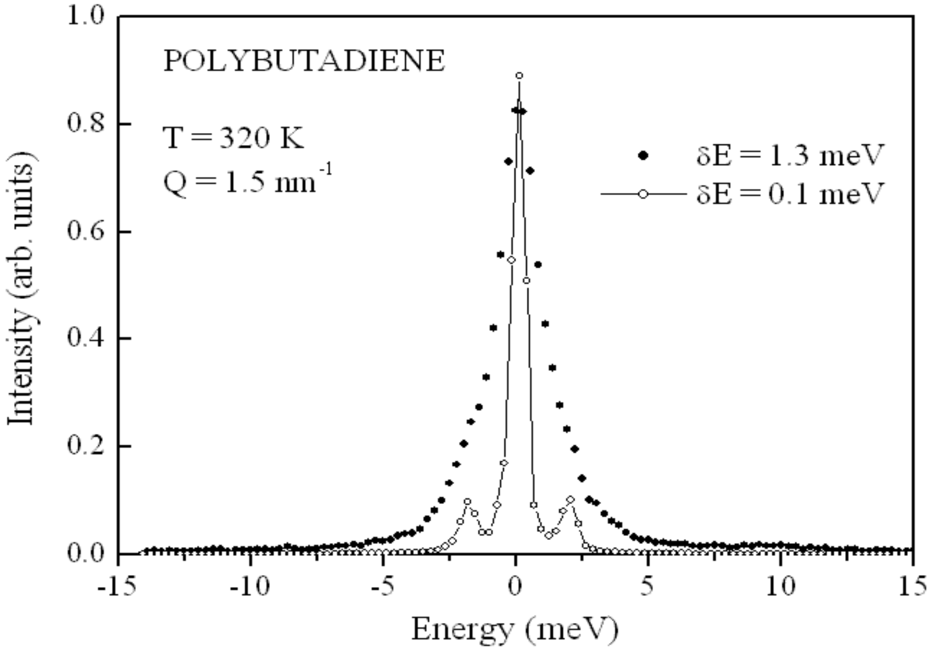
Do we really need 0.1 meV ?

