What Happens inside a Unit Cell Matters – Effect of Umklapp Process

Wei-Cheng Lee
Department of Physics
University of Illinois at Urbana-Champaign

In collaboration with Anthony J. Leggett (UIUC)

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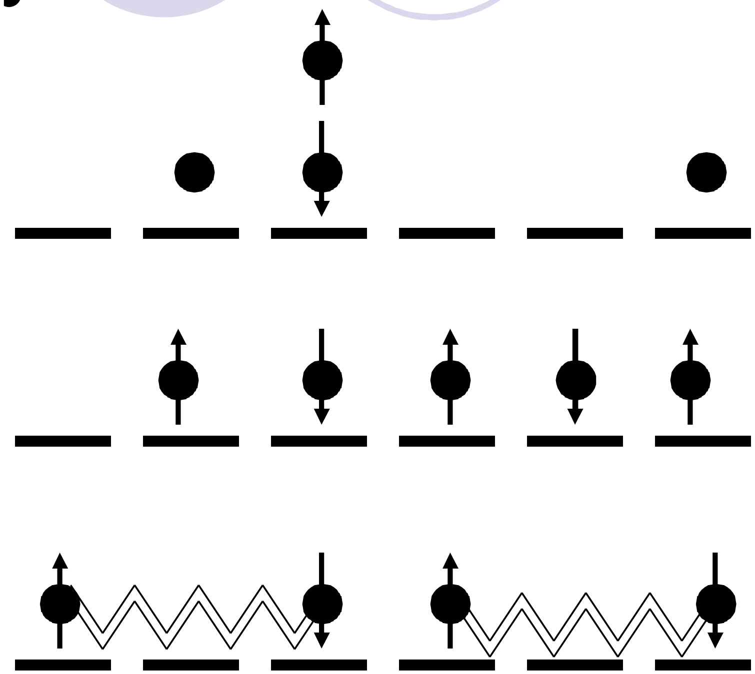
Energy Scales in Strongly Correlated Systems



$\text{Charge}: U \approx 10^3\, meV$

$\text{Magnetic}: J \approx 10^2\, meV$

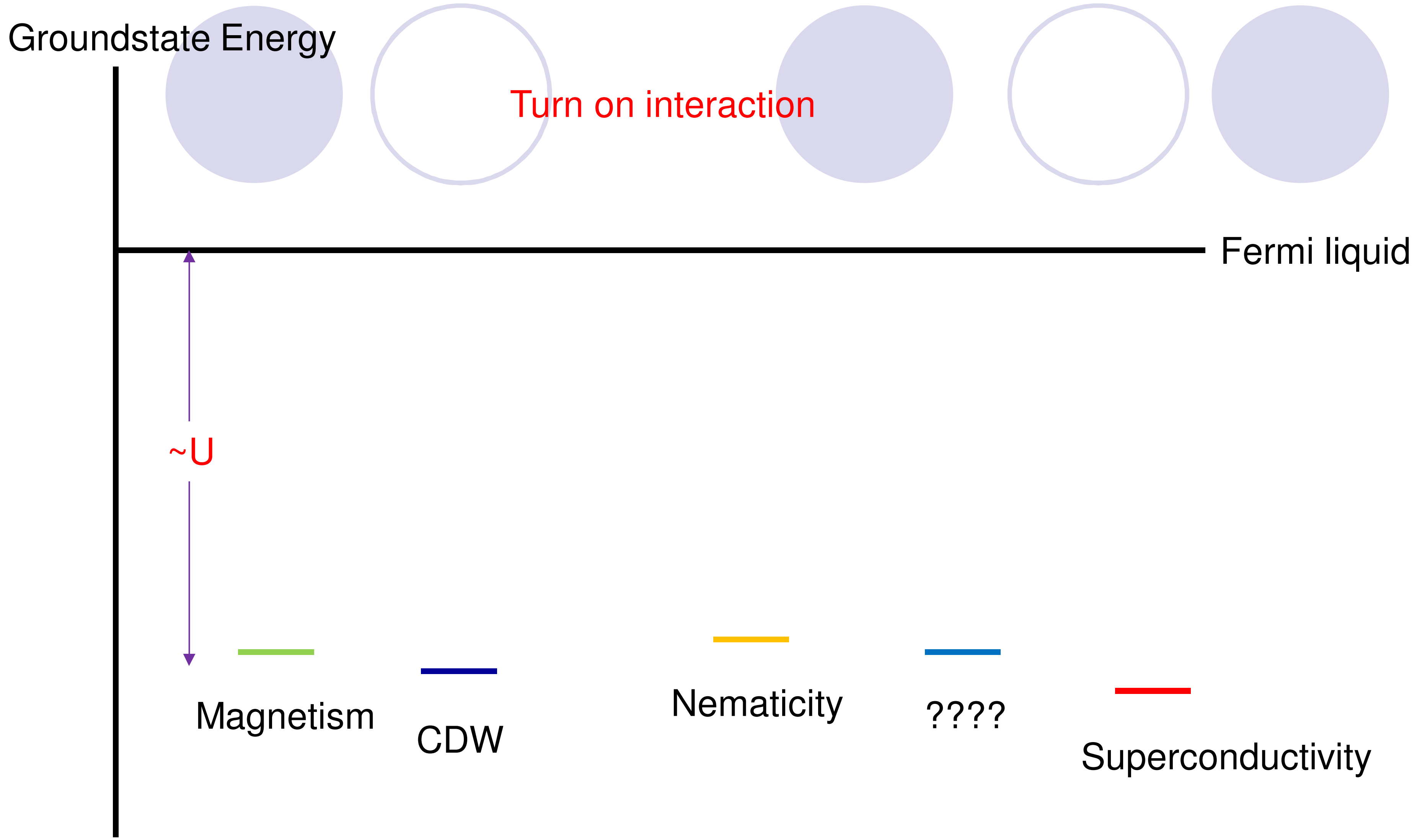
$Pairing: \Delta \approx 10^1\, meV$

$k_B T_c$

BCS Theory

Still true in strongly correlated systems?

