

$$(H/2U\Gamma)^{1/2} = \exp(-\pi(b-Q))/\pi e q_*^{1/2}.$$

Therefore, the expansion is performed in powers of $H/H_1$.

$$H_1 = \left(\frac{\Gamma U}{q_*}\right)^{1/2} \sim \Gamma \frac{U}{U+2\epsilon_d}. \tag{8.2.110}$$

The terms of this series are determined by iterations. Another parameter arises in the region of the localized moment: $H/T_K$. In this region, with the exponential accuracy, one can neglect corrections of the order of $H/\Gamma$. The dependence of the magnetization on $H/T_K$ is universal, in other words, all the physical quantities depend on the parameters $\epsilon_d$, $\Gamma$ and $U$ only through $T_K$. Therefore, the universal part of the magnetization is given by the function $M_{\text{Kondo}}(H/T_K)$ calculated previously for the s–d model (see § 5.1.3). To obtain this function it is sufficient to retain the whole term $s(z-1/I)$ in formula (8.2.72).

Equations (8.2.99) with accuracy up to $O(H/\Gamma)$ coincide with (5.1.20). Performing the replacement $p_h(z) \to Ap_h(z)$ according to (8.2.71), (8.2.72) and (8.2.99) we have

$$p_{h,i}(z) - \int_b^\infty R(z-z')p_{h,i}(z')\,dz' = \exp(-\pi z) + \frac{1}{L}s\left(z - \frac{1}{I}\right),$$

where $H/2\pi A = \int_b^\infty p_h(z)\,dz$.

An important difference arises on comparison of the functions $b(H)$ in the Anderson and s–d exchange models. All the integrals for the Anderson model are normalized with respect to $(U\Gamma)^{1/2}$, and with respect to $\epsilon_F$ for the s–d model. This circumstance together with formulae (8.2.86) and (8.2.107) solves the problem of the pre-exponential multiplier in the dependence of $T_K$ on $I$ which we have discussed. Remember, that despite the results of the perturbation theory (see § 5.1.5), on solution of the s–d model we have obtained $T_K = 2\epsilon_F/\pi \exp(-\pi/I)$ (see eqn. 5.1.23) instead of $T_K = \epsilon_F I^{1/2} \exp(-\pi/I)$. As has been assumed this divergence is an artefact of the linear spectrum and the point-like potential approximations. A consequence of these approximations—an independence of the scattering phase of the scattered particle energy—leads to an incorrect pre-exponential dependence of $T_K$ on $I$. In the Anderson model, even in the linear spectrum approximation, the scattering phase is a function of the energy, which leads to a correct pre-exponent

$$T_K = \frac{U}{2\pi} I^{1/2} \exp\left(-\frac{\pi}{I}\right). \tag{8.2.111}$$

The pre-exponential dependence of the magnetic susceptibility and the dependence of $T_K$ on $\Gamma$ and $U$ has been found numerically by the renormalization group

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

procedure (Krishna-Murthy *et al.* 1980 a, b). The numerical result for the magnetic susceptibility is

$$\chi_{\rm sp}=\frac{0{\cdot}103}{0{\cdot}182}U^{-1}\left(\frac{\pi U}{8\Gamma}\right)^{1/2}\exp\left(\frac{\pi U}{8\Gamma}\right),$$

which, with brilliant accuracy, coincides with the exact value of (8.2.85): $0{\cdot}103/0{\cdot}82\simeq\pi^{-1/2}$

### 8.3. *Thermodynamic properties of the Anderson model at finite temperatures*

#### 8.3.1. *The theory of a finite but large system*

Previously, in § 8.2.1, we have given a classification of solutions of the Bethe-Ansatz equations (8.2.A) and (8.2.B). Let us stress again that this classification is valid with accuracy up to $O(\exp(-\delta N))$, where $\delta N$ is the number of excitations above the ground state. This is the accuracy that is required for the thermodynamical limit $\delta N/N=\text{const}$ at $N\to\infty$ (see the Appendix to § 8.2.1). At finite temperatures we must take into consideration all types of excitations. Then, above all, we must express eigenvalues of the hamiltonian in terms of rapidities of possible types of excitations. Let us assume that in the system there are $N-2M'$ unbounded charge particles with rapidities $k_j$ $(J=1,\ldots,N-2M')$, $M_n$ spin complexes of the order $n$ with rapidities $\lambda_\alpha^n$ and $M_n'$ bounded spin complexes of the order $n$ with rapidities $\lambda_\alpha'^n$ which are related to $2M_n'$ pair charge complexes (see (8.2.4)).

The numbers $M'$, $M_n'$ are explicitly related as

$$M'=\sum_{n=1}^{\infty}nM_n'. \tag{8.3.1}$$

Equations (8.2.A) and (8.2.B) in terms of $k_j$, $\lambda_\alpha^n$, $\lambda_\alpha'^n$ are

$$\exp(ik_jL+i\delta(k_j))=\sum_{n=1}^{\infty}\sum_{\alpha=1}^{M_n}e_n(g(k_j)-\lambda_\alpha^n)\prod_{m=1}^{\infty}\prod_{\beta=1}^{M_m'}e_m(g(k_j)-\lambda_\beta'^m), \tag{8.3.2}$$

$$\exp\left(iL\sum_{\substack{p=1\\ \tau=\pm1}}^{2n}k_\alpha^{(\tau,n,p)}+i\sum_{\substack{p=1\\ \tau\pm1}}^{2n}\delta(k_\alpha^{(n,p,\tau)})\right)$$
$$=\prod_{j=1}^{N-2M'}e_n(\lambda_\alpha'^n-g(k_j))\sum_{m=1}^{\infty}\prod_{\beta=1}^{M_m'}E_{nm}(\lambda_\alpha'^n-\lambda_\beta'^m), \tag{8.3.3}$$

$$\prod_{j=1}^{N-2M'}e_n(\lambda_\alpha^n-g(k_j))=-\prod_{m=1}^{\infty}\prod_{\beta=1}^{M_m}E_{nm}(\lambda_\alpha^n-\lambda_\beta^m), \tag{8.3.4}$$

where $e_n(\lambda)=(\lambda+in/2)/(\lambda-in/2)$; $E_{nm}=e_{|n-m|}e_{|n-m|+2}^2\cdots e_{n+m-2}^2e_{n+m}$. Logarithmizing eqns. (8.3.2)–(8.3.4) we have

$$k_jL+\delta(k_j)=2\pi N_j-\sum_{n=1}^{\infty}\sum_{\alpha=1}^{M_n}\theta_n(g(k_j)-\lambda_\alpha^n)-\sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m'}\theta_m(g(k_j)-\lambda_\beta^m), \tag{8.3.5 a}$$

$$-2L(2U\Gamma)^{1/2}\,\mathrm{Re}\left(\lambda_\alpha'^n+\frac{in}{2}\right)^{1/2}-2\,\mathrm{Re}\,\delta[(2U\Gamma)^{1/2}(\lambda_\alpha'^n+in/2)^{1/2}]$$
$$=2\pi J_\alpha'^n+\sum_{j=1}^{N-2M'}\theta_n(\lambda_\alpha'^n-g(k_j))+\sum_{m-1}^{\infty}\sum_{\beta=1}^{M_m}\Xi_{nm}(\lambda_\alpha'^n-\lambda_\beta'^m), \tag{8.3.5 b}$$

$$\sum_{j=1}^{N-2M'}\theta_n(\lambda_\alpha^n-g(k_j))=2\pi J_\alpha^n+\sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m}\Xi_{nm}(\lambda_\alpha^n-\lambda_\beta^m), \tag{8.3.5 c}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where

$$\theta_n(\lambda) \equiv i \ln e_n(\lambda) = 2 \tan^{-1}(2\lambda/n)$$

and

$$\Xi_{nm}(\lambda) \equiv i \ln E_{nm}(\lambda) = \theta_{|n-m|}(\lambda) + 2 \sum_{k=1}^{\min(n,m)-1} \theta_{|n-m|+2k}(\lambda) + \theta_{n+m}(\lambda).$$

The integers $2N_j$, $2J_\alpha'^n$ and $2J_\alpha^n$ are quantum numbers of the system.

The energy and the projection of the spin are

$$E = \sum_{j=1}^{N-2M'} k_j + 2(2U\Gamma)^{1/2} \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_n} \left[ \operatorname{Re}(\lambda_\alpha'^n + in/2)^{1/2} + n\left(\epsilon_d + \frac{U}{2}\right)\right], \tag{8.3.6}$$

$$S^z = N/2 - \sum_{n=1}^{\infty} n(M_n' + M_n). \tag{8.3.7}$$

8.3.2. *Integral equations*

In the limit $N, L \to \infty$; $N/L$, $M_n/L$, $M_n'/L = \text{const}$ solutions of eqns. (8.3.5) $k_j$, $\lambda_\alpha^n$, $\lambda_\alpha'^n$ should be described by the distributions of particles $\rho(k)$, $\sigma_n(\lambda)$, $\sigma_n'(\lambda)$ and the appropriate 'holes' $\tilde{\rho}(k)$, $\tilde{\sigma}_n(\lambda)$, $\tilde{\sigma}_n'(\lambda)$.

Equations (8.3.8) relate the distributions of particles and 'holes' as

$$\frac{1}{2\pi} + \frac{\Delta(k)}{L} = \tilde{\rho}(k) + \rho(k) - g'(k) \sum_{n=1}^{\infty} \int a_n(g(k) - \lambda)(\sigma_n'(\lambda) + \sigma_n(\lambda))\, d\lambda, \tag{8.3.8 a}$$

$$\tilde{\sigma}_n(\lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma_m(\lambda) = \int a_n(\lambda - g(k))\rho(k)\, dk, \tag{8.3.8 b}$$

$$\tilde{\sigma}_n'(\lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma_m'(\lambda) + \int a_n(\lambda - g(k))\rho(k)\, dk$$
$$= -\frac{(2U\Gamma)^{1/2}}{2\pi} \operatorname{Re}\left(\lambda + \frac{in}{2}\right)^{-1/2} - \frac{1}{\pi L}\frac{d}{d\lambda} \operatorname{Re}\delta\left[(2U\Gamma)^{1/2}\left(\lambda + \frac{in}{2}\right)^{1/2}\right]. \tag{8.3.8 c}$$

Here the sign $*$ means a convolution,

$$a_n(\lambda) = (1/2\pi)(d/d\lambda)\theta_n(\lambda), \text{ and } A_{nm}(x) = \delta_{nm} + (1/2\pi)(d/dx)\Xi_{nm}(x)$$

is the same matrix that arose in s–d model thermodynamics. The useful formulae for the Fourier transforms of $A_{nm}$ and the inverse operator $(A^{-1})_{nm}$ which we shall require below are written in § 6.1.2 (eqns. (6.1.24) and (6.1.25)).

For further transformations of eqns. (8.3.8) the formulae for the right-hand side of (8.3.8 *c*) generalizing the relations (8.2.28) and (8.2.29) are of great use. It is easy to check that

$$-(2U\Gamma)^{1/2} \operatorname{Re}(\lambda + in/2)^{-1/2} = \int_{-\infty}^{+\infty} a_n(\lambda - g(k))\, dk, \tag{8.3.9}$$

$$\left\{-\frac{1}{\pi}\frac{d}{d\lambda} \operatorname{Re}\delta((2U\Gamma)^{1/2}\left(\lambda + \frac{in}{2}\right)^{1/2}\right\} = \int_{-\infty}^{+\infty} a_n(\lambda - g(k))\Delta(k)\, dk, \tag{8.3.10}$$

where $\Delta(k) = d\delta(k)/dk$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

8.3.3. *Thermodynamic equilibrium*

To find the equilibrium values of particle–hole distribution one should, according to the statistical mechanics principles, find the minimum of the thermodynamical potential

$$\Omega = E - TS - HS^z - AN, \tag{8.3.11}$$

where $H$ is a magnetic field, $A$ is the chemical potential calculated with respect to the bandwidth and the entropy $S$ is

$$S = \int \{(\rho+\tilde{\rho})\ln(\rho+\tilde{\rho}) - \rho\ln\rho - \tilde{\rho}\ln\tilde{\rho} + (\sigma_n+\tilde{\sigma}_n)\ln(\sigma_n+\tilde{\sigma}_n)$$
$$-\sigma_n\ln\sigma_n - \tilde{\sigma}_n\ln\tilde{\sigma}_n + (\sigma'_n+\tilde{\sigma}'_n)\ln(\sigma'_n+\tilde{\sigma}'_n) - \sigma'_n\ln\sigma'_n - \tilde{\sigma}'_n\ln\tilde{\sigma}'_n\}\,d\lambda, \tag{8.3.12}$$

The condition

$$\frac{\delta\Omega}{\delta\rho} = \frac{\delta\Omega}{\delta\sigma_n} = \frac{\delta\Omega}{\delta\sigma'_n} = 0$$

with (8.3.8) gives an equation for the energy of elementary excitations. (All algebra is quite analogous to that of § 6.1.3.)

$$\varepsilon(k) = k + H + D - A + T\sum_{n=1}^{\infty}\int a_n(\lambda - g(k))\ln\left[\frac{n(-\kappa_n(\lambda))}{n(-\kappa'_n(\lambda))}\right]d\lambda, \tag{8.3.13 a}$$

$$\ln n(\kappa_n(\lambda)) - \sum_{m=1}^{\infty} A_{nm} * \ln n(-\kappa_m(\lambda))$$
$$= -\frac{nH}{T} - \int dk\, g'(k) a_n(\lambda - g(k))\ln n(-\varepsilon(k)), \tag{8.3.13 b}$$

$$\ln n(\kappa'_n(\lambda)) - \sum_{m=1}^{\infty} A_{nm} * \ln n(-\kappa'_m(\lambda)) = -\frac{2n}{T}\left(\epsilon_d + \frac{U}{2} + D - A\right)$$
$$+\frac{2}{T}\int_{-\infty}^{+\infty} a_n(\lambda - g(k))g(k)\,dk - \int dk\, g'(k) a_n(\lambda - g(k))\ln n(-\varepsilon(k)), \tag{8.3.13 c}$$

where

$$\varepsilon = T\ln\tilde{\rho}/\rho; \qquad \kappa_n = T\ln\tilde{\rho}_n/\sigma_n; \qquad \kappa'_n = T\ln\tilde{\sigma}'_n/\sigma'_n$$

and

$n(\varepsilon) = (\exp(\varepsilon/T)+1)^{-1}$ is the Fermi distribution.

The thermodynamical potential in terms of $\varepsilon$, $\kappa_n$ and $\kappa'_n$ is of the form

$$\Omega = \Omega_{\mathrm{h}} + \Omega_{\mathrm{i}},$$

where $\Omega_{\mathrm{h}}$ is the thermodynamical potential of the host metal and $\Omega_{\mathrm{i}}$ is the impurity part of the thermodynamical potential.

$$\Omega_{\mathrm{h}}/L = T\int \ln n(-\varepsilon(k))\frac{dk}{2\pi} - T\int\frac{dk}{2\pi}\int d\lambda\sum_{n=1}^{\infty} a_n(\lambda - g(k))$$
$$\times \ln n(-\kappa'_n(\lambda)), \tag{8.3.14 a}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\Omega_{\mathrm{i}} = T\int \ln n(-\varepsilon(k))\Delta(k)dk - T\int dk \int d\lambda \sum_{n=1}^{\infty} \Delta(k) \times a_n(\lambda - g(k)) \ln n(-\kappa_n'(\lambda)). \qquad (8.3.14\,b)$$

It is possible to derive another form of eqns. (8.3.13) and (8.3.14) which is sometimes more convenient. It is then necessary to vary the thermodynamical with respect to the 'hole' distributions $\tilde{\rho}$, $\tilde{\delta}_n$ and $\tilde{\sigma}_n'$. Using the explicit form of the matrix $\mathbf{A}^{-1}$, we have

$$\varepsilon(k) = \varepsilon_0(k) + T\int s(g(k)-\lambda) \ln [n(\kappa_1(\lambda))/n(\kappa_1'(\lambda))]\, d\lambda, \qquad (8.3.15\,a)$$

$$\kappa_n(\lambda) = -Ts * \ln n(\kappa_{n-1}(\lambda))n(\kappa_{n+1}(\lambda)) + \delta_{n1} T\int s(\lambda - g(k)) \ln n(-\varepsilon(k))g'(k)\, dk, \qquad (8.3.15\,b)$$

$$\kappa_n'(\lambda) = -Ts * \ln n(\kappa_{n-1}'(\lambda))n(\kappa_{n+1}'(\lambda)) + \delta_{n1} T\int s(\lambda - g(k)) \ln n(\varepsilon(k)g'(k)\, dk, \qquad (8.3.15\,c)$$

with the conditions

$$\kappa_0 = \kappa_0' = -\infty; \qquad \lim_{n\to\infty} \frac{\kappa_n}{n} = H, \qquad \lim_{n\to\infty} \frac{\kappa_n'}{n} = \epsilon_d + \frac{U}{2} - A, \qquad (8.3.15\,d)$$

where

$$\varepsilon_0(k) = k - \epsilon_d - U/2 + \int_{-\infty}^{+\infty} R(g(k) - g(p))pg'(p)\, dp + D - A,$$

Then there occurs another form of the thermodynamical potential

$$\Omega_{\mathrm{h}}/L = E_{\mathrm{h}}^{(0)} + T\int \rho_{\mathrm{h}}^{(0)}(k) \ln n(-\varepsilon(k))\, dk + \frac{T}{2\pi}\int dk \int d\lambda s(g(k)-\lambda) \ln n(\kappa_1'(\lambda)), \qquad (8.3.16\,a)$$

$$\Omega_{\mathrm{i}} = E_{\mathrm{i}}^{(0)} + T\int \rho_{\mathrm{i}}^{(0)}(k) \ln n(-\varepsilon(k))\, dk + T\int dk \int d\lambda \Delta(k) s(g(k)-\lambda) \ln n(\kappa_1'(\lambda)), \qquad (8.3.16\,b)$$

where $\rho_{\mathrm{h}}^{(0)}(k)$ and $\rho_{\mathrm{i}}^{(0)}(k)$ are determined by the right-hand side of formulae (8.2.36) and (8.2.37) and $E_{\mathrm{h}}^{(0)}$, $E_{\mathrm{i}}^{(0)}$ are the energies of the ground state of the host metal and of the impurity, respectively.

Equations (8.3.15) and (8.3.16) completely describe thermodynamical properties of the Anderson model at arbitrary $U$, $\Gamma$, $\epsilon_d$, $H$, $T \ll \epsilon_{\mathrm{F}}$. They have been obtained by Kawakami and Okiji (1982 c) Okiji and Kawakami (1982 b), Filyov *et al.* (1982) and Tsvelick and Wiegmann (1982). Therefore, (8.3.15) and (8.3.16 *a*) describe the free particle gas. Therefore,

$$\frac{\Omega_{\mathrm{h}}}{L} = -\frac{H^2}{8\pi} - \frac{\pi T^2}{12} - \frac{A^2}{8\pi}. \qquad (8.3.17)$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

As for the s–d models (see § 6.1.4) (Filyov *et al.* 1981) there is a relation characteristic of free particles between the distributions $\rho$, $\sigma_n$, $\sigma'_n$ and the elementary excitation energies $\varepsilon$, $\kappa_n$, $\kappa'_n$ in the leading order with respect to $1/L$. It is the consequence of the linear spectrum $E=P$. Comparison of the results of (8.3.15) and (8.3.8) yields, for the host parts of the distributions:

$$\left.\begin{aligned}
\rho(k)&=\frac{1}{2\pi}\frac{\partial\varepsilon(k)}{\partial k}n(\varepsilon(k)); & \tilde{\rho}(k)&=\frac{1}{2\pi}\frac{\partial\varepsilon(k)}{\partial k}(1-n(\varepsilon(k)));\\
\sigma_n(\lambda)&=\frac{1}{2\pi}\frac{\partial\kappa_n(\lambda)}{\partial\lambda}n(\kappa_n(\lambda)); & \tilde{\sigma}_n(\lambda)&=\frac{1}{2\pi}\frac{\partial\kappa_n(\lambda)}{\partial\lambda}(1-n(\kappa_n(\lambda)));\\
\sigma'_n(\lambda)&=-\frac{1}{2\pi}\frac{\partial\kappa'_n(\lambda)}{\partial\lambda}n(\kappa'_n(\lambda)); & \tilde{\sigma}'_n(\lambda)&=-\frac{1}{2\pi}\frac{\partial\kappa'_n(\lambda)}{\partial\lambda}(1-n(\kappa'_n(\lambda))).
\end{aligned}\right\}\tag{8.3.18}$$

By means of these formulae, as for the s–d model, one can make sure of the validity of (8.3.17) through a direct calculation which we do not give here.

In Appendix B to 8.3.3 we have studied low- and high-temperature limits for a specific case and have shown how eqns. (8.2.33) and (8.2.34) follow from (8.3.13)–(8.3.16) for $T/H\to 0$, $T/\Gamma\to 0$.