Tullio Scopigno

University of Rome "La Sapienza" – I

Towards 0.1 meV energy resolution

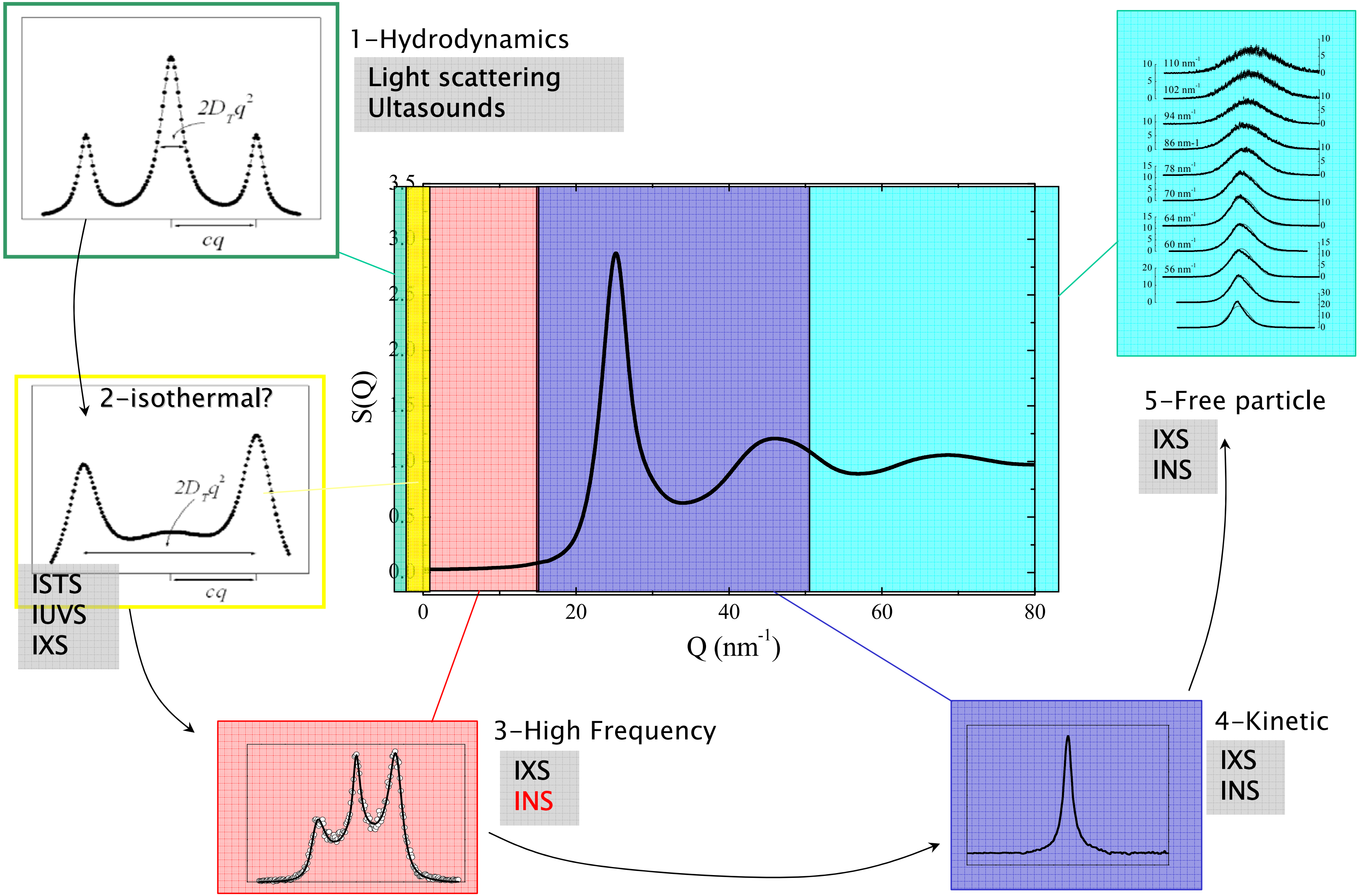


•**Position**: viscoelastic transitions in liquids, dispersion curves in xals

•**Linewidth**: dynamical heterogeneities in glasses, phonon lifetimes

•**Lineshape**: other that LA modes, non hydrodynamic behaviours

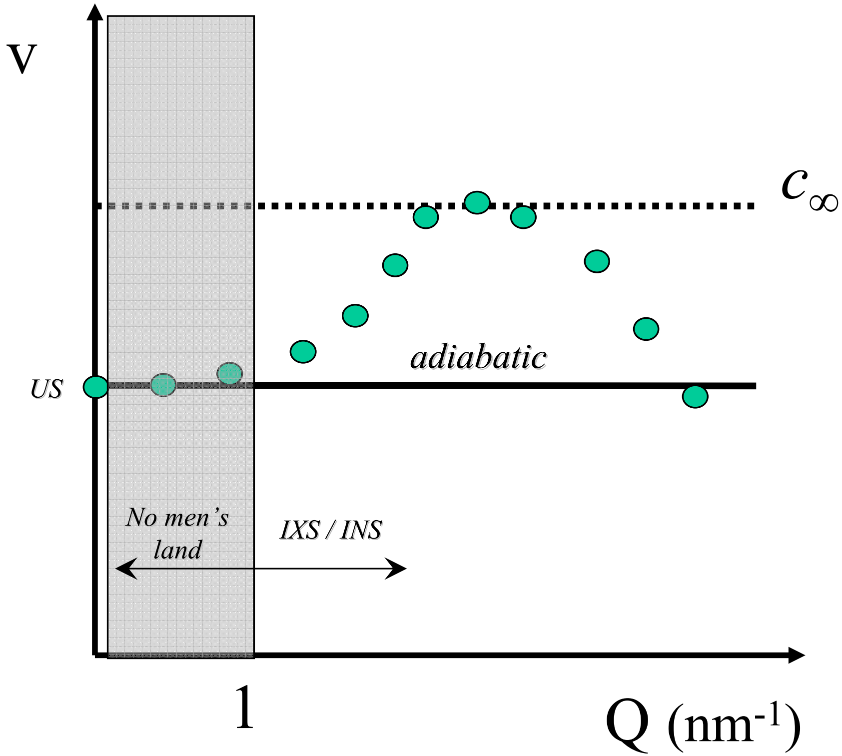
A few open issues for the physics of disordered systems



Tullio Scopigno, Giancarlo Ruocco, Francesco Sette, REVIEWS OF MODERN PHYSICS, 77, 881 (2005)

Where does positive dispersion come from?