$\text{condensation Energy } E_c < 10^0\, meV$



Why can superconductivity often win this battle in some range of phase diagram in a variety of materials?

Any interaction that is much smaller but just enough to help superconductivity to win?

Energetic Consideration

- Chester, Phys. Rev. **103**, 1693 (1956)

$$\langle \hat{H} \rangle = \langle \hat{K} \rangle + \langle \hat{V} \rangle = \frac{1}{2}\langle \hat{V} \rangle \ , \ \langle \hat{K} \rangle = -\frac{1}{2}\langle \hat{V} \rangle \ \text{(Virial Theorem)}$$

$$E_{cond} = \langle \hat{H} \rangle_N - \langle \hat{H} \rangle_S > 0 \Rightarrow \langle \hat{V} \rangle_s < \langle \hat{V} \rangle_N$$

- Leggett's extension:

$$\hat{V} = \frac{1}{2}\frac{1}{4\pi\varepsilon_0}\sum_{ij}\frac{e^2}{\varepsilon\left|\vec{r}_i - \vec{r}_j\right|} + \ldots, \quad \varepsilon = \text{dielectric constant renormaliz ed by the ionic cores}$$

If ε is the only parameter that can change,

$$\frac{\partial E_{cond}}{\partial \varepsilon} = \left\langle \frac{\partial \hat{V}}{\partial \varepsilon} \right\rangle_N - \left\langle \frac{\partial \hat{V}}{\partial \varepsilon} \right\rangle_s = \frac{1}{\varepsilon}\left(\langle \hat{V} \rangle_s - \langle \hat{V} \rangle_N \right) < 0$$

- Stronger Coulomb interaction (smaller ε) leads to larger superconducting condensation energy!!!

Short Range Coulomb Interaction

Strongly correlated systems

Electrons need to rearrange themselves locally to compromise the short range interaction

'Extended' description, e.g., band structure description, is likely breaking down and new phases like AFM, nematicity, Mottness, etc. can emerge.

How can superconductivity, a delocalized state, comprise the short range interaction??

Savings of Short Range Part of Coulomb Energy (Large q)

- Coulomb Energy:

$$H_{Coul} = \frac{1}{2\Omega}\sum_{q\neq 0} U_q \hat{\rho}_q \hat{\rho}_{-q} \equiv \frac{1}{2\Omega}\sum_{q\neq 0}\hat{V}_q \quad , \quad \hat{\rho}_q = \sum_{k,\sigma} c^{+}_{k-q,\sigma} c_{k,\sigma}$$

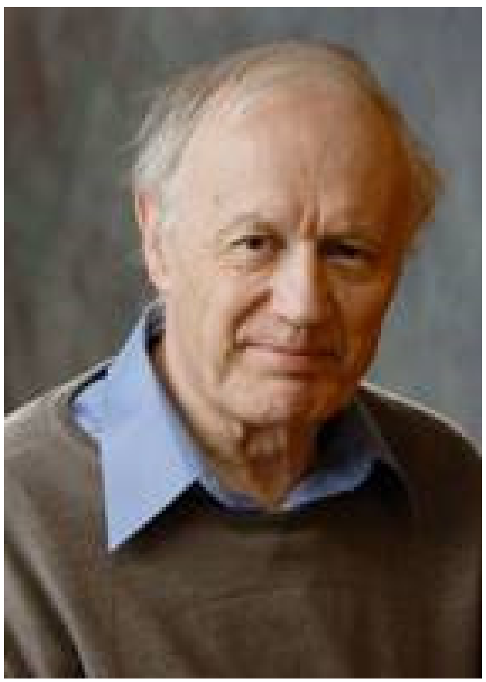
$$U_q^{3D} = \frac{e^2}{\varepsilon_0 \varepsilon_\infty q^2} \quad , \quad U_q^{2D} = \frac{e^2}{2\varepsilon_0 \varepsilon_\infty q}$$

- Superconducting condensation energy in this region:

$$E_C(\delta\langle \hat{V}_q \rangle) = U_q \langle \hat{\rho}_q \hat{\rho}_{-q} \rangle_N - U_q \langle \hat{\rho}_q \hat{\rho}_{-q} \rangle_S \approx -U_q \sum_k \Delta^*_{k+\frac{q}{2}} \Delta_{k-\frac{q}{2}}$$

- Short Range Part of Coulomb Energy can be saved in superconducting state by sign-changing gap function (for example, d-wave in cuprates)

What about long-range Coulomb Energy?