In the high-temperature limit $T\gg\Gamma$ it is evident that

$$\Omega_{\mathrm{i}}=-T\ln(1+2\cosh H/2T\exp(-\epsilon_d/T)+\exp(-(2\epsilon_d+U)/T).\tag{8.3.19}$$

This formula is derived from (8.3.13)–(8.3.16) in Appendix A to § 8.3.3. In the asymmetric case one should also bear in mind the renormalization of $\epsilon_d\to\epsilon_d^{**}$ (Appendix to § 8.3.7).

### 8.3.4. *Symmetries of charge and spin excitations*

The symmetry discussed in § 8.2.3 manifests itself most explicitly in eqns. (8.3.15) and (8.3.16). To make sure of it let us transform (8.3.16). According to (8.3.15 *a*) we have

$$T\ln n(-\varepsilon(k))=\varepsilon(k)+T\ln n(\varepsilon(k))=T\ln n(\varepsilon(k))+k+\mathscr{F}(g(k)).$$

Inserting it into (8.3.16) we get another formula for $\Omega_{\mathrm{h}}$:

$$\Omega_{\mathrm{h}}/L=T\int\rho_{\mathrm{h}}^{(0)}(k)\ln n(\varepsilon(k))\,dk+\frac{T}{2\pi}\int dk\int d\lambda s(g(k)-\lambda)\ln n\,\kappa_1(\lambda))+E'_n.$$

Similarly, for the impurity part we have

$$\Omega_{\mathrm{i}}=T\int\rho_{\mathrm{i}}^{(0)}\ln n(\varepsilon(k))\,dk+T\int dk\int d\lambda\Delta(k)s(g(k)-\lambda)\ln n(\kappa_1(\lambda))+E'_i.$$

Hence, it becomes clear that the replacement

$$U\to -U,\qquad H\to\epsilon_d+U/2-A,\qquad k-\epsilon_d-U/2\to -k+\epsilon_d+U/2$$
$$(\kappa_n\to\kappa'_n,\ \varepsilon(k)\to-\varepsilon(k))$$

does not affect eqns. (8.3.15)–(8.3.17).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

8.3.5. *Low-temperature thermodynamics*

The free energy at low temperatures is expanded in series over integer powers of $T$. Outside the region $T \sim T_K \ll \min((U\Gamma)^{1/2}, \Gamma(U/(U+2\epsilon_d))$, where the Kondo effect is observed, this expansion is performed in powers of $T/(U\Gamma)^{1/2}$ in the symmetric case and in powers of $T((U+2\epsilon_d)/\Gamma U)$ in the asymmetric case. In the Kondo region at $T \ll T_K$ the terms $T/T_K$ are exponentially large in comparison with $T/(U\Gamma)^{1/2}$ or $T(U+2\epsilon_d/\Gamma U)$. In the following, we shall obtain the linear term in the heat capacity, with respect to temperature at $T \to 0$, outside the Kondo region and in the Kondo region we shall obtain the entire universal dependence on $T/T_K$ as well as the non-universal linear contribution with respect to temperature (at arbitrary $\Gamma$, $\epsilon_d$, $U$).

In the low-temperature limit the main contribution comes from the region $\varepsilon_0(k) \sim T$, i.e. the region of energies near the Fermi level. Then certain simplifications arise. Above all, it is sufficient to confine ourselves only to the leading asymptotics of the terms related to charge degrees of freedom in the right-hand side of (8.3.15 *a*)

$$\left.\begin{aligned} -T\int s(g(k)-\lambda)\ln n(\kappa_1'(\lambda))\,d\lambda &= T\exp(-\pi g(k))\mathscr{A}, \\ \mathscr{A} = \frac{1}{2}\int_{-\infty}^{Q}\exp(\pi\lambda)\kappa_1'(\lambda)d\lambda - \frac{T}{2}\int_{-\infty}^{+\infty}\exp(\pi\lambda)\ln n(-|\kappa_1'(\lambda)|)\,d\lambda. \end{aligned}\right\} \quad (8.3.20)$$

To preserve the principal terms with respect to $T$ suffice it to take $\mathscr{A}(T=0)$ in (8.3.20). The value of $\mathscr{A}(0)$ coincides with the one calculated in (8.2.103). Thus at $T \to 0$ the principal contribution comes from the momenta at which

$$A\exp(-\pi g(k)) \sim T.$$

Therefore, the accuracy of the approximation (8.3.20) is $O(T/A)$.

The region $k > \epsilon_d + U/2$ leads to exponentially small corrections to the free energy. Outside this region $g(k)$ is monotonical and it is possible to pass over to the variable $z = g(k)$ and, with the indicated accuracy, to extend the integral over $z$ on the whole real axis. With the same accuracy let us, according to (8.2.71) and (8.2.72), replace in (8.3.16) $p_i^{(0)}(z)$ and $p_h^{(0)}(z)$ by their asymptotics at $z \to +\infty$:

$$p_h^{(0)}(z) = \frac{(2U\Gamma)^{1/2}}{2\pi}\exp(-\pi z) + \ldots, \quad (8.3.21\,a)$$

$$p_i^{(0)}(z) = \left(2\cosh\pi\left(z - \frac{1}{I}\right)\right)^{-1} + \exp(-\pi z)\frac{\Gamma}{\pi}\int_{-\infty}^{\infty} dp\exp\left(\frac{-\pi p^2}{2U\Gamma}\right)\left[\left(ip + \frac{U}{2}\right)^2 + \Gamma^2\right]^{-1}. \quad (8.3.21\,b)$$

In (8.3.21 *a*) along with the second term $\sim\exp(-\pi z)$ we have deliberately retained all the terms $\sim\exp(-\pi z n)$ $(n = 1, 2, \ldots)$ with the coefficients exponentially large with respect to $U/\Gamma$ at $U \gg \Gamma$. Those terms are responsible for the universal

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

behaviour of the physical quantities in the Kondo effect region $U \gg \Gamma$, $T \ll (U\Gamma)^{1/2}$. After these simplifications eqns. (8.3.15) and (8.3.16) acquire the form

$$\varepsilon(z) = 2A \exp(-\pi z) + Ts * \ln n(\kappa_1, (z)); \tag{8.3.22 a}$$

$$\kappa_n(\lambda) = -Ts * \ln[n(\kappa_{n-1}(\lambda))n(\kappa_{n+1}(\lambda))] - \delta_{n1} Ts * \ln n(-\varepsilon(\lambda)); \quad \lim_{n\to\infty} \kappa_n/n = H; \tag{8.3.22 b}$$

$$\kappa'_n(\lambda) = -Ts * \ln[n(\kappa'_{n-1}(\lambda))n(\kappa'_{n+1}(\lambda))] + \delta_{n1}\left[Ts * \ln n(\varepsilon(\lambda)) - 2\int s(\lambda - g(k))g(k)\,dk\right]; \quad \lim_{n\to\infty} \kappa'_n/n = \epsilon_d + U/2; \tag{8.3.22 c}$$

$$\Omega_i = \Omega_i^{sp} + \Omega_i^{ch}; \tag{8.3.23 a}$$

$$\Omega_i^{sp} = T\int\left\{s(z - 1/I) + \exp(-\pi z)(\Gamma/\pi)\int dp \exp(-\pi p^2/2U\Gamma)[(ip + U/2)^2 + \Gamma^2]^{-1}\right\}\ln n(-\varepsilon(z))\,dz; \tag{8.3.23 b}$$

$$\Omega_i^{ch} = T\int d\lambda \int dk \Delta(k) s(\lambda - g(k) \ln n(\kappa'_1(\lambda)). \tag{8.3.23 c}$$

Note that eqns. (8.3.22 *a*, *b*) now completely determine the functions $\varepsilon$ and $\kappa_n$.

### 8.3.6. *The Kondo limit*

At $U + \epsilon_d \gg \Gamma$, $-\epsilon_d \gg \Gamma$ and $T \ll A$ one should neglect the contribution of charge fluctuations and the non-universal contribution of spin fluctuations, i.e. retain only the first term in (8.3.23 *b*). Thus, we neglect the terms of the order $(T/A)^2$ in the free energy in comparison with $(T/T_K)^2$ at $T \ll T_K$ or in comparison with $(\ln T/T_K)^{-1}$ at $T \gg T_K$. Thus, eqns. (8.3.22 *a*, *b*) determine the universal behaviour of the physical quantities in the Kondo limit. Introducing the dimensionless quantities

$$\left.\begin{aligned} \varphi_1(x) &= -\frac{1}{T}\varepsilon\left(-z + \frac{1}{\pi}\ln\frac{2A}{T}\right), \\ \varphi_n(x) &= \frac{1}{T}\kappa_{n-1}\left(-\lambda + \frac{1}{\pi}\ln\frac{2A}{T}\right), \end{aligned}\right\} \tag{8.3.24}$$

we have

$$\varphi_n(x) = -s * \ln[n(\varphi_{n-1}(x))n(\varphi_{n+1}(x))] - \delta_{n1}\exp(\pi x); \quad \lim_{n\to\infty} \varphi n/n = H/T. \tag{8.3.25}$$

Then

$$\Omega_i = T\int s\left(x + \frac{1}{\pi}\ln\frac{T}{T_K}\right)\ln n(\varphi_1(x))\,dx,$$

where $T_K$ is defined by (8.2.107).

Equations (8.3.25) have been derived in § 6.1.5 for the s–d model. It has been shown that these equations also determine the thermodynamics of free electrons

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

with a constant density of states and the bandwidth $T_K/\pi$. This circumstance makes it possible to assert that

$$-\int_{-\infty}^{+\infty} \exp(\pi x) \ln n(\varphi_1(x)\, dx = \frac{\pi}{6} + \frac{1}{4\pi}\left(\frac{H}{T}\right)^2, \tag{8.3.26}$$

which has been rigorously proved in § 6.1.6 by direct calculations. This result will be used below.

8.3.7. *Specific heat at* $T \ll \epsilon_d + U/2$, $\Gamma$, $U$

We shall calculate below the specific heat at $T \to 0$, $T \ll \epsilon_d + U/2$. The method of calculation enables one to subsequently find the coefficients of the expansion in powers of $T/\sigma_1'(Q)$. If $\epsilon_d + U/2 \ll (U\Gamma)^{1/2}$ then $\sigma_1'(Q) \simeq \epsilon_d + U/2$. Therefore, this method is formally inapplicable to the symmetric case. However, the expression obtained for the specific heat

$$\frac{C_i}{T} = \frac{f(\Gamma/U, (\epsilon_d + U/2)/(U\Gamma)^{1/2})}{\epsilon_d + U/2}$$

is regular at $\epsilon_d \to -U/2$. At $\epsilon_d = -U/2$ this formula gives an expression for the specific heat of the symmetric model. To make sure of the validity of this assertion we propose in § 8.3.8 another method of calculation suitable for the symmetric case and show that, as should be expected:

$$\lim_{\epsilon_d + U/2 \to 0} \lim_{T \to 0} = \lim_{T \to 0} \lim_{\epsilon_d + U/2 \to 0} \tag{8.3.27}$$

To derive the formula for the specific heat it is convenient to use the Fermi-liquid approach already used in the analogous situation for the s–d exchange model (§ 6.1.5). The other trick relating to the commutativity of limits $T \to 0$ and $H \to 0$ was used by Kawakami and Okiji (1982 b) for the symmetric model. We considered it in § 6.1.10 for the s–d exchange model. Above all, let us calculate the contribution of spin excitations at $T \to 0$. Retaining only the principal terms with respect to $\exp(-\pi z)$ in eqn. (8.3.23) we have

$$\Omega_i^{sp} = \frac{T^2}{2} \int_{-\infty}^{+\infty} \exp(\pi x) \ln n(\varphi_1(x))\, dx \left( \exp\left(\frac{\pi}{I}\right) + \frac{\Gamma}{\pi} \int_{-\infty}^{+\infty} dp \right.$$
$$\left. \times \exp\left(-\frac{\pi p^2}{2U\Gamma}\right) \left[ \left(ip + \frac{U}{2}\right)^2 + \Gamma^2 \right]^{-1} \right) A^{-1}$$

or, according to (8.3.26),

$$\Omega_i^{sp} = -A^{-1} \left( \frac{\pi}{12} T^2 + \frac{1}{8\pi} H^2 \right) \left\{ \exp(\pi/I) + \frac{\Gamma}{\pi} \int_{-\infty}^{+\infty} dp \right.$$
$$\left. \times \exp\left(-\frac{\pi p^2}{2U\Gamma}\right) \left[ \left(ip + \frac{U}{2}\right)^2 + \Gamma^2 \right]^{-1} \right\}, \tag{8.3.28}$$

where $A$ is given by (8.2.103).

Let us now take the charge part of the thermodynamical potential. It follows from (8.3.22) that at $\epsilon_d + U/2 \gg T$, $n > 1$ at $\kappa_n' \gtrsim (n-1)(\epsilon_d + U/2)$. Therefore, with the

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

exponential accuracy $O(\exp(-(\epsilon_d+U/2)/T))$ in eqn. (8.3.13) one should neglect all $\kappa_n'$ except $\kappa_1'$. Designating $\kappa_1'(\lambda)=\xi(\lambda)$ we have

$$\xi(\lambda)+T\int_{-\infty}^{+\infty}R(\lambda-\lambda')\ln n(\xi(\lambda'))\,d\lambda'=\epsilon_d+U/2 - \int_{-\infty}^{+\infty}dk g'(k)s(\lambda-g(k))(k-T\ln n(-\varepsilon(k))). \quad (8.3.29)$$

The function $\xi(\lambda)$ monotonically decreases and turns to zero at the point $\lambda=Q$. Let us expand $\xi(\lambda)$ in powers of $T^2$: $\xi(\lambda)=\xi_0(\lambda)+T^2\xi_1(\lambda)$. For this purpose it is convenient to rewrite the second term in the left-hand side of (8.3.31) as

$$TR*\ln n(\xi(\lambda))=-\int_{-\infty}^{Q}R(\lambda-\lambda')\xi(\lambda')\,d\lambda'+TR*\ln n(-|\xi(\lambda)|). \quad (8.3.30)$$

At $T\to 0$

$$-TR*\ln n(-|\xi(\lambda)|)=\frac{\pi^2T^2}{6}\frac{R(\lambda-Q)}{|\partial\xi(\lambda)/\partial\lambda|_{\lambda=Q}}+O(T^4).$$

Retaining only the linear terms with respect to $T$ in the right-hand side of (8.3.29) we get

$$T\int s(\lambda-g(k)\ln n(-\varepsilon(k))g'(k)\,dk \simeq \exp(\pi\lambda)\,T\int\exp(-\pi g(k))\ln n(-\varepsilon(k))g'(k)\,dk. \quad (8.3.31)$$

Taking into account (8.3.26) we get the linear equation for $\xi_1$:

$$\xi_1(\lambda)-\int_{-\infty}^{Q}R(\lambda-\lambda')\xi_1(\lambda')\,d\lambda' = \frac{\pi^2}{6}\frac{R(\lambda-Q)}{|\partial\xi_0(\lambda)/\partial\lambda|_{\lambda=Q}}+\exp(\pi\lambda)\left(\frac{\pi}{12}+\frac{1}{8\pi}\left(\frac{H}{T}\right)^2\right)A^{-1}. \quad (8.3.32)$$

The function

$$\xi_0(\lambda)=\frac{1}{2\pi}\int_{\lambda}^{Q}\tilde{\sigma}(\lambda')\,d\lambda',$$

where $\tilde{\sigma}$ satisfies eqn. (8.2.44).

Let us represent the solution of (8.3.32) as

$$\xi_1(\lambda)=f_1(\lambda)\left(\frac{\pi}{12}+\frac{1}{8\pi}\left(\frac{H}{T}\right)^2\right)A^{-1}+f_2(\lambda)\frac{\pi}{12}[\tilde{\sigma}(Q)]^{-1},$$

where $f_1(\lambda)$ and $f_2(\lambda)$ satisfy (8.3.32), in the right-hand side of which there are either $\exp(\pi\lambda)$ or $R(\lambda-Q)$. The function $f_1(\lambda)$ can be defined from formula (8.2.46)

$$f_1(\lambda)=\frac{1}{2\sqrt{(\pi e)}}\int_{-\infty}^{+\infty}\exp(-i\omega(\lambda-Q))G^{(-)}(\omega)\frac{d\omega}{i\omega+\pi}\exp(\pi Q).$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Let us now take the thermodynamic potential. At $T \to 0$ we have:

$$\Omega_i^{ch}(T,H)-\Omega_i^{ch}(0,0)=-\frac{\pi}{12}\frac{T^2}{\tilde{\sigma}(Q)}\left(\sigma_0(Q)-\int_{-\infty}^{Q} d\lambda\sigma_0(\lambda)f_2(\lambda)\right)$$
$$-\int_{-\infty}^{Q}\sigma_0(\lambda)f_1(\lambda)\,d\lambda\left(\frac{T^2\pi}{12}+\frac{H^2}{8\pi}\right)A^{-1}, \qquad (8.3.33)$$

where

$$\sigma_0(\lambda)=\int_{-\infty}^{+\infty} dk\Delta(k)s(g(k)-\lambda).$$

The last term in (8.3.33) has been calculated above—it is the non-Kondo part of the magnetic susceptibility (8.2.106).

To calculate the first term in (8.3.53) we apply the technique proposed by Takahashi (1973). Let us study the equation:

$$T(\lambda)-\int_{-\infty}^{Q} R(\lambda-\lambda')T(\lambda')\,d\lambda'=\sigma_0(\lambda)\equiv\int_{-\infty}^{+\infty} s(\lambda-g(k))\Delta(k)\,dk.$$

It is easy to check that

$$\int_{-\infty}^{Q}\sigma_0(\lambda)f_2(\lambda)\,d\lambda=\int_{-\infty}^{Q} R(\lambda-Q)T(\lambda)\,d\lambda=T(Q)-\sigma_0(Q).$$

Therefore,

$$\Omega_i^{ch}(T,H)-\Omega_i^{ch}(0,0)=-\frac{\pi}{12}\frac{T(Q)}{\tilde{\sigma}(Q)}T^2$$
$$-\left(\frac{\pi}{12}T^2+\frac{H^2}{8\pi}\right)A^{-1}\int_{-\infty}^{Q}\sigma_0(\lambda)f_1(\lambda)\,d\lambda. \qquad (8.3.34)$$

Making use of the relation

$$T(Q)=\lim_{\omega\to\infty} i\omega T(\omega) \qquad (8.3.35)$$

we have

$$T(Q)/4\pi\tilde{\sigma}(Q)=\chi_{ch},$$

where $\chi_{ch}$ (see (8.2.52) or (8.2.56)) is the charge susceptibility.

Combining (8.3.28) and (8.3.34) we get

$$\Omega_i(T,H)-\Omega_i(0,0)=-\frac{T^2\pi^2}{3}(\chi_{sp}+\chi_{ch})-\frac{H^2}{2}\chi_{sp}, \qquad (8.3.36)$$

where $\chi_{sp}$ is the spin susceptibility. This almost explicit Fermi-liquid formula

$$\lim_{T\to 0}\frac{C_i}{T}=\frac{2\pi^2}{3}(\chi_{sp}+\chi_{ch}) \qquad (8.3.37)$$

is obtained for the symmetric Anderson model by Yamada (1975) (see § 3.2.2). It holds for arbitrary $H$ and $\epsilon_d+U/2$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

8.3.8. *The specific heat of the symmetric Anderson model*

It is useful to derive (8.3.36) for the symmetric case. If $\epsilon_d + U/2 = 0$ all the functions $\kappa_n'$ are essential. At $T \ll (U\Gamma)^{1/2}$ the main contribution comes from the region $\lambda \to -\infty$:

$$\int_{-\infty}^{+\infty} s(\lambda - g(k)) \ln n(\varepsilon(k)) g'(k)\, dk \simeq \exp(\pi\lambda) \int_{-\infty}^{+\infty} \exp(-\pi g(k)) \ln n(\varepsilon(k)) g'(k)\, dk.$$

When calculating this integral at $T \to 0$ one should take into consideration only the region $k \gg (U\Gamma)^{1/2}$ where $\varepsilon(k) \simeq 2k$. Therefore,

$$-T \int_{-\infty}^{+\infty} \exp(-\pi g(k)) \ln n(\varepsilon(k)) g'(k)\, dk \simeq 2 \int_0^{\infty} \exp(-\pi g(k)) k g'(k)\, dk = \frac{(2U\Gamma)^{1/2}}{\pi}.$$

Equations (8.3.22 *c*) rewritten in terms of the dimensionless function

$$\zeta_n(\lambda) = \frac{1}{T} \kappa_n' \left( \lambda + \frac{1}{\pi} \ln \frac{(2U\Gamma)^{1/2}}{\pi T} \right)$$

coincide with the universal eqns. (8.3.25), where $H$ is replaced by $\epsilon_d + U/2$.