Outside hydrodynamics: the sound velocity



Example: Liquid-like to solid-like transition

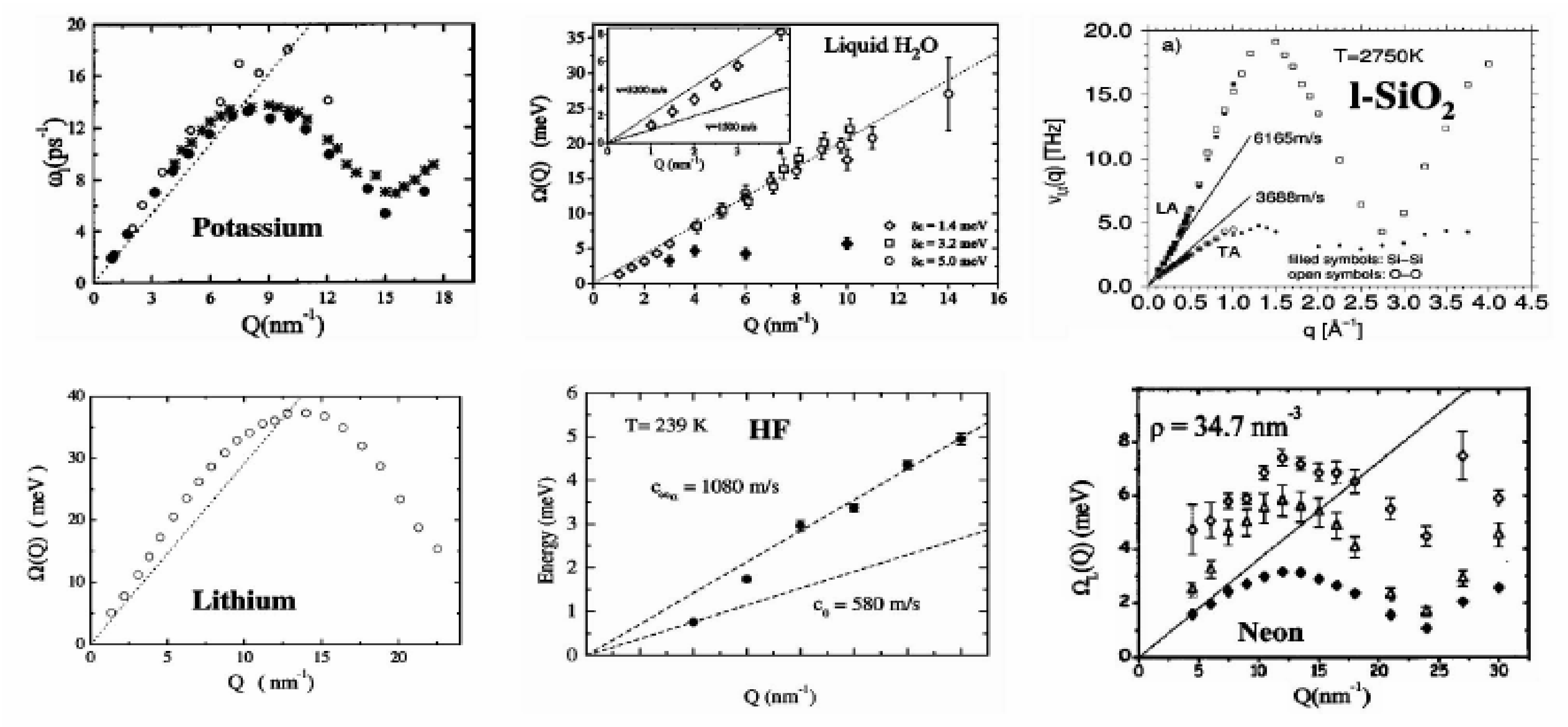
But not only!!!

Disorder-induced relaxations

Often occurs around ~2 nm^{-1} → ω~1.3 meV @ 1000 m/s

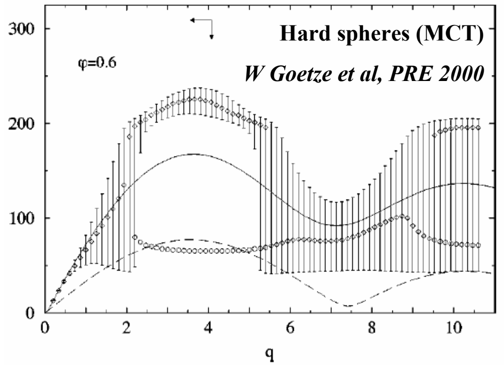
Where does the positive dispersion come from?

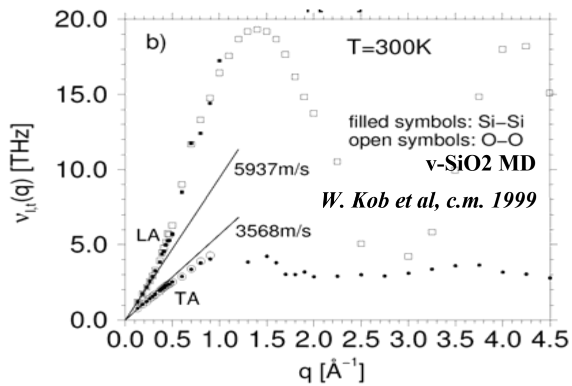
Ubiquity of positive dispersion in LIQUIDS

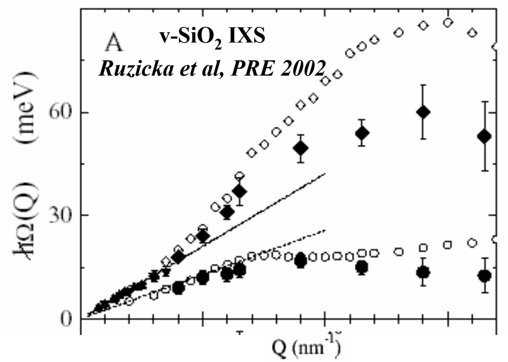


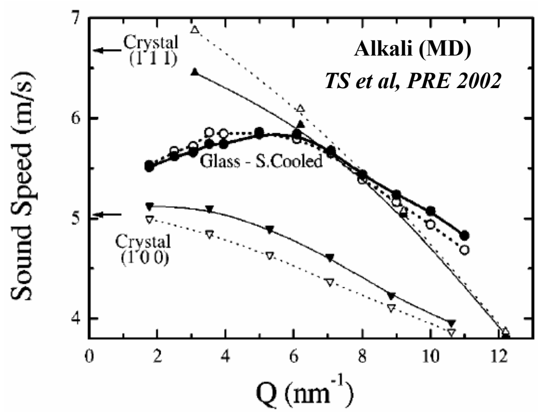
Where does the positive dispersion come from?