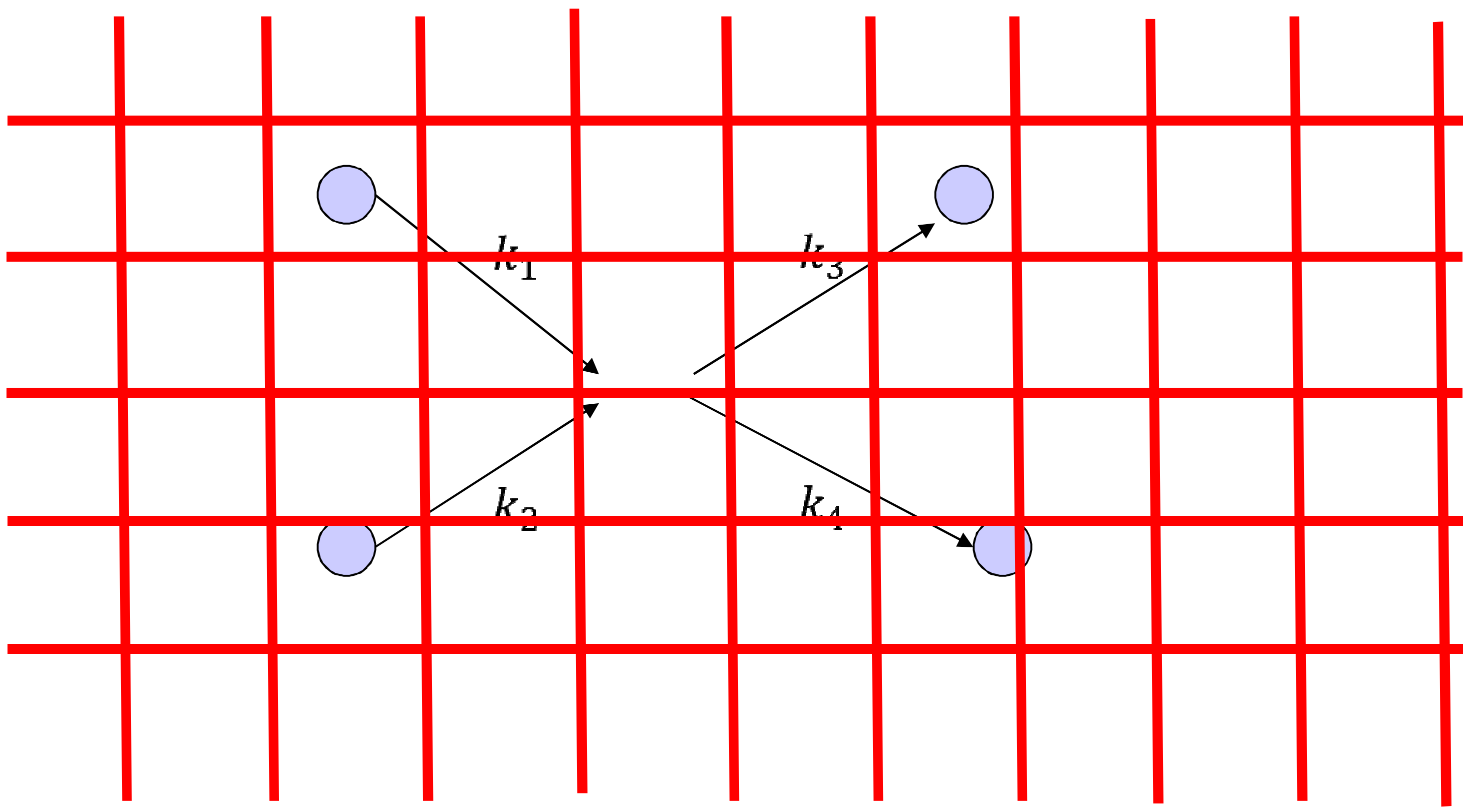


Some Arguments about the Long Range Part of Coulomb Energy

- Screening??
  - 3D → Yes, screening is effective.
  - 2D → Not necessary!!!

- Anderson’s theory (Phys. Rev. 110, 827(1958), Phys. Rev. 112, 1900(1958))
  - For small q, the plasma mode is still the only excitation in superconducting state, and its frequency is the same as the one in normal state. No change in Long-ranged Coulomb energy due to superconductivity.

Unconventional Superconductors are all built on 2D Lattice!!!



$$k_1 + k_2 + k_3 + k_4 = \boldsymbol{nK}$$

Role of Umklapp Scattering I → Sum Rule Analysis

- Rigorous sum rules for density-density response function:

$$J_{-1} \equiv \frac{2}{\pi}\int_0^{\infty} d\omega \frac{\operatorname{Im}\chi(q,\omega)}{\omega} = \chi(q,\omega=0) \quad \text{KK relation}$$

$$J_{1} \equiv \frac{2}{\pi}\int_0^{\infty} d\omega\omega \operatorname{Im}\chi(q,\omega) = \frac{nq^2}{m} \quad \text{f - sum rule}$$

$$J_{3} \equiv \frac{2}{\pi}\int_0^{\infty} d\omega\omega^3 \operatorname{Im}\chi(q,\omega) = \frac{q^2}{m^2}\langle A\rangle + q^4\frac{n^2}{m^2}\langle V_q\rangle + o(q^4)$$

$$\langle A\rangle = -\frac{1}{\pi\Omega}\sum_k (k\cdot\hat{q})^2\langle U_{-k}\rho_k\rangle \quad \text{Umklapp scattering}$$

- Applying Cauchy-Schwartz inequalities places limits on the Coulomb Energy at small q

$$\frac{\hbar\omega_p}{2} + o(q^2) \geq \langle V_q\rangle \geq \frac{\hbar\omega_p}{2}\frac{1}{\sqrt{1+\langle A\rangle/nm\omega_p^2}} + o(q^2)$$

M. Turlakov and A.J. Leggett, Phys. Rev. B 67, 044517 (2003)

Take Away Message

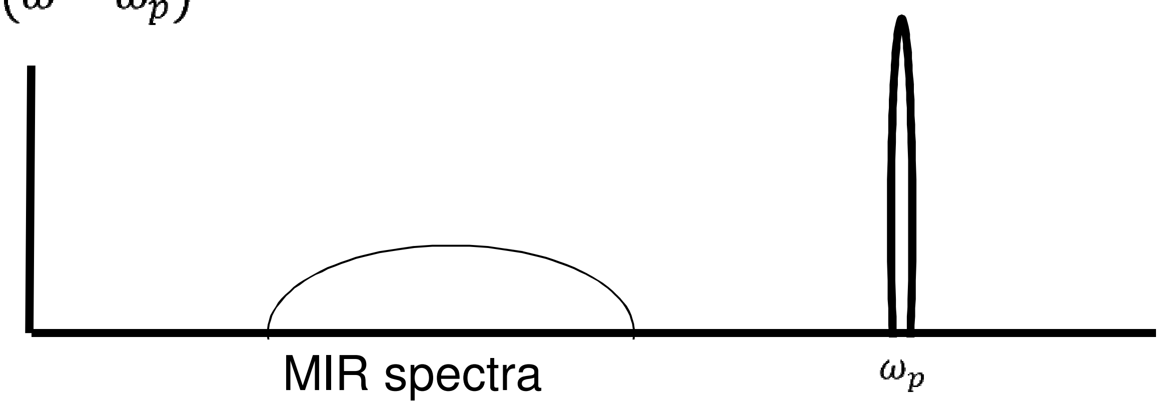
Without periodic potential, plasmon mode is IMMORTAL at small q.