Therefore, the charge part of the thermodynamic potential may be written

$$\begin{aligned} \Omega_{\mathrm{i}}^{\mathrm{ch}} &= \frac{\pi T^2}{(2U\Gamma)^{1/2}} \int_{-\infty}^{\infty} \exp(-\pi g(k)) \Delta(k)\, dk \int_{-\infty}^{\infty} \exp(\pi\lambda) \ln n(\zeta(\lambda))\, d\lambda \\ &= -\int_{-\infty}^{\infty} \frac{dk}{(2U\Gamma)^{1/2}} \Delta(k) \exp(-\pi g(k)) \left( \frac{\pi^2}{6} T^2 + \frac{1}{4} \left( \epsilon_d + \frac{U}{2} \right)^2 \right) \\ &= -\chi^{\mathrm{ch}} \left( \frac{\pi^2}{3} T^2 + \frac{1}{2} (\epsilon_d + U/2)^2 \right). \end{aligned} \tag{8.3.38}$$

Combining (8.3.28) and (8.3.38) we have (8.3.36).

Note, in conclusion, that as we have already discussed in § 2.3 the condition for the application of the non-degenerate Anderson model $\Delta_{\mathrm{CF}} \gg (2J+1)\Gamma$ is not usually valid for alloys which exhibit mixed-valence behaviour; the crystal field splitting is more than the resonance width. Therefore, the degenerate Anderson model is more realistic. The solution of this model is the subject of the following section.

*Appendix to § 8.2.1. Solutions with complex rapidities for the Bethe-Ansatz equation for the Anderson model*

(a) Let us consider the accuracy of the string (8.2.7) forming the ground state of the Anderson model:

$$k_\alpha^{(\pm)} = x(\lambda_\alpha) \mp i y(\lambda_\alpha) + \gamma^{(\pm)}(\lambda_\alpha). \tag{1}$$

At $T = 0$ from eqn. (8.2.9) we have

$$|\gamma^{(\pm)}(\lambda)| = \exp(-L y(\lambda)) \prod_{\beta=1}^{M} \left| \frac{\lambda - \lambda_\beta + i}{\lambda - \lambda_\beta} \right|. \tag{2}$$

Passing to the continuous limit, we have

$$|\gamma^{(\pm)}(\lambda)| = \exp\left\{ L \left[ \int \sigma(\lambda') \ln \left( \frac{(\lambda - \lambda')^2 + 1}{(\lambda - \lambda')^2} \right) d\lambda' - y(\lambda) \right] \right\}. \tag{3}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Using the explicit form of $\sigma(\lambda)$ in the ground state

$$\sigma(\lambda)=\frac{1}{2\pi}\int s(\lambda-g(k)\,dk \tag{4}$$

eqn. (1) yields

$$|\gamma^{(\pm)}(\lambda)|=\exp\{-L(U\Gamma)^{1/2}\tau(\lambda)\}, \tag{5}$$

where

$$\tau(\lambda)=\int_{-\infty}^{+\infty}\frac{d\omega}{\omega-i0}\,\frac{\exp(-|\omega|-i\omega\lambda)}{2\cosh\omega/2}\,\frac{1}{(-i\omega+0)^{1/2}}. \tag{6}$$

Then the string solution (1) is valid with accuracy $O(\exp(-L(U\Gamma)^{1/2}))$.

(b) Now let us consider the strings (8.2.3). Repeating the calculation of Appendix A to § 6.2.1 we obtain

$$|\gamma_n|=O\left(\exp\left\{+LT\int\frac{d\lambda'}{2\sinh\pi(\lambda-\lambda')}\ln n(\kappa_{n-2}(\lambda'))n(\kappa_n(\lambda'))\right\}\right).$$

This estimate proves the string hypothesis (8.2.3) in the thermodynamic limit $\lim_{L\to\infty}\gamma_n=0$.

*Appendix to § 8.2.6. Evaluation of the magnetic susceptibility and the occupation number in the mixed-valence region* ($|\epsilon_d^*|\ll\Gamma$)

To evaluate the integrals (8.2.57) and (8.2.106) for $|\epsilon_d^*|\ll\Gamma$ let us transform the integrands using the relation $1+\exp(-|\omega|)=G^{(+)}(\omega)G^{(-)}(\omega)$. At $I^*<0$

$$n_d=1+\frac{i}{\sqrt{2}\,\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i0}\left(\frac{1}{G^{(-)}(\omega)}-\frac{1}{G^{(-)}(0)}\right)\exp\left(\frac{-i\omega}{I^*}\right). \tag{1}$$

At $I^*>0$

$$n_d=2-\frac{i}{\pi\sqrt{2}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i0}\,G^{(+)}(\omega)\exp\left(\frac{-i\omega}{I^*}\right). \tag{2}$$

Similarly at $I^*>0$

$$\chi_{\rm sp}=\frac{\sqrt{(2\pi e)}}{8\Gamma}\left(\frac{2\epsilon_d+U}{U}\right)\left[\exp\left(\frac{\pi}{I^*}\right)-\frac{i}{2\sqrt{(\pi e)}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i\pi}\right.$$
$$\left.\times\left(\frac{1}{G^{(-)}(\omega)}-\frac{1}{G^{(-)}(-i\pi)}\right)\exp\left(\frac{i\omega}{I^*}\right)\right], \tag{3}$$

and at $I^*<0$

$$\chi_{\rm sp}=\frac{\sqrt{(2\pi e)}}{8\Gamma}\left(\frac{2\epsilon_d+U}{U}\right)\left[\frac{i}{2\sqrt{(\pi e)}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i\pi}G^{(+)}(\omega)\exp\left(\frac{i\omega}{I^*}\right)\right]. \tag{4}$$

Let

$$f^{(\pm)}(x)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp(-i\omega x)\tilde{f}^{(\pm)}(\omega)\,d\omega,$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

where $\tilde{f}^{(\pm)}(\omega)$ is an analytical function in the upper (lower) half-plane. Then the following relations exist:

$$\left.\begin{aligned} &\lim_{x\to\pm 0} f^{(\pm)}(x) = \mp \lim_{\omega\to\infty} i\omega \tilde{f}^{(\pm)}(\omega), \\ &\lim_{x\to\pm 0} \frac{d}{dx} f^{(\pm)}(x) = \mp \lim_{\omega\to\infty} \omega^2 \left( \tilde{f}^{(\pm)}(\omega) - \frac{i}{\omega} \lim_{x\to\pm 0} f^{(\pm)}(x) \right) \end{aligned}\right\} \tag{5}$$

and so on. Applying these relations to (1)–(4) it is easy to obtain eqns. (8.2.64) and (8.2.109). Note that using this trick one may expand the magnetization of the $S=1$ spin impurity in the s–d exchange model in powers of $\ln H/T_H$.

*Appendix A to §8.2.7. Proof of the relations (8.2.71) and (8.2.72)*

(a) Let us calculate the Fourier transform of the function

$$\frac{1}{2\pi}\left[\theta(z)\left(\frac{U\Gamma}{2z}\right)^{1/2} - \int_{-\infty}^{+\infty} R(z-g(k))\,dk\right]:$$

$$\frac{1}{2\pi}\left(\int_0^{\infty} \exp(i\omega z)\left(\frac{U\Gamma}{2z}\right)^{1/2} dz - \frac{1}{1+\exp(|\omega|)}\int_{-\infty}^{+\infty} \exp(i\omega g(k))\,dk\right) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}$$
$$\times \exp(i\omega g(k))\,dk\left(\frac{1}{2} - \frac{1}{1+\exp(|\omega|)}\right) = \frac{i}{4\sqrt{\pi}}\left(\frac{2U\Gamma}{i\omega - 0}\right)^{1/2} \tanh\frac{\omega}{2}. \tag{A 1}$$

(b) The Fourier transform of the impurity part of the right-hand side of eqn. (8.2.70) is

$$\int_{-\infty}^{\epsilon_d + U/2} \exp(i\omega g(k))\Delta(k)\,dk - \frac{1}{1+\exp(|\omega|)}\int_{-\infty}^{+\infty} \exp(i\omega g(k))\Delta(k)\,dk. \tag{A 2}$$

One can rewrite the integrals as follows:

$$\int_{-\infty}^{\epsilon_d + U/2} \exp(i\omega g(k))\Delta(k)\,dk = \exp\left(-\frac{|\omega|}{2} + \frac{i\omega}{I}\right) - \frac{i\Gamma}{2\pi}\operatorname{sign}\omega \int_{-\infty}^{-\infty}$$
$$\times \exp(-i\omega k^2/2U\Gamma)[(ik+U/2)^2+\Gamma^2]^{-1}\,dk + f^{(-)}(\omega), \tag{A 3}$$

where $f^{(-)}(\omega)$ is the analytical function in the lower half-plane.

$$\int_{-\infty}^{+\infty} \exp(i\omega g(k))\Delta(k)\,dk = \exp\left(-\frac{|\omega|}{2} + \frac{i\omega}{I}\right) - i\operatorname{sign}\omega\frac{\Gamma}{\pi}\int_{-\infty}^{+\infty}$$
$$\times \exp\left(-\frac{i\omega k^2}{2U\Gamma}\right)\left[\left(ik+\frac{U}{2}\right)^2+\Gamma^2\right]^{-1} dk. \tag{A 4}$$

Summing up expressions (A 3) and (A 4) one obtains

$$\text{eqn. (A 2)} = \left(2\cosh\frac{\omega}{2}\right)^{-1} \exp\left(\frac{i\omega}{I}\right) - \frac{i\Gamma}{2\pi}\tanh\frac{\omega}{2}\int_{-\infty}^{+\infty}$$
$$\times \exp\left(-\frac{i\omega k^2}{2U\Gamma}\right)\left[\left(ik+\frac{U}{2}\right)^2+\Gamma^2\right]^{-1} dk + f^{(-)}(\omega), \tag{A 5}$$

and after inverse transformation we have (8.2.72).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

*Appendix B to §8.2.7. Expansion in inverse powers of the magnetic field at $H \gg (U\Gamma)^{1/2}$*

Let us study the host part of eqn. (8.2.89):

$$\tilde{p}_{\mathrm{h}}(z) - \int_0^\infty R(z-z')\tilde{p}_{\mathrm{h}}(z')\,dz' = \frac{1}{2\pi}\left(\frac{U\Gamma}{2(z+b)}\right)^{1/2}\theta(z+b). \tag{B 1}$$

We find the solution in the following form

$$\tilde{p}_{\mathrm{h}}(z) = \frac{1}{2\pi}\left(\frac{U\Gamma}{2}\right)^{1/2}(z^{-1/2}+\mathscr{P}(z)).$$

For $\mathscr{P}$ we get

$$\mathscr{P}(z) - \int_0^\infty R(z-z')\mathscr{P}(z')\,dz' = \frac{\theta(z+b)}{(z+b)^{1/2}} - \frac{\theta(z)}{z^{1/2}} - \mathscr{Q}(z), \tag{B 2}$$

where

$$\mathscr{Q}(z) = \theta(z)z^{-1/2} - 2\int_0^\infty R(z-z')z'^{-1/2}dz'.$$

Let $\mathscr{P}_0(z)$—a $b$-independent function—satisfy eqn. (B 2), the right-hand side of which contains only $\mathscr{Q}(z)$. For the function $X(z) = \mathscr{P}(z) - \mathscr{P}_0(z)$ we have

$$X(z) - \int_0^\infty R(z-z')X(z')\,dz' = \frac{\theta(z+b)}{(z+b)^{1/2}} - \frac{\theta(z)}{z^{1/2}}. \tag{B 3}$$

Solving this equation we get

$$\int_0^\infty X(z)\,dz = \frac{i}{\sqrt{(2\pi)}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega - i0}G^{(-)}(\omega)\frac{\exp(-i\omega b)-1}{(-i\omega+0)^{1/2}}. \tag{B 4}$$

Let us close the integration path into the lower half-plane where $(-i\omega+0)^{1/2}$ has a cut. Then we obtain eqn. (8.2.91).

The solution of eqn. (8.2.89) gives the following expression for the impurity moment:

$$\frac{1}{2} - M_{\mathrm{i}} = -\frac{i}{2^{3/2}\pi}\int_{-\infty}^{+\infty}\frac{G^{(-)}(\omega)}{\omega - i0}\beta(\omega)\exp(-i\omega b)\,dw. \tag{B 5}$$

The function

$$\beta(\omega) = \int_0^\infty \exp(i\omega g(k))\Delta(k)\,dk$$

has a cut in the lower half-plane. The discontinuity on this cut is

$$\mathrm{Disc}\,\beta(\omega)|_{\omega=-it} = \left(\frac{2U\Gamma}{t}\right)^{1/2}\int_{-\infty}^{+\infty}\exp(-k^2)\Delta\left(ik\left(\frac{2U\Gamma}{t}\right)^{1/2}\right)dk$$

and can be expanded in powers of $t$:

$$\mathrm{Disc}\,\beta(-it) = \sum_{n=0}^{\infty}\beta_n t^{n+1/2}\Gamma(-1/2-n).$$

Closing the integration path in (B 4) and (B 5) into the lower half-plane we get (8.2.91) and (8.2.92).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

*Appendix A to §8.3.3. High-temperature limit ($T \gg \Gamma$)*

When $\Gamma$ tends to zero one should consider the kernels in eqns. (8.3.13) and (8.3.14) as delta-functions. Thus one obtains:

$$\Omega_i = \frac{T}{2} \ln [n(-\varepsilon(\epsilon_d)) n(\kappa_1'(U/8\Gamma))] \tag{A 1}$$

and

$$\eta_n'^2 = (1+\eta_{n+1}')(1+\eta_{n-1}'), \qquad n = 1, 2, \ldots, \tag{A 2}$$

with the boundary conditions

$$1+\eta_0' = \exp\left(-\frac{U}{T}\right)(1+\zeta), \tag{A 3}$$

$$\lim_{n\to\infty} \frac{1}{n} \ln \eta_n' = \frac{\epsilon_d + U/2}{T}, \tag{A 4}$$

and

$$\eta_n^2 = (1+\eta_{n+1})(1+\eta_{n+1}), \qquad n = 0, 1, \ldots, \tag{A 5}$$

with the boundary conditions

$$\eta_0 = \zeta; \qquad 1+\eta_{-1} = (1+\eta_1')^{-1}, \tag{A 6}$$

$$\lim_{n\to\infty} \frac{1}{n} \lim \eta_n = \frac{H}{T}. \tag{A 7}$$

Here $\zeta = \exp(-\varepsilon(\epsilon_d)/T)$, $\eta_n' = \exp(\kappa_n'(U/8\Gamma)/T)$, and $\eta_n = \exp(\kappa_n(U/8\Gamma)/T)$.

The general solutions of eqns. (A 2) and (A 5) are

$$\left.\begin{aligned} &1+\eta_n = p_n^2, \qquad 1+\eta_n' = q_n^2 \\ &p_n = \frac{\sinh(\alpha_n+\beta)}{\sinh\alpha}, \qquad q_n = \frac{\sinh(\gamma_n+\delta)}{\sinh\gamma} \end{aligned}\right\} \tag{A 8}$$

From (A 4) and (A 6) one obtains

$$\alpha = \frac{H}{T}, \qquad \gamma = \frac{\epsilon_d + U/2}{T}. \tag{A 9}$$

Conditions (A 3) and (A 7) give us the equations for the unknown parameters $\beta$ and $\delta$:

$$\left.\begin{aligned} &\frac{\sinh\delta}{\sinh\left(\dfrac{\epsilon_d+U/2}{T}\right)} = \exp\left(-\frac{U}{2T}\right)\frac{\sinh\beta}{\sinh H/T}; \\ &\frac{\sinh\dfrac{\epsilon_d+U/2}{T}}{\sinh\left(\dfrac{\epsilon_d+U/2}{T}+\delta\right)} = \frac{\sinh(\beta-H/T)}{\sinh H/T}. \end{aligned}\right\} \tag{A 10}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The solution of this system is

$$\left.\begin{aligned}
&\exp(2\beta)=\exp\left(\frac{H}{T}\right)\frac{z_+}{z_-};\\
&\sinh\delta=\exp(-U/2T)\sinh\left(\frac{\epsilon_d+U/2}{T}\right)\\
&\qquad\times\left(\frac{2\cosh H/2T+\exp(\epsilon_d/T)+\exp(-(\epsilon_d+U)/T)}{z_+z_-}\right);\\
&z_\pm=\exp(\pm H/2T)+\exp(\epsilon_d/T)+\exp(-(\epsilon_d+U)/T).
\end{aligned}\right\}\tag{A 11}$$

Using formulae (A 1), (A 8) and (A 11) we obtain formula (8.3.19).

*Appendix B to §8.3.3. Low-temperature limit* ($T\ll\Gamma, H, \epsilon_d+U/2$)

It follows from eqns. (8.3.15) that the functions $\kappa_n(\lambda)$ and $\kappa'_m(\lambda)$ ($m\neq 1$) are positive and finite at $T/H$, $T/(\epsilon_d+U/2)\to 0$. Therefore, at $T\to 0$ all the terms in eqn. (8.3.13) which contain $\exp(-\kappa_n/T)$ or $\exp(-\kappa'_m/T)$ ($m\neq 1$) vanish and eqns. (8.3.13) become linear:

$$\varepsilon(k)=k-\int_Q^\infty a_1(g(k)-\lambda)\kappa'_1(\lambda)\,d\lambda;\tag{B 1}$$

$$\kappa'_1(\lambda)+\int_Q^\infty a_2(\lambda-\lambda')\kappa'_1(\lambda')\,d\lambda'=2x(\lambda)+\int_{-\infty}^B a_1(\lambda-g(k))\varepsilon(k)\,dk.\tag{B 2}$$

Remember that $\kappa'_1(\lambda)$ is a monotonously decreasing function, $\kappa'_1(Q)=0$, and $\varepsilon(k)$ is a monotonously increasing function, $\varepsilon(B)=0$. Differentiating (B 1) and (B 2) with respect to $k$ and $\lambda$ and using (8.3.18) we obtain eqns. (8.2.15) and (8.2.16).

*Appendix to §8.3.7. Thermodynamics of the asymmetric Anderson model*

The thermodynamics equations (8.3.13) become simpler in the asymmetric limit $U\gg|\epsilon_d|$, $\Gamma, T, H$. In this regime $\kappa'_n\geqslant(n-1)(\epsilon_d+U/2)$, consequently one should replace all terms $T\ln n(-\kappa'_n)$ by 0 except for $n=1$. The equation in $\kappa'_1\equiv\xi$ has the form (see also eqn. (8.3.29))

$$\begin{aligned}\xi(\lambda)-\int_{-\infty}^Q R(\lambda-\lambda')\xi(\lambda')\,d\lambda'&=\epsilon_d+U/2-2\int s(\lambda-g(k))g(k)\,dk\\&\quad-T\int s(\lambda-g(k))\ln n(-\varepsilon(k))g'(k)\,dk-TR*\ln n(-|\xi(\lambda)|).\end{aligned}\tag{1}$$

The integration limit $Q$ is very large: $Q\sim U/8\Gamma\gg 1$. The main contribution to $Q$ gives the first term in the right-hand side of eqn. (1). Let

$$\xi(\lambda)=\xi_0(\lambda)+\xi_1(\lambda-Q),\tag{2}$$

where $\xi_0(\lambda)$ satisfies the equation:

$$\xi_0(\lambda)-\int_{-\infty}^Q R(\lambda-\lambda')\xi_0(\lambda')\,d\lambda'=\epsilon_d+U/2-2\int_{-\infty}^{+\infty}s(\lambda-g(k))g(k)\,dk.\tag{3}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

A similar equation has been solved (see eqn. (8.2.44)). Using the functions $\tilde{\sigma}(\lambda)$ and $\sigma(\lambda)$ one can find the solution of eqn. (3):

$$\left.\begin{aligned} \xi_0(\lambda) &= 2\pi \int_{\lambda}^{Q} \tilde{\sigma}(\lambda')\, d\lambda' \qquad (\lambda < Q), \\ \xi_0(\lambda) &= -2\pi \int_{Q}^{\lambda} \sigma(\lambda')\, d\lambda' \quad (\lambda > Q). \end{aligned}\right\} \tag{4}$$

Taking into account eqn. (8.2.57) and (2) we have the following equation in $Q$:

$$Q - \frac{U}{8\Gamma} = \frac{\epsilon_d}{2\Gamma} + \frac{1}{2\pi} \ln \frac{\pi e U}{4\Gamma} + \xi_1(0), \tag{5}$$

where $\xi_1(\lambda)$ is the solution of the equation:

$$\begin{aligned} \xi_1(\lambda) - \int_{-\infty}^{Q} R(\lambda - \lambda')\xi_1(\lambda')\, d\lambda' = &- TR * \ln n(-|\xi_1(\lambda) \\ &+ \xi_0(\lambda + Q)|) - T \int_{-\infty}^{+\infty} s(\lambda + Q - g(k)) \ln n(-\varepsilon(k)) g'(k)\, dk. \end{aligned} \tag{6}$$

Now we are ready to perform the limit $U \to \infty$. First, the main contribution to the second integral in the right-hand side of eqn. (6) is due to the region $g(k) \sim Q$ or $|k - \epsilon_d| \ll U$. In this region one can replace

$$g(k) - Q \to -\frac{k}{2\Gamma} - \frac{1}{2\pi} \ln \frac{\pi e U}{4\Gamma} - \xi_1(0). \tag{7}$$

Second, only the region $\lambda \sim 1$ is essential for the first integral in the right-hand side of eqn. (6). Therefore, one can restrict oneself to asymptotic behaviour

$$\xi_0(\lambda + Q) \sim \lambda^*(\lambda) \qquad (Q \to \infty), \tag{8}$$

where

$$\lambda^* + \frac{1}{2\pi} \ln \frac{\lambda}{2\pi e} = \lambda. \tag{9}$$

In approximations (7) and (8), after inserting the new variables, we obtain the universal thermodynamic equations, which contain only the renormalized quantity $\epsilon_d^*$ as a parameter:

$$\begin{aligned} \xi_1(\lambda) - \int_{-\infty}^{0} R(\lambda - \lambda')\xi_1(\lambda')\, d\lambda' = &- TR * \ln n(-|\xi_1(\lambda) + \lambda^*(\lambda)|) \\ &- T \int_{-\infty}^{+\infty} s(\lambda - k) \ln n(-\varepsilon(k))\, dk; \end{aligned} \tag{10}$$

$$\begin{aligned} \varepsilon(k) = -2\Gamma\varphi_0(k) - \int_{-\infty}^{0} s(k - \lambda)\xi_1(\lambda)\, d\lambda + Ts * \ln n(&-|\xi_1(k) \\ &+ \lambda^*(k)|) + Ts * \ln n(\kappa_1(k)); \end{aligned} \tag{11}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\left.\begin{aligned}\kappa_n(\lambda) &= -Ts * \ln[n(\kappa_{n-1}(\lambda))n(\kappa_{n+1}(\lambda))] - \delta_{n1} T \int_{-\infty}^{+\infty} s(\lambda-k)\ln n(-\varepsilon(k))\,dk \\ \varphi_0(k) &= \int_{-\infty}^{+\infty} \frac{d\omega}{(\omega-i0)^2}\frac{G^{(-)}(\omega)}{\cosh\omega/2}\exp(-i\omega k).\end{aligned}\right\} \quad (12)$$

The universal form of the thermodynamical potential in the asymmetric case is:

$$\Omega_i(T,H) = T\int_{-\infty}^{+\infty} s\left(k+\frac{\epsilon_d^*(T)}{2\Gamma}\right)\ln n(-\varepsilon(k))\,dk - \int_{-\infty}^{0} R\left(\lambda+\frac{\epsilon_d^*(T)}{2T}\right)\xi_1(\lambda)\,d\lambda$$
$$+T\int_{-\infty}^{+\infty} R\left(\lambda+\frac{\epsilon_d^*(T)}{2T}\right)\ln n(-|\xi_1(\lambda)+\lambda^*(\lambda)|\,d\lambda + \Omega_i(0,0), \quad (13)$$

where we introduced

$$\epsilon_d^*(T) = \epsilon_d^* + \xi_1(0) \quad (14)$$

and $\Omega_i(0,0)$ is the ground-state energy.