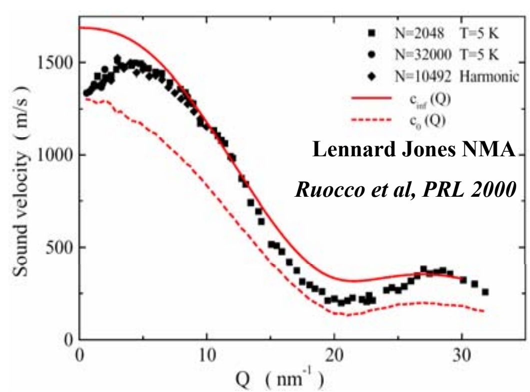
Ubiquity of positive dispersion in GLASSES

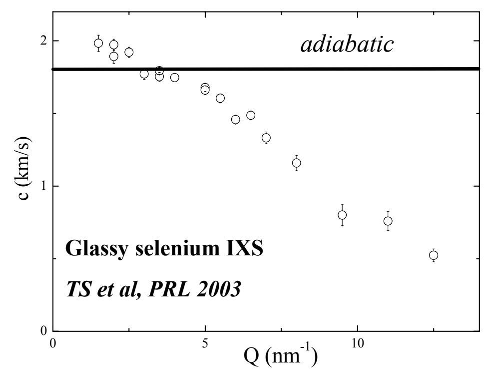








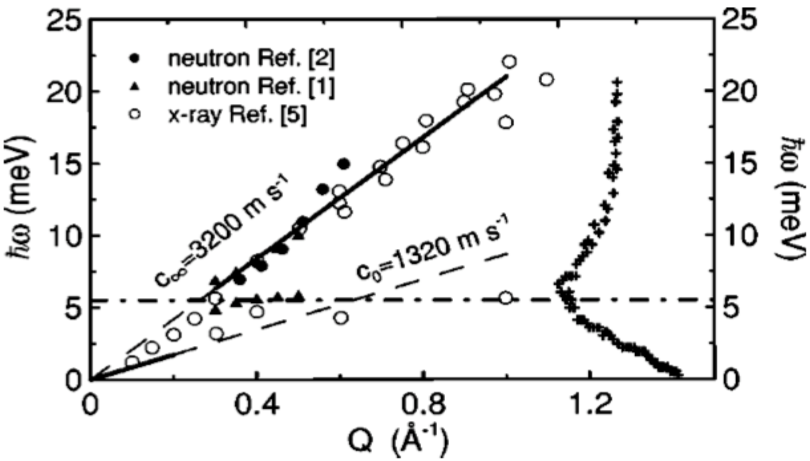




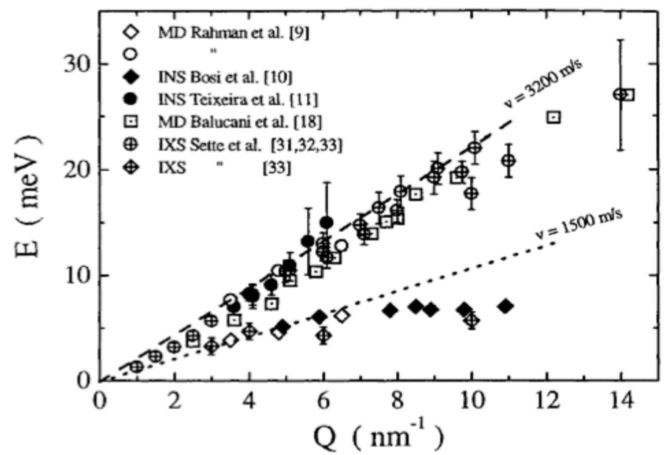
Other than LA modes…

Other than LA modes

Dispersion in liquids: viscoelasticity and transverse modes



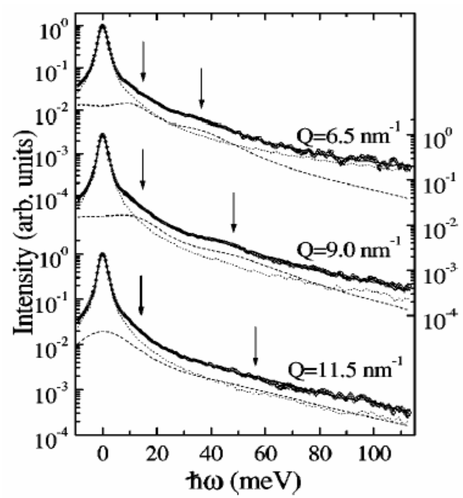
C.Petrillo et al., PRE **62**, 3611 (2000)
F.Sacchetti et al., PRE **69**, 061203 (2004)