$$Im\chi(q,\omega) \sim \delta(\omega - \omega_p)$$

With periodic potential (Umklapp scattering), plasmon mode is no longer IMMORTAL at small q.

$$Im\chi(q,\omega) \neq \delta(\omega - \omega_p)$$

=



$$\langle V_q \rangle = \int d\omega \, Im\chi(q,\omega) \rightarrow Could\ be\ reduced\ if\ MIR\ spectra\ is\ reduced$$

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Physics

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A "midinfrared" scenario for cuprate superconductivity

A. J. LEGGETT[a]

Department of Physics, University of Illinois, 1110 West Green Street, Urbana, IL 61801, and Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106

$\Delta\langle V_q\rangle$ *is comparable to superconducting condensate energy*!!!

Microscopic theory of the density-density correlation function with Umklapp process

Warm Up – Plasmon Excitation in Fermi Liquid

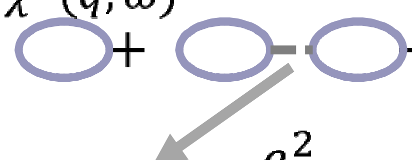
$$\chi(q, t - t') = -i\langle T_t\, \rho_q(t)\rho_q^{+}(t')\rangle$$

$$\rho_q = \sum_{k,\sigma} c_{k+q,\sigma}^{+} c_{k,\sigma}$$

Random phase approximation (RPA)

$\chi^0(q,\omega)$

$$\chi^{RPA}(q,\omega) =$$



$$+ \cdots = \frac{\chi^0(q,\omega)}{1 - v_q \chi^0(q,\omega)}$$

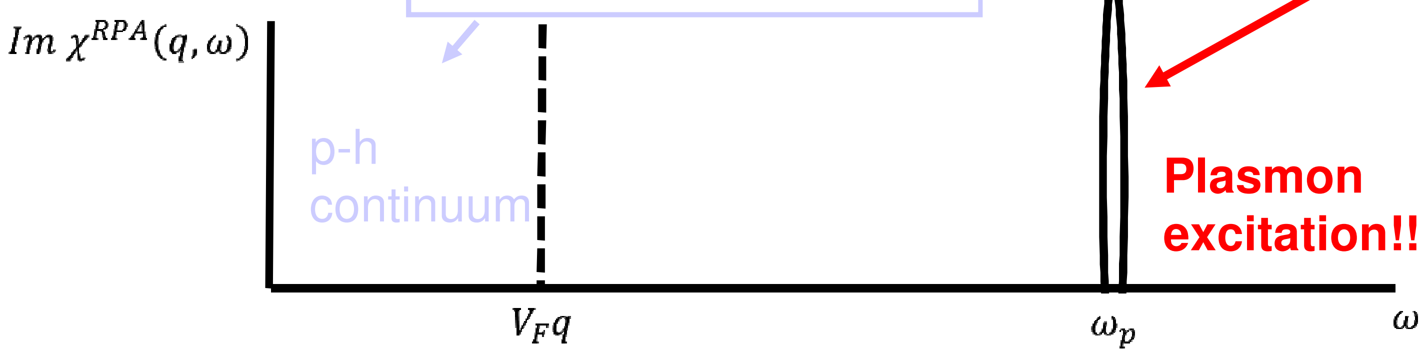
$$v_q = \frac{e^2}{4\pi\epsilon q} \quad (2D)$$

Warm Up – Plasmon Excitation in Fermi Liquid

$$\chi^0(q,\omega) = \sum_k \frac{n_F(E(k+q)-\mu) - n_F(E(k)-\mu)}{\omega + E(k) - E(k+q)}$$

$$\chi^{RPA}(q,\omega) = \frac{\chi^0(q,\omega)}{1 - v_q\chi^0(q,\omega)}$$

$$Im\ \chi^{RPA}(q,\omega) = \boxed{Re\left(\frac{1}{1 - v_q\chi^0(q,\omega)}\right) Im\chi^0(q,\omega)} + \boxed{Re\chi^0(q,\omega) Im\left(\frac{1}{1 - v_q\chi^0(q,\omega)}\right)}$$



Periodic Potential

$$H = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} c^+_{k\sigma} c_{k\sigma} + \sum_q V_q \rho_q \rho_{-q} + \sum_K \sum_{k\sigma} U_K c^+_{k\sigma} c_{k+K\sigma} + h.c.$$

$$\chi^0(q,\omega) = \sum_k \frac{n_F(E(k+q)-\mu) - n_F(E(k)-\mu)}{\omega + E(k) - E(k+q)}$$