The universal equations (10)–(14) describe the thermodynamics of the asymmetric Anderson model completely.

## § 9. Introduction to the exact solution of the degenerate Anderson model

The degenerate Anderson model, as has been explained in § 2.1.3, describes the rare-earth alloys in the mixed-valence region. In this region the crystal field splitting should be compared with a large quantity $(2J+1)\Gamma$ and prescribes the impurity atomic shell as degenerate.

We give below the solution of the Bethe-Ansatz equation (4.6.A)–(4.6.C) at zero temperatures for the model

$$\mathscr{H} = \sum_{k,\gamma}\epsilon_k c_{k\gamma}^+ c_{k\gamma} + V\sum_{k,\gamma}(c_{k\gamma}^+ X_{0\gamma} + X_{\gamma 0}c_{k\gamma}) + \sum_{\gamma}\epsilon_f X_{\gamma\gamma}. \quad (9.1.1)$$

In particular cases the hamiltonians reduces to the non-degenerate asymmetric Anderson model ($n=2$), or to the degenerate Kondo model ($-\epsilon_f \gg \Gamma$), the solutions of which are presented in §§ 7 and 8. We assume that the reader is acquainted with these sections, which we shall often refer to. The present section is based on the results obtained by Schlottmann (1982, 1983) and Ogievetskii and the present authors (1983).

### 9.1. *Basic equations*

The Bethe-Ansatz equations obtained in § 4.6 have the form (Schlottmann 1982)

$$\exp(ik_\alpha L) = \prod_{\beta=1}^{m_1}\left(\frac{k_\alpha/2\Gamma+\lambda_\beta-i/2}{k_\alpha/2\Gamma+\lambda_\beta+i/2}\right)\exp(-i\Phi(k_\alpha)), \quad (9.1.2)$$

$$\prod_{\tau=\pm 1}\prod_{\beta=1}^{m_{j+\tau}}\left(\frac{\lambda_\alpha^{(j)}-\lambda_\beta^{(j+\tau)}+i/2}{\lambda_\alpha^{(j)}-\lambda_\beta^{(j+\tau)}-i/2}\right)$$
$$= -\prod_{\beta=1}^{m_j}\left(\frac{\lambda_\alpha^{(j)}-\lambda_\beta^{(j)}+i}{\lambda_\alpha^{(j)}-\lambda_\beta^{(j)}-i}\right); \qquad j=1,\ldots,n-1. \quad (9.1.3)$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The energy of the state $\{k_\alpha, \lambda_\beta^{(1)}, \ldots, \lambda_\gamma^{(n-1)}\}$ is

$$E = \sum_{\alpha=1}^{N} k_\alpha. \tag{9.1.4}$$

$$\Phi(k) = 2\tan^{-1}\left(\frac{k-\epsilon_f}{\Gamma}\right), \tag{9.1.5}$$

$n=2J+1$, the quantities $m_j = \sum_{k=j}^{n-1} N_k$, where $N_k$ is the number of particles with momentum projection $J-k$, $m_0 = N$ is the total number of particles $m_n = 0$, and $\lambda_\alpha^{(0)} = -k_\alpha/2\Gamma$. The Bethe-Ansatz equations (9.1.2) and (9.1.3) for the host metal are just the same as the Bethe-Ansatz equations for the one-dimensional $n$-colour Fermi gas with the $\delta$-function attractive interaction. The Bethe-Ansatz equations for the ground state of this problem were obtained by Takahashi (1970 a). He showed that in contrast to the repulsive case the rapidities of the ground state are grouped in complexes of a special type. This result also holds for the Anderson model (Schlottmann 1982).

Let us describe the space of the solutions of eqns. (9.1.3) and (9.1.4). As in the $SU(n)$ Kondo model (§ 7) the spin rapidities $\lambda^{(j)}$ $(j=1,\ldots,n-1)$ are grouped into spin complexes or 'strings'.

$$\lambda_{p,k;\alpha}^{(j)} = \lambda_{p,k;\alpha}^{(j)} + i\left(\frac{p+1}{2} - k\right); \qquad k=1,\ldots,p, \tag{9.1.6}$$

but, in addition, the rapidities with neighbouring colours $j$ and $j+1$ can form the bound state

$$\lambda^{(j)} = \lambda^{(j+1)} \pm i/2; \qquad j=0,\ldots,n-1, \tag{9.1.7}$$

where $\lambda^{(0)} = -k/2\Gamma$.

The fact is that paired rapidities prove to be energetically favourable compared to unpaired rapidities, and the degrees of pairing is maximum in the ground state.

Let us define the numbers $r_k$ $(k=1,\ldots,n)$

$$m_{k-1} = r_k + 2r_{k+1} + \ldots + r_n(n+1-k), \tag{9.1.8}$$

which is illustrated by fig. 9.1. It is expected that in the ground state the $pr_{j+p-1}$ rapidities $\lambda_{(p-1)r_{j+p-2}+1}^{(j)}, \ldots, \lambda_{(p-1)r_{j+p-2}+pr_{j+p-1}}^{(j)}$ form the $p$ complexes with the centres $\lambda_1^{(j+p-1}, \ldots, \lambda_{r_{j+p-1}}^{(j+p-1)}$

$$\lambda_{(p-1)r_{j+p-2}+pk-q}^{(j)} = \lambda_k^{(j+1)} + i\left(\frac{p+1}{2} - q\right); \qquad q=1,\ldots,p; \qquad k=r_{j+p-1}. \tag{9.1.9}$$

Let us illustrate, according to Takahashi (1970 a) the structure of the ground state in the case $n=3$. In this case

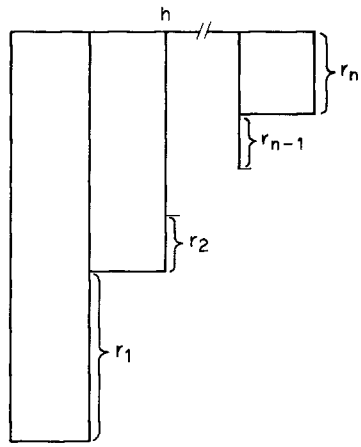
$$N = r_1 + 2r_2 + 3r_3; \qquad m_1 = r_2 + 2r_3; \qquad m_2 = r_3.$$

All $\lambda_1^{(2)}, \ldots, \lambda_{r_3}^{(2)}$ are real. Among the $\lambda^{(1)}$'s only $\lambda_1^{(1)}, \ldots, \lambda_{r_2}^{(1)}$ are real, the remaining $\lambda^{(2)}$'s form the complexes of the order 2:

$$\lambda_{r_2+1}^{(1)}, \ldots, \lambda_{r_2+2r_3}^{(1)} = \lambda_1^{(2)} \pm i/2, \ldots, \lambda_{r_3}^{(2)} \pm i/2.$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 9.1




Young tableau which corresponds to the irreducible representation $[n^{r_n}, \ldots, 2^{r_2}, 1^{r_1}]$.

The rapidities $\lambda^{(0)}$ are divided into three groups: $\lambda_1^{(0)}, \ldots, \lambda_{r_1}^{(0)}$ are real

$$\lambda_{r_1+1}^{(0)}, \ldots, \lambda_{r_1+2r_2}^{(0)} = \lambda_1^{(1)} \pm i/2, \ldots, \lambda_{r_2}^{(1)} \pm i/2,$$

$$\lambda_{r_1+2r_2-1}^{(0)}, \ldots, \lambda_{r_1+2r_2+3r_3}^{(0)} = \lambda_1^{(2)} + \begin{cases} i, \\ 0, \\ -i, \end{cases} \ldots, \lambda_{r_3}^{(0)} + \begin{cases} i, \\ 0, \\ -i, \end{cases}$$

The scheme is given in fig. 9.2.

Following Takahashi (1970 a) one can easily derive the Bethe-Ansatz equations for the independent real rapidities $\lambda_1^{(j)}, \ldots, \lambda_{r_j}^{(j)}$ $(j=0, \ldots, n-1)$. Here we omit the calculations which are conventional but cumbersome. As a result we have

$$\left.\begin{aligned} &\exp\left(i\frac{\Gamma}{\pi}L\lambda_\alpha^{(0)}\right) = \prod_{j=0}^{n-1}\prod_{\beta=1}^{m_j} e_j(\lambda_\alpha^{(0)} - \lambda_\beta^{(j)}) \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ &\exp\left(i\frac{\Gamma}{\pi}L\lambda_\alpha^{(j)}(j+1)\right) = \prod_{k=0}^{j}\prod_{i=k}^{n-1}\prod_{\beta=1}^{m_i} e_{i+j-2k}(\lambda_\alpha^{(j)} - \lambda_\beta^{(i)}), \quad j=0,1,\ldots,n-1. \end{aligned}\right\} \quad (9.1.10)$$

As usual, we define the distributions of particles and holes describing the system in the continuous limit $\rho_j(\lambda)$ and $\tilde{\rho}_j(\lambda)$, respectively. The integral equations are

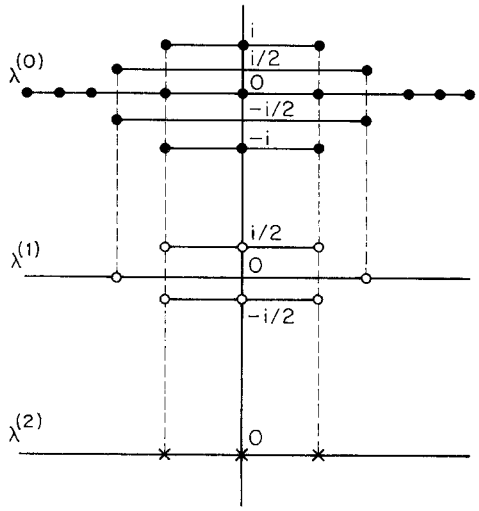
$$\frac{\Gamma}{\pi}(j+1) + \frac{1}{L}a_{j+1}\left(\lambda + \frac{\epsilon_f}{2\Gamma}\right) = \tilde{\rho}_j(\lambda) + \sum_{k=0}^{j}\sum_{i=k}^{n-1} a_{i+j-2k} * \rho_i(\lambda), \quad j=0,1,\ldots,n-1. \quad (9.1.11)$$

where

$$a_n(\lambda) = \frac{2}{\pi}\frac{n}{4\lambda^2+n^2}, \quad (9.1.12)$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Fig. 9.2




Distribution of rapidities on the complex plane. In this case $r_1=6$, $r_2=2$ and $r_3=3$.

or, in a more compact form

$$\frac{\Gamma}{\pi}(j+1)+\frac{1}{L}a_{j+1}\left(\lambda+\frac{\epsilon_f}{2\Gamma}\right)=\tilde{\rho}_j(\lambda)+\mathscr{F}_{jk}*\rho_k(\lambda) \tag{9.1.13}$$

with the matrix

$$\mathscr{F}_{jk}(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega\exp(-i\omega\lambda)\mathscr{F}_{jk}(\omega); \qquad j,k=0,\ldots n-1, \tag{9.1.14}$$

where

$$\mathscr{F}_{jk}(\omega)=\frac{\sinh(\min(j,k)+1)\omega/2}{\sinh\omega/2}\exp\left(-\frac{|\omega|}{2}\max(j,k)\right). \tag{9.1.15}$$

The energy of the state is

$$E=-2\Gamma\sum_{p=0}^{n-1}(p+1)\int\lambda\rho_p(\lambda)\,d\lambda. \tag{9.1.16}$$

In all the problems we have considered in this article the energy of the host metal is a monotonic function of the rapidities. As a consequence, in the ground state all particles occupy half-opened intervals, i.e.

$$\left.\begin{aligned}&\rho_j(\lambda)=0 \quad \text{at } B_j<\lambda<\infty; \qquad \tilde{\rho}_j(\lambda)=0 \quad \text{at } -\infty<\lambda<B_j;\\ &\sigma(\lambda)=0 \quad \text{at } -\infty<\lambda<Q; \qquad \tilde{\sigma}(\lambda)=0 \quad \text{at } Q<\lambda<\infty.\end{aligned}\right\} \tag{9.1.17}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Here we set $\rho_{n-1}=\sigma$, $\tilde{\rho}_{n-1}=\tilde{\sigma}$ to distinguish between the spin and charge variables. The parameters $Q$ and $B_j$ are determined by the conditions:

$$r_n=\int\sigma(\lambda)\,d\lambda;\qquad r_j=\int\rho_{j+1}(\lambda)\,d\lambda. \tag{9.1.18}$$

In the true ground state all $r_1,\ldots,r_{n-1}$ are zero, $B_j=\infty$. The integral equation for this case is

$$\frac{n\Gamma}{\pi}+\frac{1}{L}a_n\left(\lambda+\frac{\epsilon_f}{2\Gamma}\right)=\tilde{\sigma}(\lambda)+\mathscr{F}*\sigma(\lambda), \tag{9.1.19}$$

$$N=n\int\sigma(\lambda)\,d\lambda; \tag{9.1.20}$$

here we set $\mathscr{F}_{n-1,n-1}\equiv\mathscr{F}$.

The latter equations were obtained by Schlottmann (1982). As previously it is convenient to describe the system in terms of excitations under the true ground state. We shall use the functions $\{\rho_0,\ldots,\rho_{n-2},\tilde{\sigma}\}$. Excluding $\sigma(\lambda)$ from eqn. (9.1.14) and redefining $\rho_j\to\rho_{j+1}$ we have

$$\tilde{\rho}_j(\lambda)+D_{jk}*\rho_k(\lambda)=s_j*\tilde{\sigma}(\lambda)+\frac{1}{L}s_{n-j}(\lambda+\epsilon_f/2\Gamma), \tag{9.1.21}$$

$$\begin{aligned}D_{jk}(\omega)&=\frac{\sinh\left[(\omega/2)(n-\max(j,k))\right]\sin\left[\omega/2\min(j,k)\right]}{\sinh\omega/2\sinh n\omega/2}\exp(|\omega|/2)\\&=\frac{1}{1+a_2(\omega)}A_{jk}(\omega)\qquad\text{(see (7.1.7))}.\end{aligned} \tag{9.1.22}$$

Here

$$s_j(\omega)=\frac{\sinh\omega j/2}{\sinh\omega n/2}; \tag{9.1.23}$$

$$\sigma(\lambda)=-\mathscr{F}^{-1}*\tilde{\sigma}(\lambda)+\frac{\Gamma}{\pi}+\frac{1}{L}\mathscr{F}^{-1}*a_n\left(\lambda+\frac{\epsilon_f}{2\Gamma}\right)-s_k*\rho_k \tag{9.1.24}$$

and we have used

$$\int_{-\infty}^{+\infty}\mathscr{F}_{jn-1}(\lambda)\,d\lambda=j.$$

Note that we have met the matrix $D_{jk}$ above—it is the kernel of the integral equations (7.1.7) and (7.3.2) for the degenerate Kondo model.

The right-hand side of eqns. (9.1.22) according to expressions (9.1.22) and (9.1.23) are exponentially small at $\lambda\to+\infty$. It also means that

$$\rho_j(\lambda)=\text{const}\exp(-2\pi\lambda/n)\qquad(\lambda\to+\infty)$$

and all integrals involving $\rho_j$ in eqns. (9.1.15) and (9.1.16) converge. Quite a different situation is obtained with the function $\sigma(\lambda)$. According to (9.1.21) $\sigma(\lambda)\to\Gamma/\pi$ at $\lambda\to\infty$, therefore, the integrals are not well defined. The divergence of the integrals is a

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

consequence of the initial linear spectrum approximation which leads to an unbounded spectrum. Therefore, one should treat all $k$'s as restricted in the interval

$$-\frac{D^{(-)}}{2\Gamma}<\lambda^{(n-1)}<D^{(+)}/2\Gamma, \tag{9.1.25}$$

where $D^{(\pm)}$ are edges of the energy band. By virtue of this the density of states of the host metal, which, far from the band edges, is given by $\Gamma/\pi$ in eqn. (9.1.24), should be treated as zero beyond the interval (9.1.25). The lower edge $D^{(-)}$ is related to the total number of particles with the given colour filling the reservoir:

$$D^{(-)}=\frac{2\pi N}{nL}. \tag{9.1.26}$$

In §8 when we have dealt with the non-degenerate problem it has also been necessary to cut off at high negative energy. In fact, let us compare eqns. (8.2.34) and (9.1.24). The term

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} s(\lambda-g(k))\,dk$$

in eqn. (8.2.34) plays the role of the term $\Gamma/\pi$ in eqn. (9.1.24). The first term becomes equal to the second after the substitution $g(k)\to -k/2\Gamma$. Both lead to $\sigma(\lambda)\to$const. at $\lambda\to\infty$. However, there is a difference between these terms. The point is that the high-energy processes at the positive energy ($\lambda\to\infty$) are cut off at $\lambda=U$ in the first term, i.e. when the channel $|n_d=2\rangle$ starts participating in the real processes. Now we deal with a quite different positive high-energy cut-off. As we have assumed (§4.6) the Coulomb energy in our system is infinite compared with the conduction band width. So we cut off the positive energy processes like the negative energy processes by the band edges (9.1.25). Let us then replace the term $\Gamma/\pi$ in eqn. (9.1.24) with some realistic density of states $\eta_0(\lambda)$

$$\sigma(\lambda)+\mathscr{F}^{-1}*\tilde{\sigma}(\lambda)+S_k*\rho_k(\lambda)=\eta_0(\lambda)+\frac{1}{L}\times\mathscr{F}^{-1}*a_n(\lambda+\epsilon/2\Gamma), \tag{9.1.27}$$

where $\eta_0(\lambda)\to 0$ at $\lambda\gg D^{(+)}$ or $\lambda\ll -D^{(-)}/2\Gamma$.

Integrating eqn. (9.1.27) and using the condition

$$N=\sum_{p=1}^{n} pr_p \tag{9.1.28}$$

and (9.1.17) and (9.1.7) we have

$$\int\tilde{\sigma}(\lambda)\,d\lambda=\frac{nD^{(+)}}{2\pi}. \tag{9.1.29}$$

Equations (9.1.21) and (9.1.27) together with the conditions (9.1.17) and (9.1.29) describe the properties of the degenerate Anderson model at $T=0$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

### 9.2. *Universality*

The universal property of the asymmetric Anderson model is well known: all physical quantities depend only on the renormalized parameters:

$$\epsilon_f^* = \epsilon_f + (n-1)\frac{\Gamma}{\pi}\ln\frac{D^{(+)}}{\Gamma} \tag{9.2.1}$$

instead of on the bare parameters $\epsilon_f$, $D$. Here we prove the universality properties in the framework of eqns. (9.1.17), (9.1.21), (9.1.27) and (9..29). For this purpose we take the limit $D \to \infty$.