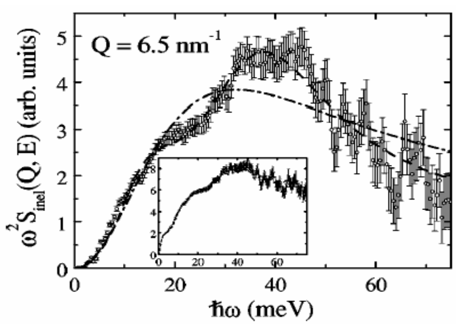


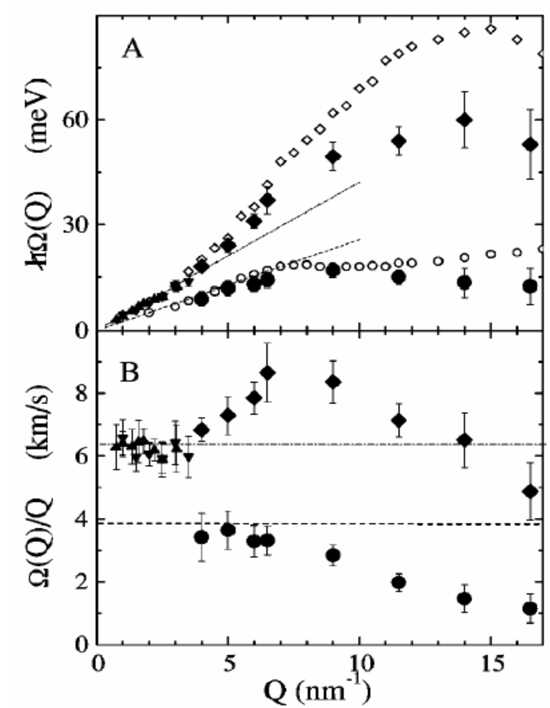
G.Ruocco et al. J. Phys.: Condens. Matter **11**, R259 (1999)
G.Monaco et al. PRE **60,** 5505 (1999)

Other than LA modes

Quasi-transverse modes in glasses





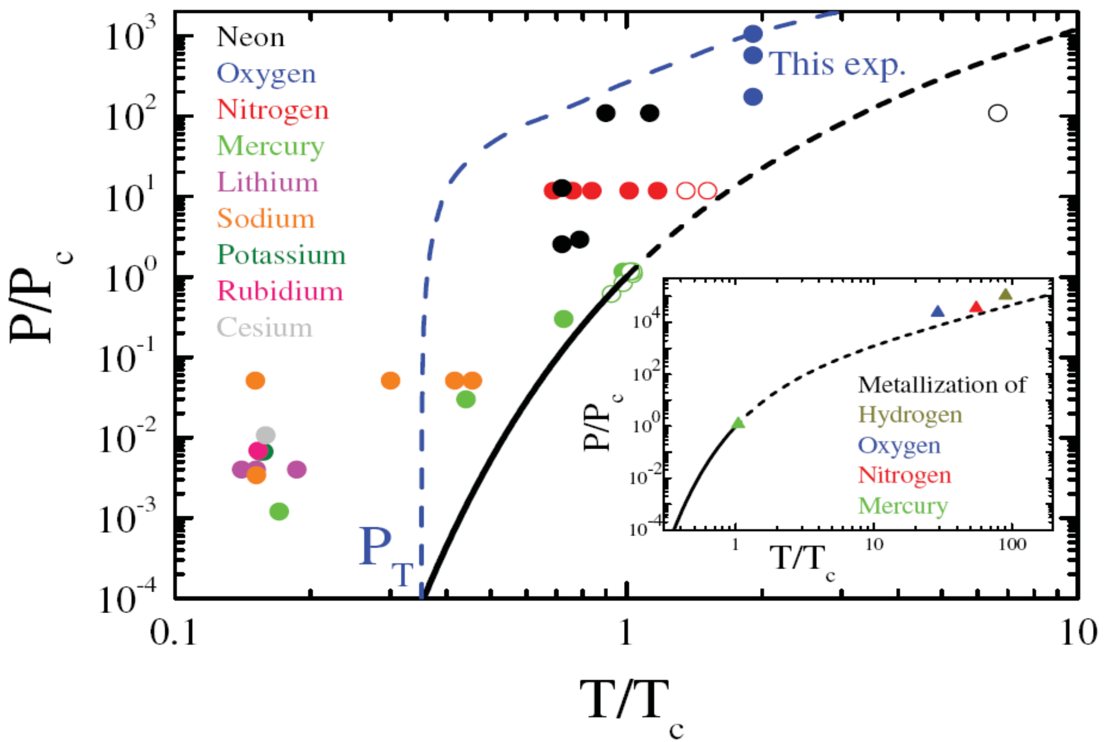


B. Ruzicka et al., Phys.Rev.B, **69** 100201 (2004)

Going extreme: towards a new "dynamical" classification of fluids?

Liquidlike Behavior of Supercritical Fluids

F. Gorelli,[1,2] M. Santoro,[1,2] T. Scopigno,[1,*] M. Krisch,[3] and G. Ruocco[4,1]



Is there an intermediate regime bridging the adiabatic and the high frequency domain?

Is there an intermediate regime bridging the adiabatic and the high frequency domain?

- Only possible in **liquid metals**

Isothermal regime?

$\omega\tau_{th} < 1$

… Of course, if DQ^2 becomes comparable with Ω, the central peak overlaps with the two side ones… But even in a typical liquid metal, where D is relatively high, this situation only arises when the wavelenght becomes comparable with the interatomic spacing…

T.E. Faber, 1972

$$\omega\tau_{th} \approx \frac{c_T Q}{D_T Q^2} < 1 \Rightarrow Q^* > c_T / D_T$$