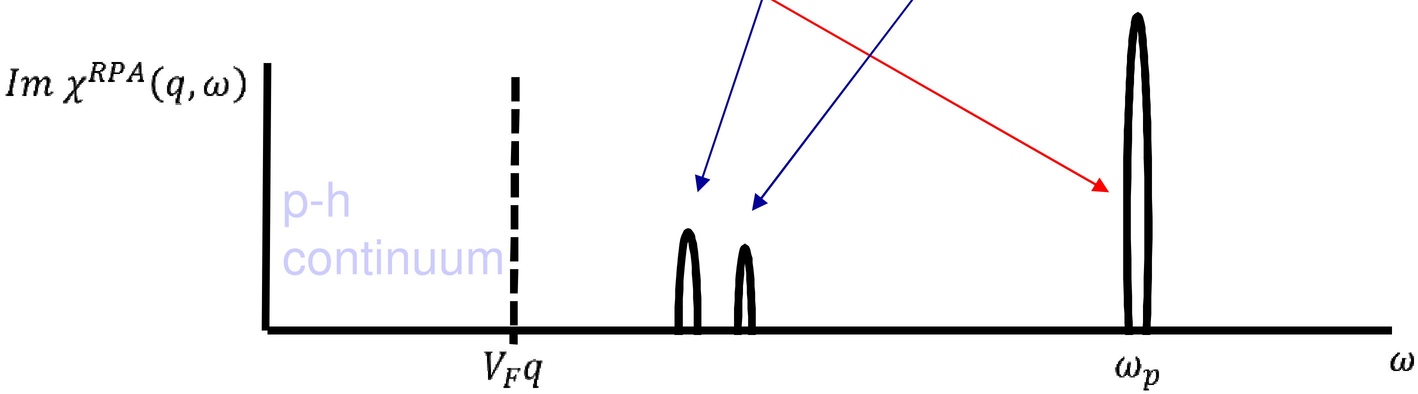
$$\chi^{RPA}(q,\omega) = \frac{\chi^0(q,\omega)}{1 - v_q \chi^0(q,\omega)}$$

$E(k+K) = E(k) \rightarrow \chi^0(q+K,\omega), \chi^0(q,\omega)$ both have p-h continuum ~ q

$\chi(q+nK, q+mK, \omega) \neq 0 \rightarrow Umklapp\ scattering$!!!

Generalized RPA with Umklapp Process

$$\hat{\chi}^{-1} = \begin{bmatrix} \chi^0(q,q,\omega) & \chi^0(q+K,q,\omega) & \cdots \\ \chi^0(q,q+K,\omega) & \chi^0(q+K,q+K,\omega) & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}^{-1} - \hat{V}$$

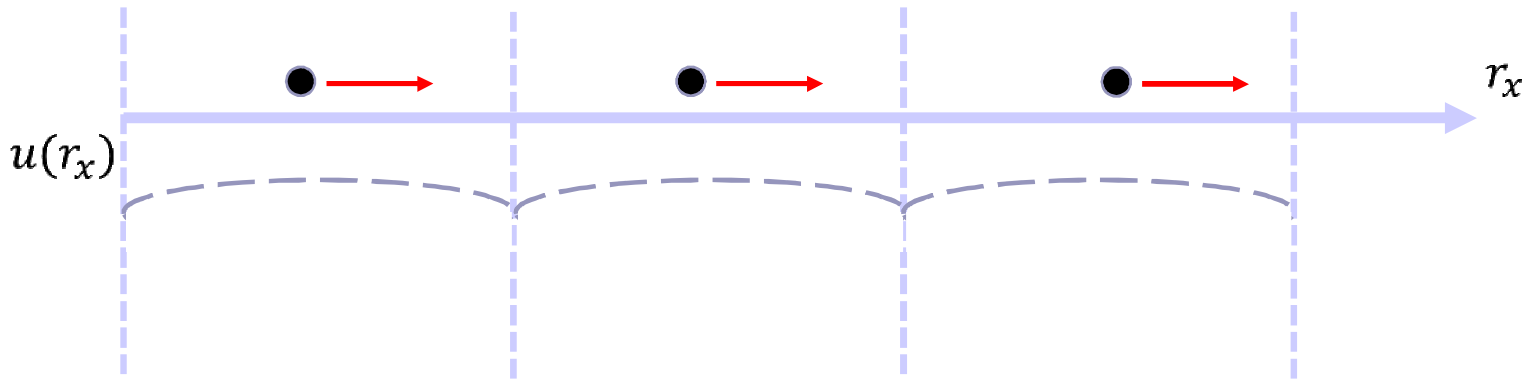


New spectral weight in Mid Infrared region appears due to the Umklapp process!!!

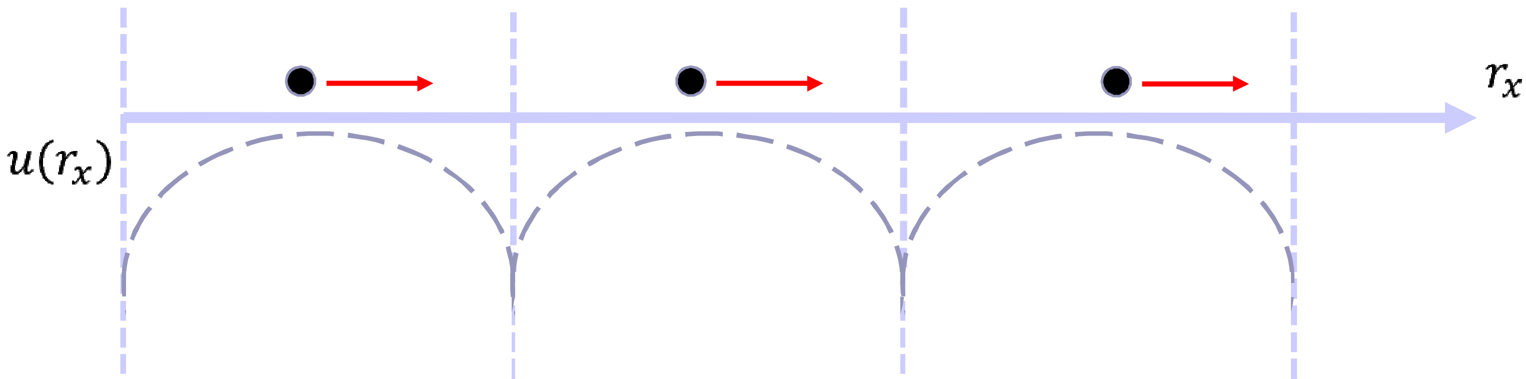
Why Plasmon Loses Spectral Weight?