Let us decompose the functions $\sigma$, $\tilde{\sigma}$ into two parts:

$$\sigma(\lambda) = \sigma_0(\lambda) - \sigma_1(\lambda - Q); \qquad \tilde{\sigma}(\lambda) = \tilde{\sigma}_0(\lambda) - \sigma_1(\lambda - Q), \tag{(9.2.2)}$$

where the functions $\sigma_0$ and $\tilde{\sigma}_0$ are the densities of particles and holes in the true ground state:

$$\sigma_0(\lambda) - \int_{-\infty}^{Q} K_n(\lambda - \lambda')\tilde{\sigma}_0(\lambda')\,d\lambda' = \eta_0(\lambda) \qquad (\lambda > Q) \tag{9.2.3}$$

$$\tilde{\sigma}_0(\lambda) - \int_{-\infty}^{Q} K_n(\lambda - \lambda')\tilde{\sigma}_0(\lambda')\,d\lambda' = \eta_0(\lambda) \qquad (\lambda < Q), \tag{9.2.4}$$

where $K_n(\omega) = 1 - \mathscr{F}^{-1}(\omega)$. To solve eqns. (9.2.3) and (9.2.4) according to the Wiener–Hopf method (see the Appendix to § 5.1.3) one must factorize the kernel

$$\mathscr{F}(\omega) \equiv \frac{\sinh n\omega/2}{\sinh \omega/2}\exp\left(-\frac{|\omega|}{2}(n-1)\right) = G^{(+)}(\omega)G^{(-)}(\omega), \tag{9.2.5}$$

where $G^{(\pm)}(\omega)$ is an analytical function in the upper (lower) half-plane. We easily find:

$$G^{(-)}(\omega) = G^{(+)}(-\omega) = \left(\frac{i\omega + 0}{2\pi e}\right)^{i\omega(n-1)/2\pi} \exp\left(i\frac{\omega}{2\pi}n\ln n\right) \times \sqrt{n}\frac{\Gamma(1 + i\omega/2\pi)}{\Gamma(1 + in\omega/2)}. \tag{9.2.6}$$

Using these functions we have:

$$\tilde{\sigma}_0(\omega) = -\frac{i}{2\pi}G^{(-)}(\omega)\exp(i\omega Q)\int_{-\infty}^{+\infty}\frac{d\omega'}{\omega - \omega' - i0}\exp(-i\omega' Q)\eta_0(\omega')G^{(+)}(\omega'), \tag{9.2.7}$$

where

$$\eta_0(\omega) = \int_{-\infty}^{+\infty}\exp(i\omega\lambda))\eta_0(\lambda)\,d\lambda.$$

To find the quantity $Q$ first note that, as we shall show below, $Q$ is a large positive value. Using this fact it is easy to find the asymptotic behaviour $\tilde{\sigma}_0(\lambda)$ at $\lambda \to \infty$. We have

$$\left.\begin{aligned} &\tilde{\sigma}_0(\lambda) = \frac{n\Gamma}{\pi}\left(1 - \frac{n-1}{2\pi}\frac{1}{|\lambda|} + \ldots\right) \quad \text{at } \frac{D^{(+)}}{2\Gamma} \gg |\lambda| \gg 1, \\ &\tilde{\sigma}_0(\lambda) = 0 \quad \text{at } |\lambda| \gg \frac{D^{(+)}}{2\Gamma}. \end{aligned}\right\} \tag{9.2.8}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Inserting (9.2.8) into (9.1.29) and using (9.1.15) we obtain the renormalization of the resonance level:

$$Q=\frac{(n-1)}{2\pi}\ln\frac{D^{(+)}}{\Gamma}+O(1)+q, \tag{9.2.9}$$

where

$$q=\int_{-\infty}^{0}\tilde{\sigma}_1(\lambda)\,d\lambda. \tag{9.2.10}$$

It is understandable that in the absence of the magnetic field $q=0$.

Consider now eqns. (9.1.21). The term $s_j*\tilde{\sigma}_0$ in the right-hand side of eqn. (9.1.21) converges without any cut-off. Therefore, in eqn. (9.1.21) one can use (9.2.7) with $\eta_0(\lambda)=\Gamma/\pi$. Shifting the arguments of the functions $\rho_j(\lambda)$, $\tilde{\sigma}(\lambda)$ in eqn. (9.1.21), for the host part of the distributions, we have:

$$\rho_j^{\mathrm{h}}(\lambda)-\int_0^{\infty}R_{jk}(\lambda-\lambda'+b_j-b_k)\rho_k^{\mathrm{h}}(\lambda')\,d\lambda'$$
$$=f_j(\lambda+b_j)-\int_{-\infty}^{0}s_j(\lambda+b_j-\lambda')\tilde{\sigma}_1^{\mathrm{h}}(\lambda')\,d\lambda'; \tag{9.2.11}$$

$$\tilde{\sigma}_1^{\mathrm{h}}(\lambda)-\int_{-\infty}^{0}R_n(\lambda-\lambda')\tilde{\sigma}_1^{\mathrm{h}}(\lambda')\,d\lambda'=\int_0^{\infty}s_k(\lambda-\lambda'-b_k)\rho_k^{\mathrm{h}}(\lambda')\,d\lambda', \tag{9.2.12}$$

where

$$R_{jk}(\omega)=1-D_{jk}(\omega),$$
$$f_j(\lambda)=-\frac{in\Gamma}{2\pi^2}\int_{-\infty}^{\infty}d\omega\exp(-i\omega\lambda)\frac{\sinh j\omega/2}{\sinh n\omega/2}\frac{G^{(-)}(\omega)}{G^{(-)}(0)}\frac{1}{\omega-i0}$$

and

$$R_n(\omega)=1-\mathscr{F}^{-1}(\omega);\qquad b_j=B_j-Q$$

depends on $\epsilon_j^*/2\Gamma$, $H/\Gamma$.

In the presence of the magnetic field the host part of the numbers $r_k$ have the form (see § 7)

$$r_k=\frac{HL}{2\pi}\qquad(k=1,\ldots,n-1).$$

Therefore, the quantities $b_k$ are determined by the conditions

$$\int_0^{\infty}\rho_j(\lambda)\,d\lambda=\frac{H}{2\pi}. \tag{9.2.13}$$

Now we shall study the impurity part of eqns. (9.1.21) and (9.1.24). They are

$$\rho_j^{\mathrm{i}}(\lambda)-\int_0^{\infty}R_{jk}(\lambda-\lambda'+b_j-b_k)\rho_k^{\mathrm{i}}(\lambda')\,d\lambda'$$
$$=s_{n-j}(\lambda+\epsilon_j^*(H)/2\Gamma+b_j)+\int_{-\infty}^{0}s_j(\lambda-\lambda'+b_j)\tilde{\sigma}^{\mathrm{i}}(\lambda')\,d\lambda', \tag{9.2.14}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

$$\tilde{\sigma}^{\mathrm{i}}(\lambda)-\int_{-\infty}^{0} R_n(\lambda-\lambda')\tilde{\sigma}^{\mathrm{i}}(\lambda')\,d\lambda'$$
$$=-\int_{0}^{\infty} s_k(\lambda-\lambda'-b_k)\rho_k^{\mathrm{i}}(\lambda')\,d\lambda'+\mathscr{F}^{-1}*a_n(\lambda+\epsilon_f^*(H)/2\Gamma), \qquad (9.2.15)$$

where we put

$$\epsilon_f^*(H)=\epsilon_f^*+q(H)2\Gamma. \qquad (9.2.16)$$

The impurity parts of the magnetization and the occupation number are given by the integrals:

$$M_{\mathrm{i}}=\frac{1}{2}\sum_{j=1}^{n-1} j(n-j)\int_{0}^{\infty}\rho_j^{\mathrm{i}}(\lambda)d\lambda, \qquad (9.2.17)$$

$$n_f=1-\int_{-\infty}^{0}\tilde{\sigma}_{\mathrm{i}}(\lambda)d\lambda. \qquad (9.2.18)$$

The universal equations (9.2.10)–(9.2.18) completely describe the equilibrium properties at $T=0$ of the degenerate Anderson model. At $n=2$ we come back to the equations for the asymmetric non-degenerate Anderson model.

### 9.3. *The occupation number*

Here we shall derive the dependence of the valence of the impurity ion on the renormalized level position at $H=0$. From eqns. (9.2.13) and (9.2.15) we have at $H=0$, $b_k=\infty$ and

$$\left.\begin{aligned}\tilde{\sigma}_{\mathrm{i}}(\lambda)-\int_{-\infty}^{0} R_n(\lambda-\lambda')\tilde{\sigma}_{\mathrm{i}}(\lambda')\,d\lambda'&=\mathscr{F}^{-1}*a_n(\lambda+\epsilon_f^*/2\Gamma),\\ n_f=1-\int_{-\infty}^{0}\tilde{\sigma}_{\mathrm{i}}(\lambda)\,d\lambda.&\end{aligned}\right\} \qquad (9.3.1)$$

Using the Wiener–Hopf method and functions (9.2.6) one can easily find the solution of eqn. (9.3.1):

$$\tilde{\sigma}_{\mathrm{i}}(\omega)=-\frac{iG^{(-)}(\omega)}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega'}{\omega-\omega'-i0}\,\frac{\exp\left(-(n|\omega'|/2)-i\omega'\epsilon_f^*/2\Gamma\right)}{G^{(-)}(\omega')} \qquad (9.3.2)$$

and obtain the valence in the explicit form:

$$n_f=1-\frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i0}\,\frac{\Gamma(1+i\omega n)}{\Gamma(1+i\omega)}\exp\left(-\pi|\omega|\right)$$
$$\times\left(\frac{-i\omega+0}{e}\right)^{-i\omega(n-1)}\exp\left(-i\omega\left(\frac{\epsilon_f^*\pi}{\Gamma}+n\ln n\right)\right). \qquad (9.3.3)$$

This formula generalizes expression (8.2.56) for arbitrary $n$ and describes the smooth transition from the localized moment regime ($n_f=1$) to the fulfilled shell ($n_f=0$) via the mixed-valence regime. Deforming the integration path in the upper (lower) half-plane if $\epsilon_f^*<0$ ($\epsilon_f^*>0$) one obtains the asymptotic behaviour at $|\epsilon_f^*|\gg\Gamma$. Let

$$\epsilon_f^{**}+\frac{(n-1)\Gamma}{\pi}\ln\left(\frac{|\epsilon_f^{**}|}{2\Gamma n^{n/n-1}}\right)=\epsilon_f^*. \qquad (9.3.4)$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

At $\epsilon_f^* < 0$

$$n_f = 1 + \frac{1}{\pi}\int_0^\infty \frac{dt}{t}\exp(-2\pi t)\sin\left(\frac{2\pi\Gamma}{\epsilon_f^{**}}t\right)\frac{\Gamma(1+(2\Gamma n/\epsilon_f^{**})t)}{\Gamma(1+(2\Gamma/\epsilon_f^{**})t)} \times\left(\frac{t}{e}\right)^{[-(2\Gamma(n-1)/\epsilon_f^{**})t]} + O\left(\exp\left(\frac{\pi\epsilon_f^{**}}{n\Gamma}\right)\right); \tag{9.3.5}$$

$$n_f = 1 + \frac{\Gamma}{\pi\epsilon_f^{**}} + O\left(n^2\left(\frac{\Gamma}{\epsilon_f^{**}}\right)^3\right). \tag{9.3.6}$$

At $\epsilon_f^* > 0$

$$n_f = \frac{1}{\pi}\int_0^\infty \frac{dt}{t}\exp(-2\pi t)\sin\left(\frac{2\pi n\Gamma}{\epsilon_f^{**}}t\right)\frac{\Gamma(1+(2\Gamma n/\epsilon_f^{**})t)}{\Gamma(1+(2\Gamma/\epsilon_f^{**})t)}\left(\frac{t}{e}\right)^{-(2\Gamma(n-1)/\epsilon_f^{**})t}; \tag{9.3.7}$$

$$n_f = \frac{n\Gamma}{\pi\epsilon_f^{**}} + O\left(\left(\frac{n\Gamma}{\epsilon_f^{**}}\right)^3\right). \tag{9.3.8}$$

Both the asymptotics (9.3.6) and (9.3.8) were obtained by the perturbation theory of Tsvelick and Barabanov (1978) and Bringer and Lustfeld (1978).

### 9.4. *Magnetic susceptibility and the Kondo limit*

Like all the problems solved in this paper we apply the Fermi-liquid approach to calculate the magnetic susceptibility.

This approach is based on the comparison of the host part, eqns. (9.2.11), and the impurity part, eqns. (9.2.14), at $H \to 0$. At $H \to 0$ one must confine oneself to only the asymptotic behaviour at $b \to \infty$ in the right-hand side of eqn. (9.2.11) and (9.2.14) and neglect the terms with $\tilde{\sigma}_1^n$ in (9.2.11) and the term with $\rho_k^{\mathrm{i}}$ in (9.2.15), which is proportional to $H^2$:

$$\rho_j^{\mathrm{h}}(\lambda) - \int_0^\infty R_{jk}(\lambda-\lambda'+b_j-b_k)\rho_k^{\mathrm{h}}(\lambda')\,d\lambda' = \exp\left(-\frac{2\pi}{n}(\lambda+b_j)\right)\sin\left(\frac{\pi j}{n}\right)\frac{\Gamma n}{\pi^2}\frac{G^{(-)}(-i2\pi/n)}{G^{(-)}(0)}; \tag{9.4.1}$$

$$\rho_j^{\mathrm{i}}(\lambda) - \int_0^\infty R_{jk}(\lambda-\lambda'+b_j-b_k)\rho_k^{\mathrm{i}}(\lambda')\,d\lambda' = \exp\left(-\frac{2\pi}{n}(\lambda+b_j)\right)\frac{2}{n}\sin\left(\frac{\pi j}{n}\right)\left[\exp\left(-\frac{\pi\epsilon_f^*}{n\Gamma}\right)+\tilde{\sigma}_{\mathrm{i}}\left(\frac{i2\pi}{n}\right)\right]. \tag{9.4.2}$$

Comparing these equations we obtain at $H=0$ the partial magnetic susceptibility $\chi_k = \partial r_k/\partial H$, where $r_k$ related to the impurity occupation number with the projection of the total moment $((n-1)/2-j)$ by eqn. (9.1.8) has the form

$$\frac{\chi_k^{(\mathrm{i})}}{\chi_k^{(\mathrm{h})}} = \frac{\exp(-\pi\epsilon_d^*/n\Gamma)+\tilde{\sigma}_{\mathrm{i}}(\omega=-i2\pi/n)}{(\Gamma n^2/2\pi^2)(G^{(-)}(-i2\pi/n)/G^{(-)}(0))}. \tag{9.4.3}$$

The total magnetic susceptibility according to (7.3.13) is

$$\chi = \frac{n(n^2-1)}{24\pi}\frac{\chi^{(\mathrm{i})}}{\chi^{(\mathrm{h})}}. \tag{9.4.4}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Using the solution (9.3.2) we come to the explicit expression for the generalized magnetic susceptibility eqn. (8.2.106),

$$\chi=\frac{\pi(n^2-1)}{12n\Gamma}\left[\frac{(en)^{(n-1)/n}}{n\Gamma(1+1/n)}\exp\left(-\frac{\pi\epsilon_f^*}{n\Gamma}\right)\right.$$
$$+\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{1-i\omega}\frac{\Gamma(1+i\omega)}{\Gamma(1+i\omega/n)}\left(\frac{-i\omega+0}{e}\right)^{-i\omega(n-1)/n}$$
$$\left.\times\exp\left(-i\omega\left(\frac{\epsilon_f^*\pi}{\Gamma n}+\ln n\right)-\frac{\pi|\omega|}{n}\right)\right]. \quad (9.4.5)$$

In the localized-moment regime $-\epsilon_f^*\gg\Gamma$ the Kondo effect takes place and

$$\chi=\frac{n(n^2-1)}{12\pi\Gamma T_K}(\mu_B g)^2, \quad (9.4.6)$$

where

$$T_K=\frac{n^2\Gamma}{\pi^2 e}(en)^{1/n}\Gamma\left(1+\frac{1}{n}\right)\exp\left(\frac{\pi\epsilon_f^*}{n\Gamma}\right). \quad (9.4.7)$$

Defining the exchange coupling as

$$I=-\Gamma/\pi\epsilon_f \quad (9.4.8)$$

we have the expression for the Kondo temperature

$$T_K=\text{const}\,\Gamma\left(\frac{D}{\Gamma}\right)^{(n-1)/n}\exp\left(-\frac{1}{nI}\right). \quad (9.4.9)$$

The pre-exponential numerical factor in (9.4.9), in contrast to the factor in (9.4.7), exceeds the logarithmic accuracy with which we have found the renormalization of the resonance level (9.2.1). However, the pre-exponential behaviour $\Gamma(D/\Gamma)^{(n-1)/n}$ is true and corresponds to the perturbation theory result. In the nonmagnetic regime $\epsilon_f^*\gg\Gamma$, the magnetic susceptibility is

$$\chi=\frac{n(n^2-1)}{12}\left(\frac{\Gamma}{\pi\epsilon_f^{*2}}+O\left(\frac{\Gamma^2}{\epsilon_f^{*3}}\right)\right). \quad (9.4.10)$$

There is a smooth transition between the regimes (9.4.6) and (9.4.10) via the mixed-valence regime $|\epsilon_f^*|\sim\Gamma$.

In conclusion let us show that eqns. (9.2.11)–(9.2.16) coincide with eqns. (7.3.2) for the degenerate Kondo model if $-\epsilon_f^*\gg\Gamma$. The procedure for the nondegenerate Anderson model has been described in detail in § 8.2.10. In the Kondo limit one must neglect all terms of the order of $H/\Gamma$ compared with $H/T_K$. Therefore, omitting the

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

terms $\tilde{\sigma}_1^{\mathrm{h}}$ and $\tilde{\sigma}_{\mathrm{i}}$ in the right-hand side of (9.2.11) and (9.2.14) we obtain the equations:

$$\left.\begin{aligned}
&\rho_j^{\mathrm{i}}(\lambda)-\int_0^\infty R_{jk}(\lambda-\lambda'+\tilde{b}_j-\tilde{b}_k)\rho_k^{\mathrm{i}}(\lambda')\,d\lambda'=s_{n-j}\left(\lambda+\tilde{b}_j-\frac{n}{2\pi}\ln\frac{H}{T_H}\right),\\
&\rho_j^{\mathrm{h}}(\lambda)-\int_0^\infty R_{jk}(\lambda-\lambda'+\tilde{b}_j-\tilde{b}_k)\rho_k^{\mathrm{h}}(\lambda')\,d\lambda'=\sin\left(\frac{\pi j}{n}\right)\exp\left(-\frac{2\pi}{n}(\lambda+\tilde{b}_j)\right);\\
&\qquad\qquad 1=\int_0^\infty \rho_j^{\mathrm{h}}(\lambda)\,d\lambda,
\end{aligned}\right\}\tag{9.4.11}$$

where $T_H=T_{\mathrm{K}}/2\pi n$, $\tilde{b}_j=b_j+n/2\pi\ln H/T_H$ are just numbers which coincide with the analogous equations for the degenerate Kondo model after replacing $\rho_k\to\rho_k$ with the Kondo temperature given by (9.4.7).

Finally, let us discuss the limit $n\to\infty$. Keeping the parameter $\epsilon_f^*/n\Gamma$ finite we have

$$n_f^\infty=1-\frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega+i0}\Gamma(1+i\omega)\left(\frac{-i\omega+0}{e}\right)^{-i\omega}\exp\left(-i\omega\frac{\epsilon_f^*\pi}{\Gamma n}\right).$$

The transition from the localized-moment regime to the mixed-valence regime sharpens as $n$ increases. At $n=\infty$ the power corrections at $-\epsilon_f^*\gg\Gamma$ disappear:

$$n_f^\infty=1\sum_{k=1}^{\infty}\frac{(-1)^k}{k!}\left(\frac{k}{e}\right)^k\exp\left(\frac{\pi\epsilon_f^*}{n\Gamma}k\right)\qquad(\epsilon_f^*<0).$$

On the other hand the transition from the unfilled-shell to the mixed valence regime remains smooth

$$n_f^\infty=\int_0^\infty dt\frac{(t/e)}{\Gamma(1-t)}\exp\left(-\frac{\pi e_f^*}{n\Gamma}t\right).$$

So in the limit $n\to\infty$ the dependence of the physical quantities on $\epsilon_f^*/n\Gamma$ is still rather complicated. Therefore, the possibility of constructing the $n$-expansion without applying the exact solution seems rather doubtful.