- > 200 nm^{-1} ordinary liquids
- > 0.1 nm^{-1} liquid metals

THE HYDRODYNAMIC LIMIT OF $S(k, \omega)$ 227

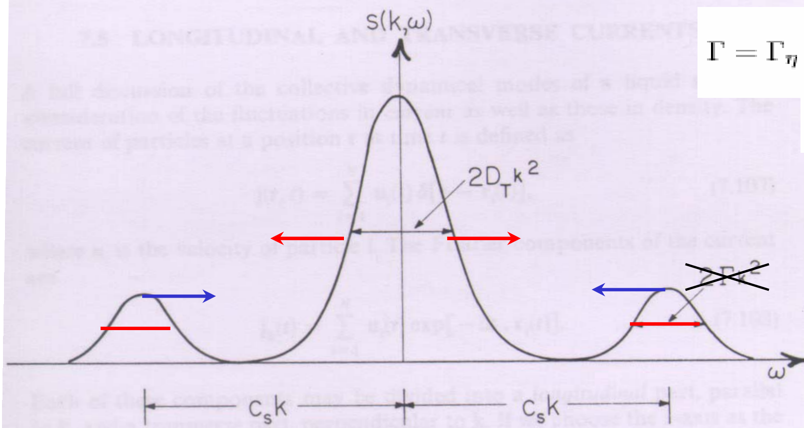


FIG. 24. Dynamic structure factor in the hydrodynamic limit. D_T is the thermal diffusivity, Γ is the sound wave attenuation coefficient and c_s is the adiabatic velocity of sound.

$$\Gamma = \Gamma_\eta + \Gamma_{th} = \frac{Q^2}{2\rho}\left[\frac{4}{3}\eta_s + \eta_B + (\gamma - 1)\lambda / C_p\right]$$

$$\Gamma_{th} = (\gamma - 1)\, c_t^2 / D_T$$

Is there an intermediate regime bridging the adiabatic and the high frequency domain?

PHYSICAL REVIEW E **67**, 012201 (2003)

Collective dynamics in liquid lithium, sodium, and aluminum

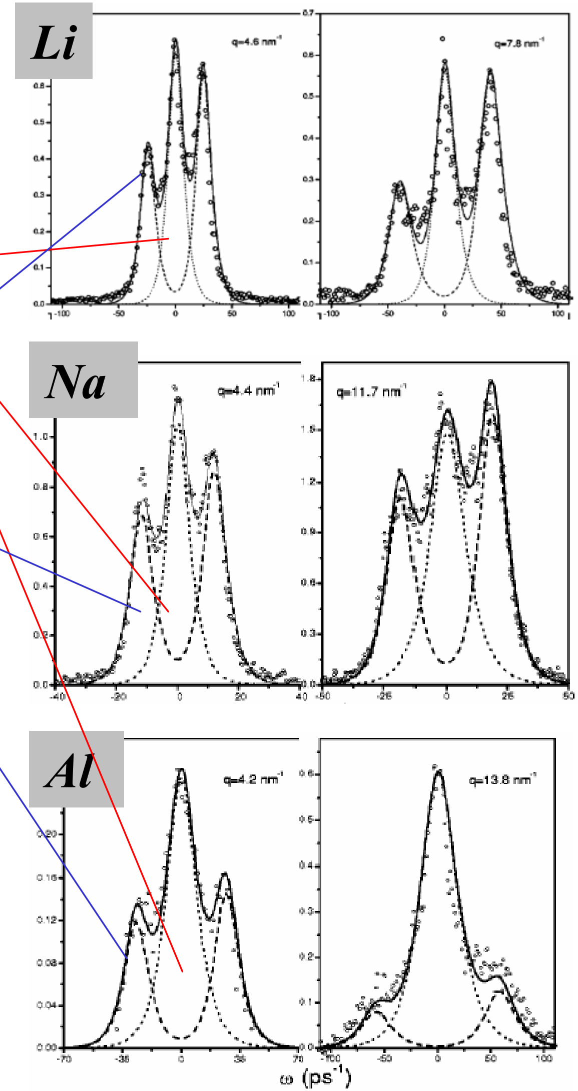
Shaminder Singh and K. Tankeshwar
Department of Physics, Panjab University, Chandigarh-160014, India
(Received 30 July 2002; published 13 January 2003)

$$F(q,t)=S(q)[a\ \mathrm{sech}(t/\tau_1)+(1-a)\mathrm{sech}(t/\tau_2)\cos(\omega_O t)], \quad (3)$$

$$S_c(q,\omega)=S(q)\left\{\frac{a\tau_1}{2}\mathrm{sech}\left(\frac{\pi\omega\tau_1}{2}\right)+\frac{(1-a)\tau_2}{4}\left[\mathrm{sech}\left(\frac{\pi(\omega+\omega_0)\tau_2}{2}\right)+\mathrm{sech}\left(\frac{\pi(\omega-\omega_0)\tau_2}{2}\right)\right]\right\}. \quad (4)$$