$$\psi_{nk}(r) = e^{ikr}u_n(r)$$

(a) No Umklapp process

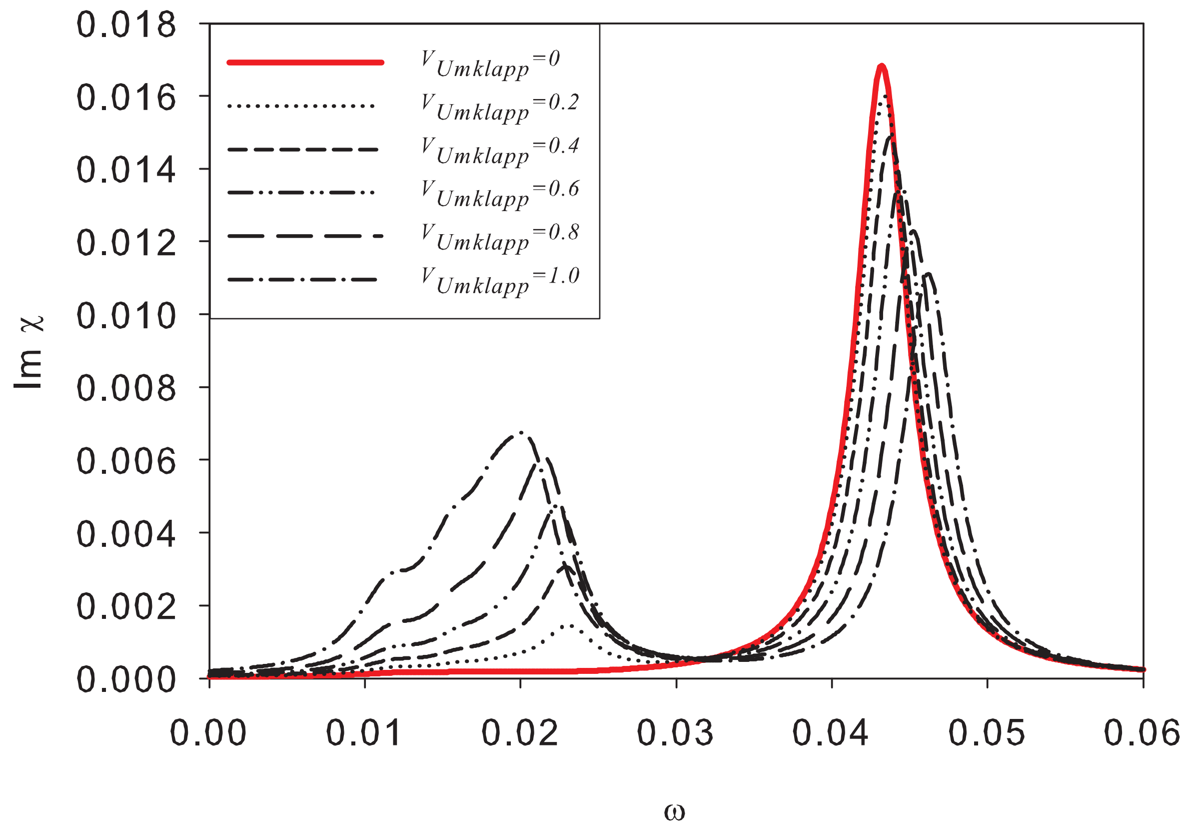


(b) With Umklapp process



What happens inside a unit cell is the key!!!

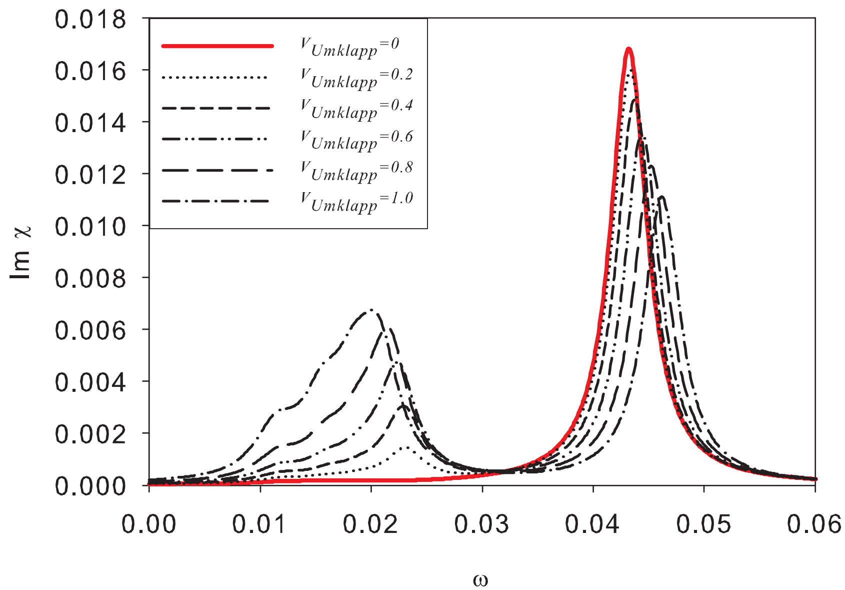
Calculations



To obtain a truly broad spectrum, we need to go beyond RPA.
Solving the Kinetic equations can do the trick.

Why Superconductivity Can Take Advantage?

Because it is not local and gapped, it has much less Umklapp scattering!!!