Unfortunately dilute magnetic systems in the mixed-valence regime have been poorly studied experimentally. We stress only the recent experimental study on the problem of the role of single impurity versus collective contributions to the mixed valence phenomena (Luszik-Bhadra *et al.* 1981).

Intermediate-valence dilute Ce ions in thorium have been investigated. The observed magnetic susceptibility shows a transition from magnetism to non-magnetism of the Ce ions and has a characteristic maximum. The behaviour of the magnetic susceptibility is like the well-known behaviour of concentrated Ce alloys which are ordered intermetallic compounds. The strong similarities make it possible to assume that valence transitions in the concentrated Ce systems are governed by the single Ce ion behaviour at least at a not very low temperature. Microscopic measurements of the single-ion behaviour in the intermediate-valence regime provide one of the best tests of the theory discussed here.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

## Supplement

### *Exact solution of the resonant-level model*

We expound below the Bethe-Ansatz technique for the resonant-level (RL) model.

$$\mathscr{H}_{\mathrm{RL}}=\sum_k \epsilon_k c_k^+ c_k + V\sum_k (c_k^+ d + d^+ c_k) + \frac{U}{4}(d^+ d - dd^+)\sum_{k,k'}(c_k^+ c_{k'} - c_k c_{k'}^+), \quad \text{(S 1)}$$

where $c_k^+$ and $d^+$ are creation operators of a spinless fermion with momentum $k$ and a spinless fermion on the local resonant level, respectively. The RL model is equivalent to the anisotropic s–d exchange model in the long-time approximation. This connection has been discussed in § 3.1.

We shall compare the Bethe-Ansatz equations for the RL model with those for the anisotropic s–d exchange model (5.2.5 and (5.2.6) and show how the equality discovered by Anderson *et al.* (1970) displays itself in the framework of the exact solution. Here we follow the papers of Filyov and Wiegmann (1980) and Wiegmann 1981).

1. *The Bethe-Ansatz technique*

In the same manner as for the Kondo hamiltonian (see § 4.2) it is easy to see that

(i) the RL problem is one-dimensional and
(ii) for small $U$ and $V^2/\epsilon_{\mathrm{F}}$ one can neglect the states lying far from the Fermi surface.

Hence

$$\varepsilon_k \simeq \epsilon_{\mathrm{F}} + v_F(k-k_F). \quad \text{(S 2)}$$

Then in the space representation $\mathscr{H}_{\mathrm{RL}}$ has the form

$$\mathscr{H}_{\mathrm{RL}}=\int dx\Big[-ic^+(x)\frac{d}{dx}c(x)+V\delta(x)(c^+(x)d+d^+c(x)) + \frac{U}{4}\delta(x)(d^+d-dd^+)(c^+(x)c(x)-c(x)c^+(x)\Big].$$

This hamiltonian conserves the total number of particles:

$$M=\int c^+(x)c(x)\,dx + d^+d.$$

Therefore, its eigenfunctions are obtained in the form

$$|\Psi\rangle_M=\int g(x_1,\ldots,x_M)\prod_{i=1}^{M} c^+(x_i)\,dx_i|0\rangle + \int e(x_1,\ldots,x_{M-1})\,d^+\prod_{i=1}^{M-1} c^+(x_i)\,dx_i|0\rangle,$$

where the vacuum is defined as follows:

$$d|0\rangle = c(x)|0\rangle = 0.$$

At first we construct the solution for $U=0$. In this case the solution is a product of one-body functions:

$$|\Psi\rangle_M=\sum_{\alpha=1}^{M}\left(\int g_0(p_\alpha|x)c^+(x)\,dx + e(p_\alpha)\,d^+\right)|0\rangle. \quad \text{(S 3)}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The functions $g_0(p|x)$ and $e(p)$ satisfy the Schrödinger equations:

$$\left.\begin{aligned} -i\frac{\partial}{\partial x}g_0(p|x)+Ve(p)\delta(x)&=pg_0(p|x),\\ Vg_0(p|0)&=pe(p),\end{aligned}\right\} \tag{S 4}$$

where $p_\alpha$ are the arbitrary unequal parameters-momenta of the particles. The energy of the state is

$$E=\sum_{\alpha=1}^{M}p_\alpha. \tag{S 5}$$

The solution of (S 4) is

$$g_0(p|x)=g_0(p|0)\exp\left(ipx+\frac{i}{2}\delta(\varepsilon)\operatorname{sign}x\right), \tag{S 6}$$

where the phase shift is

$$\delta(\varepsilon)=2\tan^{-1}(V^2/2p). \tag{S 7}$$

Now we can consider the two-body state for $U\neq 0$:

$$|\Psi\rangle_2=\left[\int g(x_1,x_2)c^+(x_1)c^+(x_2)\,dx_1dx_2+\int e(x)c^+(x)\,dx\,d^+\right]|0\rangle. \tag{S 8}$$

The Schrödinger equations for the functions $g(x_1,x_2)$ and $e(x)$ are

$$\begin{aligned} -i\left(\frac{\partial}{\partial x_1}+\frac{\partial}{\partial x_2}\right)g(x_1,x_2)+\frac{1}{2}V(e(x_2)\delta(x_1)-e(x_1)\delta(x_2))&\\ -\frac{1}{2}V[\delta(x_1)+\delta(x_2)]g(x_1,x_2)&=Eg(x_1,x_2),\end{aligned} \tag{S 9}$$

$$-i\frac{\partial}{\partial x}e(x)+2Vg(0,x)+\frac{1}{2}U\delta(x)e(x)=(E+\tilde{\varepsilon}_d)e(x), \tag{S 10}$$

where

$$\tilde{\varepsilon}_d=U\langle c^+(0)c(0)\rangle$$

is the shift of the level.

Using the property of the kinetic energy operator

$$\left(\frac{\partial}{\partial x_1}+\frac{\partial}{\partial x_2}\right)f(x_1-x_2)=0$$

for an arbitrary $f(x)$, we look for the solution of eqns. (S 9) in the following form:

$$\left.\begin{aligned} 2!\,g(x_1,x_2)&=g(p_1|x_1)g(p_2|x_2)f(x_1-x_2)-g(p|x_2)g(p_2|x_1)f(x_2-x_1),\\ e(x)&=e(p_1)g(p_2|x)f(-x)-e(p_2)g(p_1|x)f(x),\end{aligned}\right\} \tag{S 11}$$

where $g(p|x)=g_0(p|x)\exp(i(U/4)\operatorname{sign}x)$.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

The energy of this state is $E=p_1+p_2$. The first equation in (S 9) is satisfied for an arbitrary $f(x)$ and the second one defines $f(x)$:

$$e(p_1)g(p_2|x)\frac{df(-x)}{dx}-e(p_2)g(p_1|x)\frac{df(x)}{dx}$$
$$=-U\delta(x)[e(p_1)g(p_2|x)f(-x)-e(p_2)g(p_1|x)f(x)]. \qquad \text{(S 12)}$$

The right-hand side of eqn. (S 12) is badly defined. Therefore, we spread the $\delta$ function. Then we get

$$\left.\begin{aligned} f(x_1,x_2)&=f(0)\exp\left[-\frac{i}{2}\Phi(p_1,p_2)\,\mathrm{sign}\,(x_1-x_2)\right],\\ \Phi(p_1,p_2)&=2\tan^{-1}\left(\tan\frac{U}{2}\frac{p_1-p_2}{p_1+p_2+2\tilde{\epsilon}_d}\right).\end{aligned}\right\} \qquad \text{(S 13)}$$

Before constructing the $M$-particle eigenstate let us consider the two-particle solution (S 11) and (S 13). Putting $V=0$ in (S 11) we obtain the wavefunction of two free particles:

$$g(x_1,x_2)\underset{V\to 0}{\to} g^{(0)}(x_1,x_2)=\exp\left(ip_1x_1+ip_2x_2+\frac{i}{2}\Phi(p_1,p_2)\,\mathrm{sign}\,(x_1-x_2)\right)$$
$$-\exp\left(ip_1x_2+ip_2x_1+\frac{i}{2}\Phi(p_1,p_2)\,\mathrm{sign}\,(x_2-x_1)\right).$$

Note that the wavefunction of free particles includes the two-particke scattering phase. This phenomenon has been discussed in § 4.6.

Now consider the solution of the $M$-body problem for $U\neq 0$. The wavefunction of our problem is factorized in a product of two-body ones. It is the *Bethe Ansatz*:

$$N!\,g(x_1,\ldots,x_M)=\sum_Q(-1)^Q g(p_{q_1}|x_1)\ldots g(p_{q_M}|x_M)$$
$$\times\prod_{j>k}\exp\left\{-\frac{i}{2}\Phi(p_{q_j},p_{q_k})\,\mathrm{sign}\,(x_j-x_k)\right\}, \qquad \text{(S 14)}$$
$$E=\sum_{j=1}^{M}p_j.$$

The summation in (S 14) extends over all permutations $Q=\{q_1,\ldots,q_M\}$ of integers $1,\ldots,M$. One can easily verify by direct substitution that Bethe-Ansatz is valid. The eigenfunctions (S 13) are defined by the set of parameters $\{p_1,\ldots,p_M\}$. To study (S 13) are defined by the set of parameters $\{p_1,\ldots,p_M\}$. To study the spectral properties of the system, we must impose boundary conditions in the wavefunction (S 14). Let us impose the periodic boundary conditions putting the system in a sphere of radius $L/2$ around the impurity site:

$$g(x_1,\ldots,x_j=-L/2,\ldots,x_M)=g(x_1,\ldots,x_j=L/2,\ldots,x_M). \qquad \text{(S 15)}$$

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

Equation (S 14) leads to a system of algebraic equations which define the values $p_\alpha$ (Filyov and Wiegmann 1980):

$$Lp_\alpha+\delta(p_\alpha)+U/2=2\pi I'_\alpha+\sum_{\beta=1}^{M}\Phi(p_\alpha,p_\beta), \tag{S 16}$$

where the $I'_\alpha$ ($\alpha=1,\ldots,M$) are integers. They are the quantum number of system. Note that due to the boundary conditions the shift of the level energy (S 10) is equal to $\tilde{\epsilon}_d=\epsilon_d+MU/2L$.

2. *Comparison with Bethe-Ansatz equations for the anisotropic exchange model (§§5.2.5 and 5.2.6)*

Firstly, let us find the rapidity variable $\lambda=\lambda(p)$ in terms of which the two-particle phase is the function of the difference particle rapidities:

$$\Phi(p(\lambda),p(\lambda'))=\Phi(\lambda-\lambda').$$

The two-particle phase $\Phi(p,q)$ is a uniform function. Therefore, one can choose the rapidities as follows

$$p(\lambda)+\tilde{\epsilon}_d=-D\exp(2\mu\lambda), \tag{S 17}$$

where $D$ is an ultraviolet cut-off and we put

$$\cot\mu=-\tan U/2. \tag{S 18}$$

The linear spectrum approximation (S 2), which was an important step towards the integrability in the RL model, is valid for $U\ll 1$ and for the low-energy processes with the energy $p\ll V^2\ll D$. That is why only the linear term in $p/V^2$ in the one-particle scattering phase shift on impurity (S 7) is universal

$$\delta(p)\simeq\pi\left(\frac{p+\tilde{\epsilon}_d}{V^2}\right). \tag{S 19}$$

In this approximation the replacement (S 17) and (S 18) leads to the Bethe-Ansatz equations for the RL model at $-\lambda\gg 1$

$$\begin{aligned}DL\exp(2\mu\lambda)+\exp(2\mu(\lambda+f/\mu))+MU+U/2\\ =2\pi I'_\alpha+2\sum_{\beta=1}^{M}\tan^{-1}(\cot\mu\tanh\mu(\lambda_\alpha-\lambda_\beta)),\end{aligned} \tag{S 20}$$

where

$$\frac{V^2}{2D}=\exp(-2f). \tag{S 21}$$

Now let us compare eqn. (S 20) with the Bethe-Ansatz equations for the anisotropic s–d exchange model (5.2.5–6). Recall that the mission of the RL model is to describe equivalently the spin subsystem of the s–d exchange model (see § 3.1). Therefore, it was expected that the coordinate Bethe Ansatz for the RL model must be equivalent to the spin Bethe Ansatz for the s–d exchange model (Wiegmann 1981) (see also § 4.3). In fact eqns. (5.2.6) and (S 20) are just the same in the limit $-\lambda\gg 1$. In this

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

limit the momentum of the spin-density wave and the scattering phase of this wave on impurity (the left-hand side of eqn. (5.2.5 *b*)) has the form

$$\left.\begin{aligned} p(\lambda) &\equiv 2\tan^{-1}(\cot\mu/2\tanh\mu\lambda) \simeq -\pi/2 + U/2 + 2\sin\mu\exp(2\mu\lambda), \\ \delta(\lambda) &\equiv 2\tan^{-1}(\cot\mu/2\tanh\mu(\lambda+f/\mu)) \simeq -\pi/2 + U/2 + 2\sin\mu\exp(2\mu(\lambda+f/\mu)). \end{aligned}\right\} \quad \text{(S 22)}$$

Comparing (S 22), (S 20) and (5.2.5) we see that the number of particles $M$ in the RL model is equal to the number of the spin-down particles in the s–d model, and the cut-off $D = 2\sin\mu(N/L)$. Equations (S 18), (S 21) and (4.3.8) give the relations between the parameters $I_{\parallel}$, $I_{\perp}$ and $V$, $U$ of the models. Note that these relations are not universal.

## Conclusion

The reader who has followed the development of the problem from the interaction of one bare particle with a magnetic impurity to the solution of the many-body problem and the derivation of concrete physical results should note the adequacy of the Bethe method for application to the problems concerning magnetic impurities.

The method has enabled us to reduce the thermodynamics of the many-body problem to a system of integral equations. Yet these equations are non-linear and the number of them is infinite. However, this does not prevent us from getting the necessary data on the analytical character of particularly interesting limit cases leaving the crossover region in temperatures open to numerical calculations.

We do not think that a numerical solution of eqns. (8.3.15) which describe the thermodynamics of the Anderson model will be too complicated. Most likely a small computer will manage to do it as in the case of the Kondo model. At $T=0$ it is possible to obtain the explicit dependence of the magnetic and charge susceptibilities on parameters $U$, $\Gamma$, $\epsilon_d$ for the Anderson model and also the explicit dependence on the magnetic field for the symmetric Anderson model. Looking back we may construct a very simple physical picture. This picture corresponds in many respects to the Anderson–Nozières ideas. We emphasize that not only is the physics simple in the vicinity of fixed points at low and high energies and may be describable either by perturbation or phenomenological theories, but various crossover regimes which are not controlled by qualitative arguments are not very complicated and are described by simple mathematics.

In the 1970s one had to hear many times that 'the Kondo problem is solved'. It really was for those interested only in the impurity ground state and the qualitative behaviour at low temperatures. Those who wished to know something about the analytical structure of crossover between the weak and strong-coupling regions can only now get the solution to the Kondo problem.

However, the exact solution derived above has a limited domain of application. It describes the thermodynamics of magnetic alloys, but, apart from not-yet resolved problems within the model itself, it does not enable us to extend a new style of theory to numerous interesting and important applications of the Kondo effect. Finally, we do not analyse the experimental situation in detail. Thus we cannot say that the problem is completely solved.

We enumerate some unsolved problems below. The Bethe-Ansatz approach is extremely sensitive to the choice of the quantity to be calculated. Within the framework of the Bethe Ansatz it is relatively easy to calculate a thermodynamic

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

potential. The situation is different for the kinetic coefficients and dynamical characteristics. Therefore, we now know only the kinetic coefficients related to the equilibrium quantities. For example, such a quantity is resistivity at $T=0$ and arbitrary $H$. It is given by eqn. (3.2.11).

However, the temperature dependence of the electrical resistivity is still unknown except for the Fermi-liquid $T^2$-term. This is just as in the case of the thermoelectric power and other kinetic coefficient. The thermoelectric power $S$, Hall coefficient $R_H$, and thermal conductivity $k$ for $T\to 0$ and arbitrary values of magnetic field and the parameters $U$, $\epsilon_d$ and $\Gamma$, have the forms:

$$S=\frac{1}{e}C_i\frac{\sin \pi n_d(\cos 2\pi M_i-\cos \pi n_d)}{1-\cos \pi n_d \cos 2\pi M_i};$$

$$R_H=\frac{2}{enc}\left[1-\frac{(\cos 2\pi M_i-\cos \pi n_d)^2}{2(1-\cos \pi n_d \cos 2\pi M_i)}\right];$$

$$k=\frac{\pi^2 T}{3e^2}\sigma;$$

where $C_i$ is the impurity specific heat at $T\to 0$, $M_i$, $n_d$ and $\sigma$ are the impurity magnetization, average occupation number and electric conductivity at $T=0$ and arbitrary $H$. The temperature and frequency dependence of kinetic coefficients seems to be the principal unsolved problem.

Another interesting and important question is the effect of magnetic impurities on superconductivity. Today we know the quantities which may be calculated by perturbation theory or Fermi-liquid approach. For example, the linear term in the expansion of the superconducting transition temperature in powers of the impurity concentration is equal to

$$\frac{T_c-T_{c0}}{T_{c0}}=-c\frac{1}{4\rho_s T_K}\left(\ln\frac{T_k}{T_{c0}}\right)^2 \qquad \text{at } T_K\gg T_{c0}$$

(Sakurai 1978, Matsuura *et al.* 1978) and unknown for an arbitrary value of $T_{c0}/T_K$.

The magnetic impurity in a metal affects the conduction electron states by the exchange interaction. It is easy to show that these so-called Friedel charge and spin oscillations have, at $T=0$ and $r\gg\rho(\epsilon_F)(k_B T_K)^{-1}$, the following form (Ishii 1976)

$$\rho(r)=\frac{1}{2\pi^2 r^3}\cos^2[M_i(H)]\sin 2k_F r,$$

$$\delta(r)=\frac{1}{8\pi^2 r^3}\sin[2M_i(H)]\cos 2k_F r,$$

where the impurity magnetization $M_i(H)$ is given by eqn. (5.1.33). Such oscillations were observed by Boyce and Slichter (1974). The polarization of the conduction electrons provides an indirect exchange interaction of the RKKY type between impurities. When the impurity concentration increases the impurity–impurity interaction results in a non-linear dependence of the physical quantities on the concentration. Larkin and Khmel'nitskii (1970) and Souletie and Tournier (1969) derived a virial expansion for various physical quantities at $T\gg T_K$ and $H\gg T_K$ and established the boundaries of applicability of the single-impurity approximation. It is very interesting to derive the virial expansion at arbitrary ratios $T/T_K$ and $H/T_K$. It

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

is important for the analysis of experiments with Ce alloys and, particularly, for the superconducting re-entrant phenomenon in the La-based alloys. Such a virial expansion enables us to explain the surprising difference between $3d$ and $4f$ impurities where the values of $T_K$ are comparable in order of magnitude but the concentration at which the impurity–impurity interaction in $3d$ alloys becomes important is at least two orders of magnitude lower than that for $4f$ alloys.

The unsolved problem is the diagonalization of the exchange hamiltonian (2.2.7) (the so-called $n$-channel Kondo problem). The non-physical results which were obtained in the naive Bethe-Ansatz framework (Furuya and Lowenstein 1982) are associated with the approximation in which the bare particle–impurity scattering phase is taken as independent of the energy of a particle. It is possible that this difficulty may be overcome with the help of some special degenerate Anderson model.

Other unsolved interesting problems involve the Anderson hamiltonian describing Sm- and Tm-mixed valence alloys.

The search for new integrable hamiltonians describing magnetic impurities in metals is associated with the general progress of the Bethe method and particularly with a search for new factorizable $S$-matrices. It would be especially interesting for the theory of magnetic alloys to have the factorizable $S$ matrices corresponding to various representations of the $O(3)\otimes O(3)$ group. It would enable us to investigate the exchange hamiltonians for transition impurities (see § 2). Thus, we cannot assert that the Kondo problem is solved. However, we hope to hear this declared in future and not only once.

It is natural to wonder why the theory of §§ 4–8 has not been compared with the experiments described in § 1. Indeed it was tempting to seek quantitative agreement between theory and experiment. However, without more detailed experimental studies of these substances there is no guarantee that some of the potentially important properties of these alloys have not been ignored. Hence, we restrained ourselves from citing one more "satisfactory" agreement between the experiment and, perhaps, imperfect theory. Indeed, preliminary analyses shows that something may be missing (Melnicov 1982, Rajan *et al.* 1982). The qualitative agreement between theory and experiment was recognized before the appearance of the exact solution. Quantitative analysis requires new experiments at low temperatures and concentrations as well as special precautions to decrease the impurity–impurity interaction, and the role of the superconducting transition temperature. On the other hand theory must provide a careful estimate of effects which are not taken into consideration by the simple models, such as the detailed band structure of the host metal. We think that since the Kondo effect can now be completely taken into account, it is reasonable to work at precise experiments to understand whether only this effect is responsible for the behaviour of real magnetic alloys.