Thermal

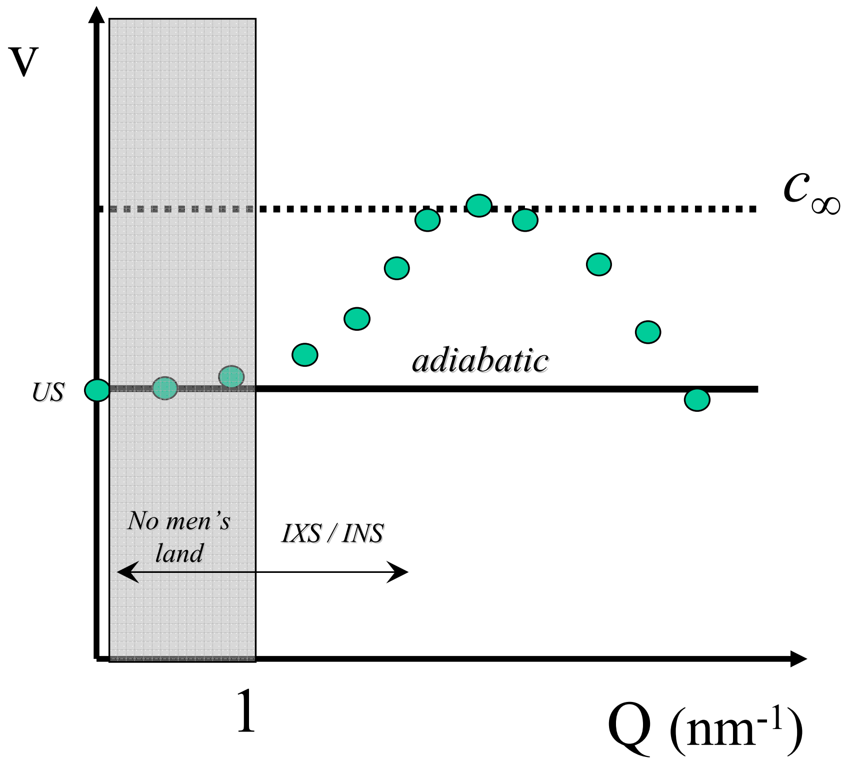
Viscous



"..But as far as the calculation of dynamical structure factor, $S(q,\omega)$ is concerned, <u>it is well known that only the ionic thermal conductivity enters into the calculation</u>."

Is there an intermediate regime bridging the adiabatic and the high frequency domain?

Speculation: the sound velocity…



Is there an intermediate regime bridging the adiabatic and the high frequency domain?

VOLUME 85, NUMBER 1 PHYSICAL REVIEW LETTERS 3 JULY 2000

Persistence of Well-Defined Collective Excitations in a Molten Transition Metal

F. J. Bermejo,[1] M. L. Saboungi,[2] D. L. Price,[2] M. Alvarez,[1] B. Roessli,[3] C. Cabrillo,[1] and A. Ivanov[4]
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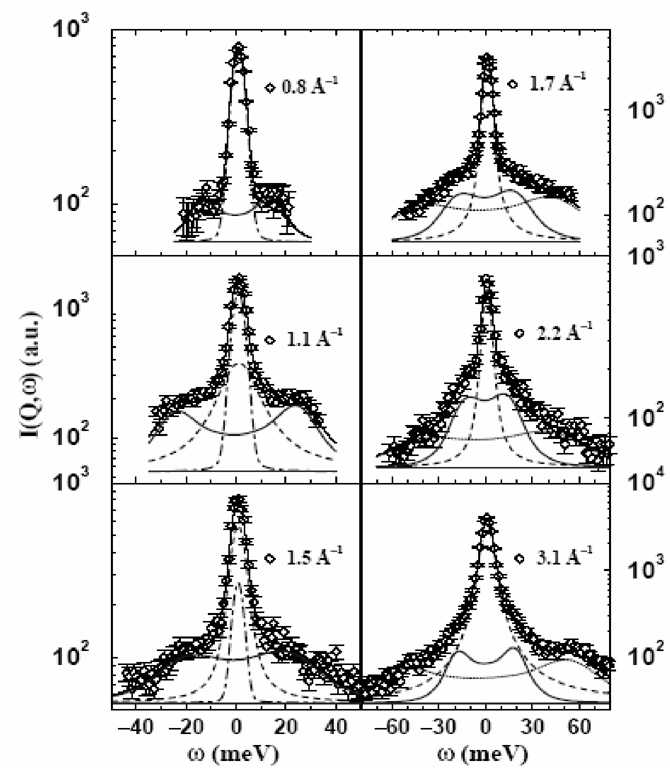
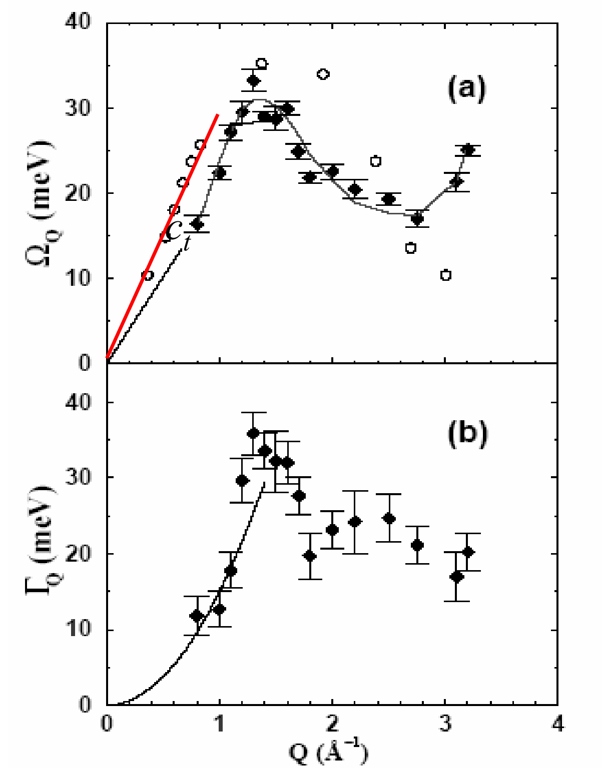
[2]*Argonne National Laboratory, Argonne, Illinois 60439*
[3]*Laboratory for Neutron Scattering, ETH Zurich & Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*
[4]*Institut Laue Langevin, BP156, F-38042 Grenoble, Cedex 9, France*
(Received 25 January 2000)