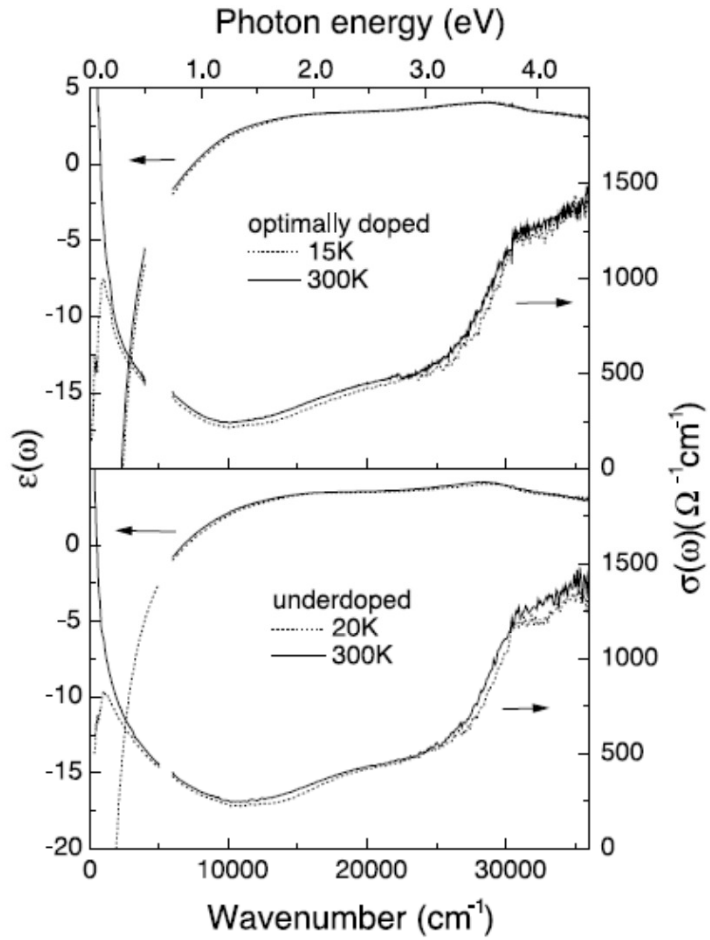


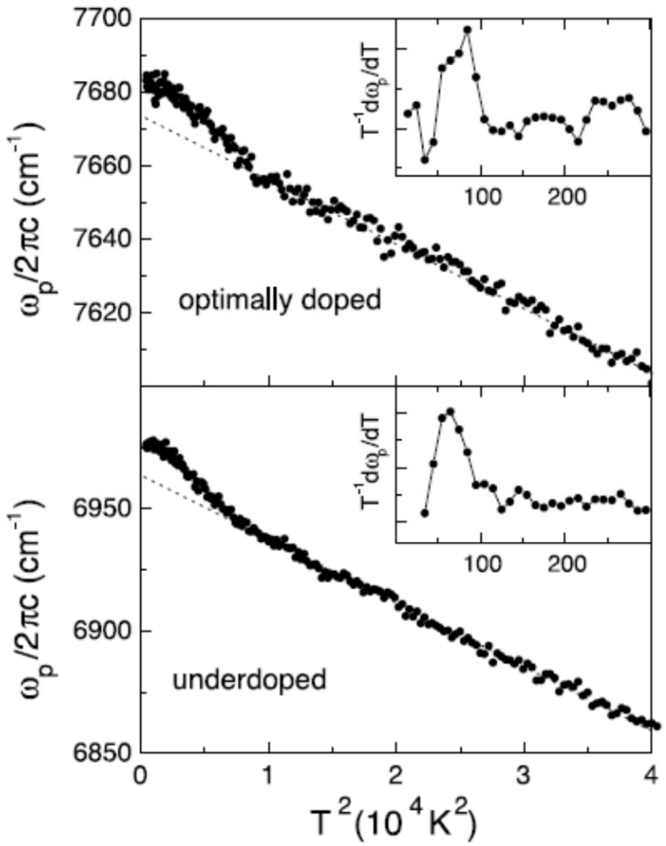
Umklapp scattering → Mid Infrared peaks →increase long-ranged Coulomb energy

Superconductivity suppresses Umklapp scattering → Mid Infrared peaks reduced→ long-ranged Coulomb energy decreased!!!

Experimental Observation in Cuprates

Fig. 1 (left). Dielectric function $\varepsilon(\omega)$ and optical conductivity $\sigma(\omega)$ of optimally doped (top) and underdoped (bottom) $Bi_2Sr_2CaCu_2O_{8-\delta}$ versus photon energy in the superconducting state and at 300 K. **Fig. 2 (right).** Temperature dependence of the screened plasma frequency ω_p for optimally doped (top) and underdoped (bottom) $Bi_2Sr_2CaCu_2O_{8-\delta}$. **(Insets)** Derivatives $T^{-1}d\omega_p/dT$.





Mole graaf, et. al., Science **295**, 2239 (2002)