## Acknowledgments

One of the authors (P.B.W.) would like to thank A. I. Larkin, who first introduced him to Bethe Ansatz and to Fateev and Filyov for their cooperation, and also to A. A. Abrisokov, I. M. Lifshitz and L. P. Pitaevsky for their support. The authors also wish to thank V. R. Chechetkin and E. E. Tsvelik for their help in preparing the text. The authors are indebted to their colleagues A. Aronovv, R. S. Arhipov, B. L. Altsuler, A. A. Belavin, A. F. Barabanov, S. A. Bulgadaev,

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

G. I. Dzhaparidze, I. E. Dzyaloshinskii, M. I. D'yakanov, L. D. Faddeev, A. M. Finkelstein, A. A. Gogolin, V. N. Gribov, D. I. Khomskii, D. E. Khmelnitskii, Yu. Kagan, V. E. Korepin, K. I. Kikoin, P. P. Kulish, I. B. Levinson, S. V. Maleev, L. A. Maximov, A. E. Meierovich, V. I. Melnikov, A. A. Nersesyan, N. N. Nikolaev, E. Ogievetskii, S. L. Pokrovskii, A. M. Polyakov, N. Reshetikhin, A. B. Zamlodchikov, Al. B. Zamolodchikov, for helpful discussions. Finally, we would like to thank Professor N. N. Nikolaev for his great contribution and Tanya Kachalova for her help and good humour.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

*Note added in proof*—Here we give the most important results supplementing the present review. These results have been obtained since the article was prepared for publication.

(1) The thermodynamic equations of the degenerate exchange model ((7.1.12), (7.1.13)) have been solved numerically by Rajan (1983, *Phys. Rev. Lett.*, **51,** 308). The magnetic susceptibility and specific heat curves have been found as a function of temperature for zero magnetic field for $I=1/2,\ldots,7/2$. It is interesting that the susceptibility exhibits an $I$-dependent peak at $I>1$. The peaks become sharper as $I$ increases. Such peaks are experimentally observed in some intermediate valence intermetallic like YbCuAl. A similar peak has been observed in the magnetic field dependence of the zero-temperature susceptibility of the model for which numerical analysis has been performed by Hewson and Rasul (1983, *J. Phys.* C, **16,** 6799). In this work the exact results for $I=7/2$ compared with the experimentally measured low-temperature magnetic isoterms for the compound YbCuAl.

(2) Kawakami and Okiji (1983, *Phys. Rev. Lett.*, **50,** 1157) have performed the numerical analysis for the temperature dependence of the impurity susceptibility and specific heat for the non-degenerate Anderson model on the basis of eqns (8.3.14)–(8.3.16).

(3) Schlottmann (*Z. Phys.*, to be published) and Tsvelick (*J. Phys.* C, to be published) have investigated thermodynamic properties of the degenerate Anderson model on the basis of the solution presented in § 9. To complete our review, we give the results obtained by them. The thermodynamic potential is

$$\Omega=-\Gamma\frac{\sqrt{n}}{\pi}\int\frac{d\omega}{\omega^2}(\exp(iq(\theta)\omega)-1-iq(0)\omega)(G^{(-)}(\omega))^{-1}\exp\left(-\frac{n|\omega|}{2}+i\omega\epsilon_f^*(T)\right)$$
$$-T\int_{-\infty}^{\sigma}d\lambda\tilde{\sigma}^i(\lambda)\ln(1+\exp(\kappa(\lambda)/T))-T\int d\lambda\sum_{j=1}^{n-1}\ln(1+\exp(\varepsilon_1^{(j)}/T))$$
$$\times\left(s_{n-j}\left(\lambda-\frac{\epsilon_f^*(T)}{2\Gamma}\right)+\rho_j^i(\lambda)\right);$$

where $\varepsilon_k^{(j)}(\lambda)$, $\kappa(\lambda)$, $q(\lambda)$ satisfy the equations

$$T\ln(1+\exp(-\varepsilon_m^{(j)}))-A^{jk}*C_{ml}*\Gamma\ln(1+\exp(\varepsilon_l^{(k)}/T))=\delta_{m1}Ts_j*\ln(1+\exp(\kappa/T)),$$

$$l,m=1\ldots\infty;\quad j=1\ldots n-1;\quad \lim_{m\to\infty}\frac{\varepsilon_m^{(j)}}{m}=h^{(j)};$$

$$\kappa=-2\Gamma\sqrt{n}\int d\omega\exp(-i\omega\lambda)\left[\frac{G^{(+)}(\omega)}{(i\omega-0)^2}-\frac{(G^{(-)}(\omega))^{-1}}{(i\omega+0)^2}\right]q(\lambda);$$

$$2\Gamma q(\lambda) = T\int A(\lambda,\lambda')\ln(1+\exp(-|\kappa(\lambda')|/T))\,d\lambda'$$
$$-T\sum_{j=1}^{n-1}\int d\lambda' B_j(\lambda,\lambda')\ln(1+\exp(\varepsilon_1^{(j)}/T)).$$

Here we use the notations of §§7 and 9 and

$$A(\lambda\lambda') = \frac{i}{(2\pi)^2}\iint d\omega\, d\omega' \exp(-i\omega\lambda + i\omega'\lambda')(G^{(+)}(\omega'))^{-1}$$
$$\times\left[\frac{G^{(+)}(\omega)}{\omega-\omega'+i0} - \frac{(G^{(-)}(\omega))^{-1}}{\omega-\omega'-i0}\right],$$
$$B(\lambda\lambda') = \frac{i}{(2\pi)^2}\iint d\omega\, d\omega' \exp(-i\omega\lambda + i\omega'\lambda')s_j(\omega')G^{(-)}(\omega')$$
$$\times\left[\frac{G^{(+)\omega}(\omega)}{\omega-\omega'+i0} - \frac{(G^{(-)}(\omega))^{-1}}{\omega-\omega'-i0}\right],$$

$$\rho_j^i(\lambda) = \frac{i}{(2\pi)^2}\int d\omega \exp(-i\lambda\omega)s_j(\omega)G^{(+)}(\omega)\int\frac{d\omega'}{\omega-\omega'-i0}(G^{(+)}(\omega'))^{-1},$$
$$\epsilon_f^*(T) = \epsilon_f^* + 2\Gamma q(0).$$

(4) The authors of the present paper have obtained the exact solution of the Kondo problem for the orbital singlet or so-called multichannel Kondo problem referred to in §2.2.2 for arbitrary number of channels $n$ and impurity spin $S$ (Wiegmann and Tsvelick, 1983, *JETP Lett.* **38,** 489, and *Z. Phys.*, to be published, and Tsvelick, *J. Phys.* C, to be published). It is amazing that the hypothesis of Nozières and Blandin (1980) that the fixed point of the hamiltonian (2.2.7) at $n>2S$ is finite and the model exhibits the scaling power law at small energy scale, proves to be valid. The basic results are as follows.

The magnetization as a function of the magnetic field and the thermodynamics equations are

$$M_{\text{imp}}(H) = S - \frac{in}{4\pi^{3/2}}\int\frac{d\omega}{\omega-i0}\exp(2i\omega\ln(H/T_H))\left(\frac{i\omega+0}{e}\right)^{i\omega n}$$
$$\times\exp(\pi|\omega|(n-\max(n,2S)))\frac{\sinh(\pi\min(n,2S)\omega)}{\sinh(\pi n\omega)}\,\frac{\Gamma(1+i\omega)\Gamma(\frac{1}{2}-i\omega)}{\Gamma(1+i\omega n)},$$
$$\varphi_n = -\delta_{n2S}\exp(\pi\lambda) + \int\frac{d\lambda'\ln(1+\exp(\varphi_{n+1}(\lambda)))(1+\exp(\varphi_{n-1}(\lambda)))}{2\cosh\pi(\lambda-\lambda')},$$
$$\varphi_0 = -\infty,\quad \lim_{n\to\infty}\frac{\varphi_n}{n} = \frac{H}{T},$$

which generalize eqns. (5.1.33) and (6.1.60)–(6.1.62).

At $n<2S$ the ground state of the impurity is $(2S+1-n)$-fold degenerate.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

At low energy scales $H, T \ll T_K$ the free energy is

$$\mathscr{F}_{\text{imp}} = -T\ln(2S-n+1) - \frac{T}{3}\left(S-\frac{n}{2}\right)\left(S-\frac{n}{2}+1\right) \times \left[\frac{H^2}{2T^2}\left(1-\frac{1}{\ln(T/T_K)}\right) - \frac{\pi^2}{\ln^3(T/T_K)}\right].$$

At $n=2S$ the ground state is singlet and the Fermi-liquid law holds at low energies:

$$\mathscr{F}_{\text{imp}} = -\frac{T^2}{2T_K}\left(\frac{\pi n}{n+2} + \frac{1}{2\pi}\left(\frac{H}{T}\right)^2\right).$$

This proves eqn. (3.1.48).

At $n>2S$ the new scaling regime arises: the ground state is also singlet but with infinite susceptibility given by the scaling law

$$\mathscr{F}_{\text{imp}} = -T\ln\left(\frac{\sin[\pi(S+1)/n+2]}{\sin(\pi/n+2)}\right) - \sum_{K=2}^{\infty} \alpha_K(H,T)(T/T_K)^{2K/n+2}$$

Note that the limits $H\to 0$, $T\to 0$ do not commute:

$$\lim_{H/T\to 0} \alpha_K(H,T) = \alpha_K; \quad \lim_{T/H\to 0} \alpha_K(H,T)\left(\frac{T}{T_K}\right)^{(2K/n+2)} = \beta_K\left(\frac{H}{T_K}\right)^{K/n}.$$

So all basic models enumerated in § 2 have been solved exactly on the basis of the Bethe-Ansatz approach.

## References


Abrisokov, A. A., 1965, *Physics*, **2**, 5; 1969, *Usp. fiz. Nauk*, **97**, 403 (*Soviet Phys. Usp.*).

Abrisokov, A. A., Gor'kov, L. P., and Dsyaloschinski, I. E., 1965, *Methods of Quantum Field Theory in Statistical Physics* (Oxford: Pergamon Press).

Abrisokov, A. A., and Migdal, A. A., 1970, *J. low-temp. Phys.*, **3**, 519.

Allen, J. W., Oh, S.-J., Lindau, I., Lawrence, J. M., Johansson, L. I., and Hangström, S. B., 1981, *Phys. Rev. Lett.*, **46**, 1100.

Anderson, P. W., 1961, *Phys. Rev.*, **124**, 41; 1970, *J. Phys.* C, **3**, 2346; 1978, *Rev. mod. Phys.*, **50**, 191.

Anderson, P. W., and Clogston, A. M., 1962, *Bull. Am. phys. Soc.*, **6**, 124.

Anderson, P. W., and Yuval, G., 1969, *Phys. Rev. Lett.*, **23**, 89; 1971, *J. Phys.* C, **4**, 607; 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 217.

Anderson, P. W., Yuval, G., and Hamann, D. R., 1970a, *Solid St. Commun.*, **8**, 1033; 1970b, *Phys. Rev.* B, **1**, 4664.

Andrei, N., 1980, *Phys. Rev. Lett.*, **45**, 379; 1982, *Phys. Lett.* A, **87**, 299.

Andrei, N., Furuya, K., and Lowenstein, J. H., 1983, *Rev. mod. Phys.*, **55**, 331.

Andrei, N., and Lowenstein, J. H., 1979, *Phys. Rev. Lett.*, **43**, 1698; 1980, *Phys. Lett.* B, **90**, 106; 1981, *Phys. Rev. Lett.*, **46**, 356.

Anselm, A. A., 1959, *Zh. éksp. teor. Fiz.*, **35**, 1522 (*Soviet Phys. JETP*).

Arinstein, A., 1980, *Phys. Lett.* B, **95**, 280.

Armbrüster, H., Lohneysen, H. V., Riblet, G., and Steglich, F., 1974, *Solid St. Commun.*, **14**, 55.

Babelon, O., de Vega, H. J., and Viallet, C. M., 1982, preprint LPTHE 82/10.

Baberschke, K., and Tsang, E., 1980, *Phys. Rev. Lett.*, **45**, 1512.

Babujan, H. M., 1982, *Phys. Lett.* A, **90**, 479.


Downloaded by [University of Chicago Library] at 18:11 18 August 2015

BADER, S. D., PHILLIPS, N. E., MAPLE, M. B., and LUENGO, C. A., C. A., 1975, *Solid St. Commun.*, **16,** 1263.
BAKANOWSKI, S., CROW, J. E., and MIHALISIN, T., 1977, *Solid St. Commun.*, **22,** 241.
BARABANOV, A. F., KIKOIN, K. A., MAKSIMOV, L. A., 1974, *Teor. Mat. Fiz.*, **20,** 364 (*Soviet Theor. Math. Phys.*).
BARABANOV, A. F., and TSVELICK, A. M., 1979, *Fiz. tverd. Tela*, **21,** 3214 (*Soviet Phys. solid St.*).
BAXTER, R. J., 1972 a, *Ann. Phys.*, **70,** 193; 1972 b, *Ibid.*, **70,** 323; 1972 c, *Ibid.*, **76,** 1; 1972 d, *Ibid.*, **76,** 25; 1972 e, *Ibid.*, **76,** 48; 1978, *Phil. Trans. R. Soc.*, **289,** 315; 1980, *Fundamental Problems of Statistical Mechanics*, Vol. V, edited by E. G. D. Cohen (Amsterdam: North-Holland).
BAXTER, R. J., and PEARCE, P. A., 1982, *J. Phys.* A, **15,** 897.
BELAVIN, A. A., 1979, *Phys. Lett.* B, **87,** 117; 1980, *Nucl. Phys.* **180**, 189.
BENOIT, A., and FLOQUET, J., 1976, *Physica* B, **86–88,** 519.
BEREZIN, F. A., and SUSCHKO, V. N., 1965, *Zh. éksp. teor. Fiz.* **48,** 1293 (*Soviet Phys. JETP*).
BEREZIN, F. A., POKHIL, G. P., and FINKELBERG, V. M., 1964, *Vest. Mosk. Gos. Univ.*, **1,** 21.
BERG, B., KAROWSKI, M., KURAK, V., and WISZ, P., 1978, *Nucl. Phys.*, **134,** 125.
BERGER, A., HAEN, P., HOLTZBERG, F., LAPIERRE, F., MIGNOT, J. M., PENNEY, T., PENA, O., and TOURNIER, R., 1979, *J. Phys. Colloque* C5, **40,** 364.
BERGNOFF, H., and THACKER, H. B., 1979, *Phys. Rev.* D, **19,** 3666.
BETHE, H., 1931, *Z. Phys.*, **71,** 205.
BLANDIN, A., 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 58.
BLOOMFIELD, P. E., and HAMANN, D. R., 1967, *Phys. Rev.*, **164,** 856.
BOYCE, J. B., and SLICHTER, C. P., 1974, *Phys. Rev. Lett.*, **32,** 61.
BRENIG, W., and GÖTZE, W., 1968, *Z. Phys.*, **217,** 188.
BRENIG, W., and ZITTARTZ, J., 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 185.
BRINGER, A., and LUSTFELD, H., 1977, *Z. Phys.* B, **28,** 213.
COQBLIN, B., and SCHRIEFFER, J. R., 1969, *Phys. Rev.*, **185,** 847.
CORNUT, B., and COQBLIN, B., 1972, *Phys. Rev.* B, **5,** 4541.
CRAGG, D. M., and LLOYD, P., 1979, *J. Phys.* C, **12,** 3301.
CRAGG, D. M., LLOYD, P., and NOZIÈRES, P., 1980, *J. Phys.* C, **13,** 803.
CROFT, M., WEAVER, J. H., PETERMAN, D. J., and FRANCIOSI, A., 1981, *Phys. Rev. Lett.*, **46,** 1104.
DAYBELL, M. D., 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 121.
DEENADAS, C., THOMPSON, A. N., CRAIG, D. K., and WALLACE, W. E., 1971, *J. Phys. Chem. Solids*, **32,** 1853.
DE GENNES, P. G., 1962, *J. Phys., Paris*, **23,** 510.
DES CLOIZEAUX, J., and GAUDIN, M., 1966, *J. Math. Phys.*, **7,** 1384.
DES CLOIZEAUX, J., and PEARSON, J. J., 1962, *Phys. Rev.*, **128,** 2131.
DESGRANGES, H.-U., and SCHOTTE, K.-D., 1982, *Phys. Lett.* A, **91,** 240.
DESTRI, C., and LOWENSTEIN, J. H., 1982, *Nucl. Phys.* B, **205,** F55, 369.
DREW, H. D., and DOEZEMA, R. E., 1972, *Phys. Rev. Lett.*, **28,** 1581.
DREYER, R., KRUG, T., and WINZER, K., 1982, *J. low-temp. Phys.*, **48,** 111.
FADDEEV, L. D., 1980, *Soviet Scientific Review of Mathematical Physics*, Vol. C1, edited by S. P. Novicov (New York: Harwood Academic), p. 107.
FADDEEV, L. D., and SKLYANIN, E. K., 1978, *Soviet Phys. Dokl.*, **243,** 902.
FADDEEV, L. D., and TAKHTAJAN, L. A., 1981, *Phys. Lett.* A, **85,** 375.
FATEEV, V. A., 1980, unpublished.
FATEEV, V. A., and WIEGMANN, P. B., 1981 a, *Phys. Lett.* A, **81,** 179; 1981 b, *Phys. Rev. Lett.*, **46,** 356.
FELSCH, W., 1977, *Physica* B, **86–88,** 501 (ICM-76); 1978, *Z. Phys.* B, **29,** 211.
FELSCH, W., and WINZER, K., 1973, *Solid St. Commun.*, **13,** 569.
FELSCH, W., WINZER, K., and MINNEGERODE, G. V., 1975, *Z. Phys.* B, **21,** 151.
FILYOV, V. M., 1977, *Teor. Mat. Fiz.*, **33,** 119.
FILYOV, V. M., TSVELICK, A. M., and WIEGMANN, P. B., 1981, *Phys. Lett.* A, **81,** 115; 1982, *Ibid.* A, **89,** 157.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