Experimental Observations in Iron Pnictides

ARTICLE

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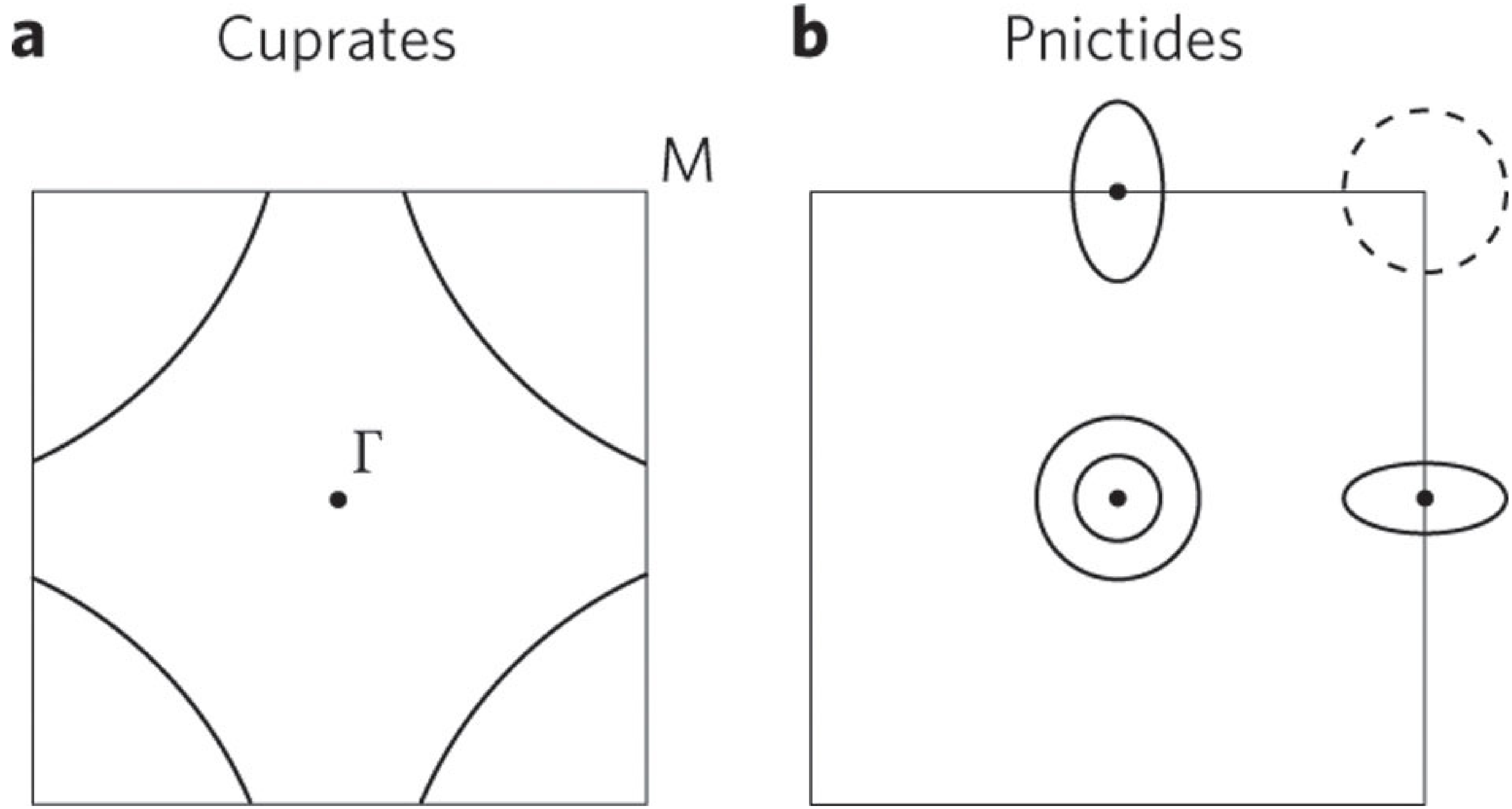
Superconductivity-induced optical anomaly in an iron arsenide

A. Charnukha[1], P. Popovich[1], Y. Matiks[1], D. L. Sun[1], C. T. Lin[1], A. N. Yaresko[1], B. Keimer[1] & A. V. Boris[1,2]

One of the central tenets of conventional theories of superconductivity, including most models proposed for the recently discovered iron-pnictide superconductors, is the notion that only electronic excitations with energies comparable to the superconducting energy gap are affected by the transition. Here, we report the results of a comprehensive spectroscopic ellipsometry study of a high-quality crystal of superconducting $Ba_{0.68}K_{0.32}Fe_2As_2$ that challenges this notion. We observe a superconductivity-induced suppression of an absorption band at an energy of 2.5 eV, two orders of magnitude above the superconducting gap energy $2\Delta \approx 20$ meV. On the basis of density functional calculations, this band can be assigned to transitions from As-p to Fe-d orbitals crossing the Fermi level. We identify a related effect at the spin-density wave transition in parent compounds of the 122 family. This suggests that As-p states deep below the Fermi level contribute to the formation of the superconducting and spin-density wave states in the iron arsenides.

Fermi Surface Consideration



Umklapp scattering also affects pairing interaction

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Breakdown of the Landau-Fermi liquid in two dimensions due to umklapp scattering

C. Honerkamp,[1] M. Salmhofer,[2] N. Furukawa,[1,3] and T. M. Rice[1]
[1]*Theoretische Physik, ETH-Hönggerberg, CH-8093 Zürich, Switzerland*
[2]*Mathematik, ETH Zentrum, CH-8092 Zürich, Switzerland*
[3]*Department of Physics, Aoyama Gakuin University, Setagaya, Tokyo 157-8572, Japan**
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We study the renormalization-group (RG) flow of interactions in the two-dimensional t-t' Hubbard model near half-filling in an *N*-patch representation of the whole Fermi surface. Starting from weak to intermediate couplings the flows are to strong coupling, with different characters depending on the choice of parameters. In a large parameter region elastic umklapp scatterings drive an instability which on parts of the Fermi surface exhibits the key signatures of an insulating spin liquid (ISL), as proposed by Furukawa, Rice, and Salmhofer [Phys. Rev. Lett. **81**, 3195 (1998)] rather than a conventional symmetry-broken state. The ISL is characterized by both strong *d*-wave pairing and antiferromagnetic correlations; however, it is insulating due to the vanishing local charge compressibility and a spin liquid because of the spin gap arising from the pairing correlations. We find that the unusual RG flow, which we interpret in terms of an ISL, is a consequence of a Fermi surface close to the saddle points at the Brillouin-zone boundaries which provides an intrinsic and mutually reinforcing coupling between pairing and umklapp channels.

Final Remarks

Why superconductivity is so competitive?

- Short-ranged Coulomb energy saved by sign-changing gap
- Long-ranged Coulomb energy saved by reducing Umklapp process
- Higher Tc superconductivity might occur in materials with 2D lattice, localized orbitals, and smaller dielectric constant.

Much more efforts should be spent on changes due to superconductivity on optical conductivity, electron energy loss spectroscopy (EELS)!!!