FILYOV, V. M., and WIEGMANN, P. B., 1980, *Phys. Lett.* A, **76,** 283.
FISHER, K., 1970, *Springer Tracts in Modern Physics*, Vol. 54, edited by G. Höhler (Berlin: Springer-Verlag).
FLICKER, M., and LIEB, E. H., 1967, *Phys. Rev.*, **161,** 179.
FLOQUET, J., 1978, *Progress in Low-Temperature Physics*, Vol. VIIB, edited by D. F. Brewer (Amsterdam: North-Holland), p. 650.
FOWLER, M., and ZAWADOWSKI, A., 1971, *Solid St. Commun.*, **9,** 471.
FOWLER, M., and ZOTOS, X., 1981, *Phys. Rev.* B, **24,** 2634.
FRIEDEL, J., 1958, *Nuovo Cim.* (Suppl.), **7,** 287.
FURUYA, K., and LOWENSTEIN, J. M., 1982, *Phys. Rev.* B, **25,** 5935.
GAUDIN, M., 1967, *Physics Lett.* A, **24,** 55; 1967, Thesis, Fac. des Sciences, d'Orsay University of Paris (unpublished); 1971 a, *Phys. Rev. Lett.*, **21,** 1301; 1971 b, *Phys. Rev.* A, **4,** 386.
GRIFFITH, R., 1964, *Phys. Rev.* A, **133,** 768.
GRÜNER, G., 1974, *Adv. Phys.*, **23,** 941.
GRÜNER, G., and ZAWADOWSKI, A., 1974, *Rep. Prog. Phys.*, **37,** 1497; 1978, *Progress in Low-Temperature Physics*, Vol. VIIB, edited by D. F. Brewer (Amsterdam: North Holland).
HAISENBERG, W., 1926, *Z. Phys.*, **49,** 619.
HALDANE, F. D. M., 1978 a, *Phys. Rev. Lett.*, **40,** 416; 1978 b, *J. Phys.* C, **11,** 5015.
HAMANN, D. R., and SCHRIEFFER, J. R., 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 237.
HEEGER, A. J., 1969, *Solid State Physics*, Vol. 23, edited by F. Seitz, D. Turnbull and H. Ehrenreich (New York: Academic Press), p. 283.
HEWSON, A. C., 1982, *J. Phys.* C, **15,** L611.
HEWSON, A. C., RASUL, J. W., and NEWNS. D. M., 1983, *Phys. Lett.* A, **92,** 311.
HIDA, K., 1981, *Phys. Lett.* A, **84,** 2634.
HIDA, K., IMADA, M., and ISHIKAWA, M., 1983, *J. Magn. magn. Mater.*, **31–34,** 541.
HIRSHKOFF, E. C., SYMKO, O. G., and WHEATLEY, J. C., 1971, *J. low-temp. Phys.*, **5,** 155.
HIRST, L. L., 1978, *Adv. Phys.*, **27,** 231.
HÖNERKAMP, J., WEBER, P., and WIESLER, A., 1979, *Nucl. Phys.* B, **152,** 266.
HUBBARD, J., 1965, *Proc. R. Soc.* A, **285,** 542.
HULTEN, L., 1938, *Arkiv. Mat. Astr. Fys.*, A, **26,** N11.
ISHII, H., 1970, *Prog. theor. Phys.*, **43,** 578; 1976, *Ibid.*, **55,** 1373.
JAPARIDZE, G., and NERSISYAN, A., 1981, *Phys. Lett.* A, **85,** 23.
JAPARIDZE, G., NERSISYAN, A., and WIEGMANN, P. B., 1982, *Physica scripta*, **27,** 5; 1983, *Nucl. Phys.*, BFS in press.
JAYAPRAKASH, C., KRISHNA-MURTHY, H. R., and WILKINS, J. W., 1981, *Phys. Rev. Lett.*, **47,** 737.
JOHNSON, J. D., 1974, *Phys. Rev.* A, **9,** 1743.
JOHNSON, J. D., KRINSKY, S., and MCCOY, B., 1973, *Phys. Rev.* A, **8,** 2526.
JOHNSON, J. D., and MCCOY, B., 1972, *Phys. Rev.* A, **6,** 1613.
KAROWSKI, M., THUN, H.-J., TRUONG, T. T., and WEISZ, P. H., 1977, *Phys. Lett.* B, **67,** 321.
KAWAKAMI, N., and OKIJI, A., 1982 a, *Phys. Lett.* A, **86,** 483; 1982 b, *J. phys. Soc. Japan*, **51,** 1145; 1982 c, *Solid St. Commun.*, **43,** 365.
KHOMSKI, D. I., 1979, *Usp. fiz. Nauk*, **129,** 443 (*Soviet Phys. Usp.*).
KONDO, J., 1962, *Prog. theor. Phys., Osaka*, **28,** 846; 1969, *Solid State Physics*, Vol. 23, edited by F. Seitz, D. Turnbull and H. Ehrenreich (New York: Academic Press), p. 183; 1964, *Prog. theor. Phys., Osaka*, **32,** 37.
KOREPIN, V. E., 1979, *Teor. Mat. Fiz.*, **41,** 169.
KRAMERS, H. A., WANNIER, G. H., 1941, *Phys. Rev.*, **60,** 252.
KREIN, M., 1962, *Am. Math. Soc. Transl.*, ser. 2, **22,** 163.
KRISHNA-MURTHY, H. R., WILKINS, K. W., and WILSON, K. G., 1975, *Phys. Rev. Lett.*, **35,** 1101; 1980 a, *Phys. Rev.* B, **21,** 1003; 1980 b, *Ibid.* B, **21,** 1044.
KRIVNOV, V. YA., and OVCHINNIKOV, A. A., 1974, *Zh. éksp. teor. Fiz.*, **67,** 1568 (*Soviet Phys. JETP*).
KULISH, P. P., and RESHETIKHIN, N. YU., 1980, *Zap. nauch. semin. LOMI*, **101,** 112; 1981, *Zh. éksp. teor. Fiz*, **80,** 214 (*Soviet Phys. JETP*).
KULISH, P. P., RESHETIKHIN, N. YU., and SKLYANIN, E. K., 1981, *Lett. Math. Phys.*, **5,** 393.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

KULISH, P. P., and SKLYANIN, E. K., 1979, *Phys. Lett.* A, **70,** 461; 1980, *Zap. nauch. semin. LOMI*, **95,** 129; 1981, *Lecture Notes in Physics*, Vol. 151, edited by J. Hietarinta and C. Montonen (New York: Springer-Verlag).
LAI, C. C., and SHI, W. Y., 1981, *J. Phys.* C, **14,** L915.
LANGRETH, D. C., 1966, *Phys. Rev.*, **150,** 516.
LARKIN, A. I., KHMEL'NITSKII, D. E., 1970, *Zh. éskp. teor. Fiz.*, **58,** 1789 (*Soviet Phys. JETP*, **31,** 958).
LIEB, E. H., 1963, *Phys. Rev.*, **130,** 1616; 1967 a, *Phys. Rev. Lett.*, **18,** 692; 1967 b, *Ibid.*, **18,** 1046; 1967 c, *Ibid.*, **19,** 108; 1967 d, *Phys. Rev.*, **162,** 162.
LIEB, E. H., and LINIGER, W., 1963, *Phys. Rev.*, **130,** 1605.
LIEB, E. H., and WU, F. Y., 1968, *Phys. Rev. Lett.*, **20,** 1445; 1972, *Phase Transitions and Critical Phenomena*, edited by S. Domband and M. S. Green (New York: Academic Press).
LIPATOV, L. N., and BUHVOSTOV, A. P., 1980, *Pis'ma Zh. éskp. teor Fiz.*, **31,** 138 (*Soviet Phys. JETP Lett.*).
LOEWENHAUPT, M., RAINFORD, B. D., and STEGLICH, F., 1979, *Phys. Rev. Lett.*, **42,** 1709.
LUENGO, C. A., HUBER, J. G., MAPLE, M. B., and ROTH, M., 1974, *Phys. Rev. Lett.*, **32,** 54.
LUSZIK-BHADRA, M., BARTH, H. J., BLOCKSCH, H. J., NETZ, G., RIEGEL, D., and BERTSCHAT, H. H., 1981, *Phys. Rev. Lett.*, **47,** 871.
LUTHER, A., and EMERY, V. J., 1974, *Phys. Rev. Lett.*, **33,** 589.
MCGUIRE, J. B., 1964, *J. Math. Phys.*, **5,** 622; 1966, *Ibid.*, **7,** 123.
MALEEV, S. V., 1966, *Zh. éskp. teor. Fiz.*, **51,** 1940 (*Soviet Phys. JETP*, **24,** 1300); 1967, *Ibid.*, **53,** 1038 (*Ibid.*, **26,** 620).
MAPLE, M. B., 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 289; 1976, *J. appl. Phys.*, **9,** 179.
MAPLE, DE LONG, L. E., and SALES, B. C., 1978, *Handbook on the Physics and Chemistry of Rare Earths*, Vol. 1, edited by K. A. Gshneider, Jr and Le Roy Eyring (Amsterdam: North-Holland), p. 797.
MAPLE, M. B., FERTING, W. A., MOTA, A. C., WOHLLEBEN, D., and FITZGERALD, R., 1972, *Solid St. Commun.*, **11,** 829.
MAPLE, M. B., and FISK, Z., 1968, *Proc. 11th Int. Conf. Low-Temp. Phys.*, St. Andrews, Scotland, Vol. 2, edited by J. F. Allen, D. M. Findlayson and D. M. McCall, p. 1288.
MAPLE, M. B., and WITTIG, J., 1971, *Solid St. Commun.*, **8,** 1611.
MATSUURA, T., ICHINOSE, S., and NAGAOKA, Y., 1978, *Prog. theor. Phys., Osaka*, **57,** 713.
MATTIS, D., 1967, *Phys. Rev. Lett.*, **19,** 1478.
MELNICOV, N. I., 1982 a, *Soviet Phys. JETP Lett.*, **35,** 414; 1982 b, unpublished.
MIHALY, L. M., and ZAWADOWSKI, A., 1978, *J. Phys. Lett., Paris*, **39,** L483.
MILLS, D. L., BEAL-MONOD, M.-T., and LEDERER, P., 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 89.
MOESER, J. H., STEGLICH, F., and VON MINNIGERODE, G., 1974, *J. low-temp. Phys.*, **15,** 91.
MORANDI, G., GALLEANI D'AGLIANO, E., NAPOLI, F., and RATTO, C. F., 1974, *Adv. Phys.*, **23,** 868.
MORANDI, G., NAPOLI, F., and RATTO, C. F., 1981, *Theoretical Review of the Friedel-Anderson Model* (Ferraro, University publishers).
MÜLLER-HARTMANN, E., and ZITTARTZ, J., 1971, *Phys. Rev. Lett.*, **26,** 428.
MURAO, T., and MATSUBARA, T., 1957, *Prog. theor. Phys., Osaka*, **18,** 215.
MYERS, H. P., WALLDEN, L., and KALSSON, A., 1968, *Phil. Mag.*, **18,** 725.
NAGAOKA, Y., 1965, *Phys. Rev.* A, **138,** 1112; 1969, *Prog. theor. Phys., Osaka*, **41,** 586.
NARATH, A., 1970, *J. appl. Phys.*, **41,** 1122; 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 149.
NOZIÈRES, P., 1974, *J. low-temp. Phys.*, **17,** 13; 1975, *Proc. 15th Conf. Low. Temp. Phys.*, Vol. 5, edited by Krusius and Vuorio (Amsterdam: North-Holland), p. 339.
NOZIÈRES, P., and BLANDIN, A., 1980, *J. Phys. Paris*, **41,** 193.
OGIEVETSKII, E., TSVELICK, A. M., and WIEGMANN, P. B., 1983, *J. Phys.* C, **16,** L797.
OKIJI, A., and KAWAKAMI, N., 1982 a, *Solid St. Commun.*, **43,** 365; 1982 b, *J. phys. Soc. Japan*, **51,** 3192.
OLIVEIRA, L. N., and WILKINS, J. W., 1981, *Phys. Rev. Lett.*, **47,** 1553.
ONSAGER, L., 1944, *Phys. Rev.*, **65,** 117.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

ORBACH, R., 1958, *Phys. Rev.*, **112,** 309.
OVCHINNICOV, A. A., 1969 a, *Zh. éskp. teor Fiz.*, **56,** 1354 (*Soviet Phys JETP*); 1969 b, *Ibid.*, **57,** 2137.
PUGA, M. W., 1980, *J. Math. Phys.*, **21,** 2307.
RAJAN, V. T., LOWENSTEIN, J. H., and ANDEI, N., 1982, *Phys. Rev. Lett.*, **49,** 497.
RASUL, J. W., 1982, *Valence Instabilities*, edited by P. Wachter and H. Boppart (Amsterdam: North-Holland).
RESHETIKHIN, N. YU., 1983, *Zh. éksp. teor Fiz.*, **84,** 1190 (*Soviet Phys. JETP*).
RIBLET, G., and WINZER, K., 1971, *Solid St. Commun.*, **11,** 175.
RIZZUTO, C., 1974, *Rep. Prog. Phys.*, **37,** 147.
SAKURAI, A., 1978, *Phys. Rev.*, **17,** 1195.
SAKURAI, A., and YOSIDA, 1979, *Prog. theor. Phys., Osaka*, **61,** 1597.
SAMWER, K., and WINZER, K., 1976, *Z. Phys.* B, **25,** 269.
SCHANKAR, R., and WITTEN, E., 1978, *Phys. Rev.* D, **17,** 2134.
SCHLOTTMANN, P. A., 1978 a, *J. Magn. magn. Mater.*, **7,** 72; 1978 b, *J. Phys., Paris*, **39,** CG-1486; 1981, *Solid St. Commun.*, **38,** 1087; 1982, *Z. Phys.* B, **49,** 109; 1983, *Phys. Rev. Lett.*, **50,** 1697.
SCHOTTE, K.-D., 1970, *Z. Phys.*, **230,** 99.
SCHOTTE, K.-D., and SCHOTTE, U., 1969, *Phys. Rev.*, **182,** 479; 1971, *Ibid.* B, **4,** 2228; 1975, *Phys. Lett.* A, **55,** 38.
SCHRIEFFER, J. R., 1967, *J. appl. Phys.*, **38,** 1143.
SCHRIEFFER, J. R., and WOLF, P. A., 1966, *Phys. Rev.*, **149,** 491.
SCHULZ, H., 1982, *J. Phys.* C, **15,** L37.
SHIBA, H., 1975, *Prog. theor. Phys., Osaka*, **54,** 967.
SKLYANIN, E. K., 1978, *Soviet Phys. Dokl.*, **241,** 107; 1980, *Zap. nauch. semin. LOMI*, **95,** 55.
SKLYANIN, E. K., TAKHTAJAN, L. A., and FADDEEV, L. D., 1979, *Teor. Mat. Fiz.*, **40,** 194.
SOULETIE, I., and TOURNIER, R., 1969, *J. low-temp. Phys.*, **1,** 95.
STASÜK, I. V., and SLOBODYAN, P. M., 1974, *Teor. Mat. Fiz.*, **19,** 423.
STEGLICH, F., 1976, *Z. Phys.* B, **23,** 331; 1977 *Festkörperproblem* (*Advances in Solid State Physics*), Vol. XVII, edited by J. Treusch (Braunschweig: Vieweg), p. 319.
STEGLICH, F., and ARMBRÜSTER, 1972, *Solid St. Commun.*, **11,** 1445.
STEGLICH, F., FRANZ, W., SENKEN, W., and LOEWENHAUPT, M., 1977, *Physica* B, **86–88,** 503.
STROGANOV, V. G., 1979, *Phys. Lett.* A, **74,** 116.
SUGAWARA, T., 1965, *J. phys. Soc. Japan.*, **20,** 2252.
SUGAWARA, T., and EGUCHI, H., 1966, *J. phys. Soc. Japan.*, **23,** 965.
SUHL, H., 1965 a, *Physics*, **2,** 39; 1965 b, *Phys. Rev.* A, **138,** 515; 1966, *Ibid.*, **141,** 483.
SUTHERLAND, B., 1968, *Phys. Rev. Lett.*, **20,** 98; 1970, *J. Math. Phys.*, **11,** 3183; 1975, *Phys. Rev.* B, **12,** 3795.
SUTHERLAND, B., and MATTIS, D., 1981, *Phys. Rev.* A, **24,** 1194.
TAKAHASHI, M., 1970 a, *Prog. theor. Phys., Osaka*, **44,** 899; 1970 b, *Ibid.*, **44,** 348; 1971 a, *Ibid.*, **46,** 401; 1971 b, *Ibid.*, **46,** 1388; 1972, *Ibid.*, **47,** 69; 1973, *Ibid.*, **50,** 1519; 1974 a, *Ibid.*, **51,** 1348; 1974 b, *Ibid.*, **52,** 103.
TAKAHASHI, M., and SUZUKI, M., 1972, *Prog. theor. Phys., Osaka*, **48,** 2187.
TAKHTAJAN, L. A., 1981, *Zap. nauch. semin. LOMI*, **101,** 158; 1982, *Phys. Lett.* A, **87,** 479.
TAKHTAJAN, L. A., and FADDEEV, L. D., 1979, *Usp. mat. Nauk*, **34,** 13 (*Soviet Math. Usp.*); 1981 a, *Zap. nauch. semin. LOMI*, **109,** 134; 1981 b, *Phys. Lett.*, **85,** 375.
TETELMAN, M., 1982, *Zh. éskp. teor Fiz.*, **82,** 528 (*Soviet Phys. JETP*).
THACKER, H. B., 1981, *Rev. mod. Phys.*, **53,** 253.
THACKER, H. B., and WILKINSON, D. W., 1979, *Phys. Rev.* D, **19,** 3660.
TOULOUSE, G., 1969, *C. r. hebd. Séanc. Acad. Sci., Paris*, **268,** 1200.
TSELFES, W., PAPASTAIKONDIS, C., and ROCOFYLLON, E., 1980, *Solid St. Commun.*, **33,** 531.
TSVELICK, A. M., 1979, *Zh. éksp. teor Fiz.*, **76,** 2260 (*Soviet Phys. JETP*, **46,** 1142).
TSVELICK, A. M., and BARABANOV, A. F., 1978, *Zh. éksp. teor Fiz.*, **75,** 153 (*Soviet Phys. JETP*).
TSVELICK, A. M., and WIEGMANN, P. B., 1981, *Physica* B, **107,** 379; 1982 a, *J. Phys.* C, **15,** 1707; 1982 b, *Phys. Lett.* A, **89,** 368; 1983, *J. Phys.* C, **16,** 2321.
UEDA, K., and APEL, W., 1983, *J. Phys.* C, **16,** L849.
VAKS, V. G., and LARKIN, A. I., 1961, *Zh. éksp. teor. Fiz.*, **40,** 1392 (*Soviet Phys. JETP*).

Downloaded by [University of Chicago Library] at 18:11 18 August 2015

VAN DAM, J. E., GUBBENS, P. C. M., VAN DEN BERG, G. J., 1972, *Physica*, **62,** 389.
VAN DEN BERG, G. J., 1964, *Progress in Low-Temperature Physics*, Vol. IV, edited by C. J. Gorter (Amsterdam: North-Holland), p. 194.
VARMA, C. N., 1976, *Rev. mod. Phys.*, **48,** 219.
VARMA, C. N., and YAFET, Y., 1976, *Phys. Rev.* B, **13,** 2950.
VOUSOVSKII, S., 1946, *Zh. éskp. teor. Fiz.*, **16,** 981 (*Soviet Phys. JETP*).
WALKER, L. R., 1959, *Phys. Rev.*, **116,** 1089.
WIEGMANN, P. B., 1980 a, *Soviet Phys. JETP Lett.*, **31,** 392; 1980 b, *Soviet Scientific Review*, Ser. A, Vol. 2, edited by I. M. Halatnikov (New York: Harwood Academic), p. 43; 1980 c, *Phys. Lett.* A, **80,** 163; 1981, *J. Phys.* C, **14,** 1463; 1982, *Quantum Theory of Solid State*, edited by I. M. Lifshitz (Moscow: Mir).
WIEGMANN, P. B., and FINKELSTEIN, A. M., 1978, *Zh. ésp. teor. Fiz.*, **75,** 204 (*Soviet Phys. JETP*).
WIEGMANN, P. B., FILYOV, V. M., and TSVELICK, A. M., 1982, *Soviet Phys. JETP Lett.*, **35,** 77.
WIEGMANN, P. B., and LARKIN, A. I., 1977, *Zh. éksp. teor. Fiz.*, **72,** 857 (*Soviet Phys. JETP*).
WIEGMANN, P. B., and TSVELICK, A. M., 1982, *Soviet Phys. JETP Lett.*, **35,** 100; 1983, *J. Phys.* C, **16,** 2281.
WILSON, K., 1974, *Nobel Symposia*, Vol. 24 (New York: Academic Press), p. 68; 1975, *Rev. mod. Phys.*, **47,** 773.
WINZER, K., 1973, *Z. Phys.*, **265,** 139; 1975, *Solid St. Commun.*, **16,** 521.
WOHLLEBEN, D. R., and COLES, B. R., 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 3.
WOYNAROVICH, F., 1982, *J. Phys.* A, **15,** 2985; *Ibid.* C, **15,** 6397; 1982, *Ibid.* C, **15,** 85, 97.
YAMADA, K., 1975, *Prog. theor. Phys., Osaka*, **53,** 970.
YANG, C. N., 1967, *Phys. Rev. Lett.*, **19,** 1312.
YANG, C. N., and YANG, C. O., 1966 a, *Phys. Rev.*, **150,** 321; 1966 b, *Ibid.*, **150,** 327; 1969, *J. Math. Phys.*, **10,** 1115.
YOSHIMORI, A., 1976, *Prog. theor. Phys., Osaka*, **55,** 67.
YOSHIMORI, A., and ZAWADOWSKI, A., 1982, preprint.
YOSIDA, K., and YAMADA, K., 1970, *Prog. theor. Phys., Osaka* (Suppl.), **N46,** 244; 1975, *Prog. theor. Phys., Osaka*, **53,** 1286.
YOSIDA, K., and YOSHIMORI, A., 1973, *Magnetism*, Vol. V, edited by H. Suhl (New York: Academic Press), p. 217.
YUVAL, G., and ANDERSON, P. W., 1970, *Phys. Rev.* B, **1,** 1522.
ZAITSEV, R. O., 1976, *Zh. éskp. teor. Fiz*, **70,** 1100 (*Soviet Phys. JETP*); 1977, *Fiz. tverd. Tela*, **19,** 3204 (*Soviet Phys. solid St.*).
ZAKHAROV, V. E., MANAKOV, S. V., NOVIKOV, S. P., and PITAEVSKY, L. P., 1980, *Theory of Solitons* (*Inverse Scattering Method*) (Moscow: Nauka) (English version, 1983 (New York: Plenum)).
ZAMOLODCHICOV, A. B., 1979, *Commun. math. Phys.*, **69,** 165; 1980, *Soviet Scientific Review*, Ser. A, Vol. 2, edited by I. M. Halatnikov (New York: Harwood Academic), p. 1.
ZAMOLODCHICOV, A. B., and FATEEV, V. A., 1980, *Yad. Fiz.*, **32,** 587 (*Soviet J. Nucl. Phys.*).
ZAMOLODCHIKOV, A. B., and ZAMOLODCHICOV, AI.B., 1978, *Physics Lett.* B, **72,** 481; 1979, *Ann. Phys.*, **120,** 253.
ZENER, C., 1951, *Phys. Rev.*, **81,** 440.
ZITTARTZ, J., and MÜLLER-HARTMANN, E., 1968, *Z. Phys.*, **212,** 380.
ZLATIĆ, V., and HORVATIĆ, B., 1983, *Phys. Rev.* B, **28,** 6904.
ZELLER, E., and DIEDRICH, M., 1971, *Phys. Rev.* B, **4,** 4357.

Downloaded by [University of Chicago Library] at 18:11 18 August 2015