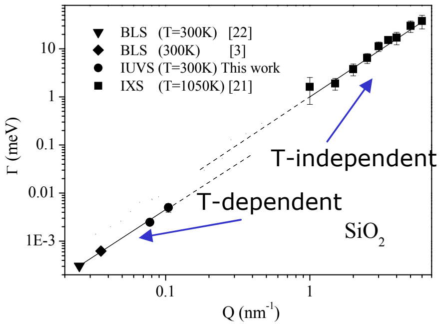
$$\gamma = 1.88$$



Acoustic damping in glasses

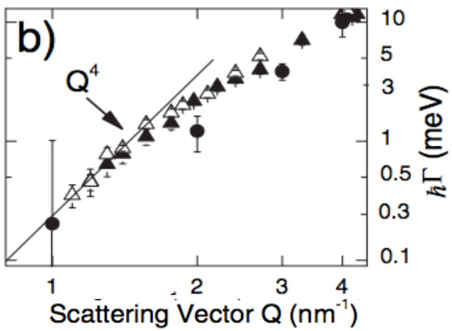
Acoustic damping in Glasses

Propagation and damping @> 1nm^{-1} is not the extrapolation of hydrodynamics



Change in acoustic damping @ 0.01meV < E < 1meV
0.1nm^{-1}< Q < 1nm^{-1}

C.Masciovecchio et al. 92 247401 (2004)

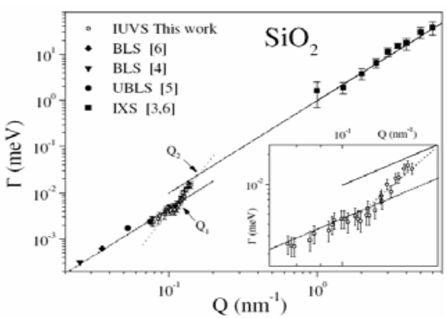


d-SiO_2 and Li_2O-$2B_2O_3$: crossover to Q^4 regime @ 1nm^{-1}

B. Rufflè et al., PRL **96**, 045502 (2006);

Comment: G.Ruocco et al., PRL **98**, 079601 (2007);

*Reply:*B. Rufflè et al., PRL **98**, 079602 (2007)



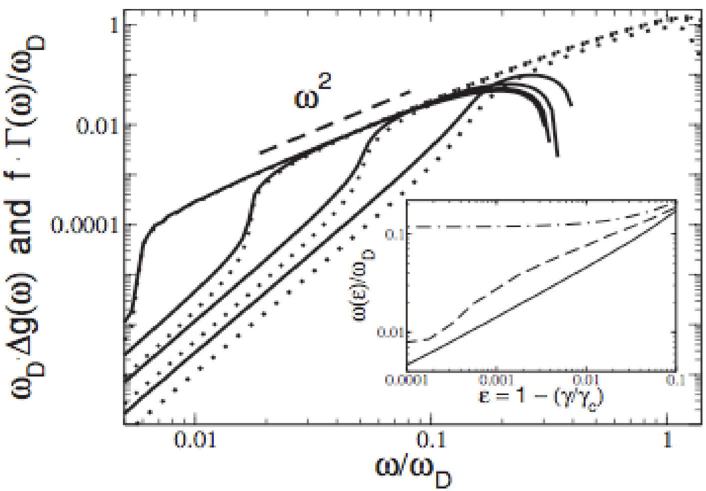
SiO_2: crossover to Q^4 (E^4) regime @ 0.1nm^{-1} (0.01meV)

C.Masciovecchio et al., PRL 97, 035501 (2006)

Acoustic Attenuation in Glasses and its Relation with the Boson Peak

W. Schirmacher,[1] G. Ruocco,[2,3] and T. Scopigno[3]
[1]Physik-Department E13, Technische Universität München, D-85747, Garching, Germany
[2]Dipartimento di Fisica, Universitá di Roma "La Sapienza", I-00185, Roma, Italy
[3]CRS SOFT-INFM-CNR c/o Universitá di Roma "La Sapienza", I-00185, Roma, Italy
(Received 24 August 2006; published 9 January 2007)

A theory for the vibrational dynamics in disordered solids [W. Schirmacher, Europhys. Lett. **73**, 892 (2006)], based on the random spatial variation of the shear modulus, has been applied to determine the wave vector (k) dependence of the Brillouin peak position (Ω_k) and width (Γ_k), as well as the density of vibrational states [$g(\omega)$], in disordered systems. As a result, we give a firm theoretical ground to the ubiquitous k^2 dependence of Γ_k observed in glasses. Moreover, we derive a quantitative relation between the excess of the density of states (the boson peak) and Γ_k, two quantities that were not considered related before. The successful comparison of this relation with the outcome of experiments and numerical simulations gives further support to the theory.



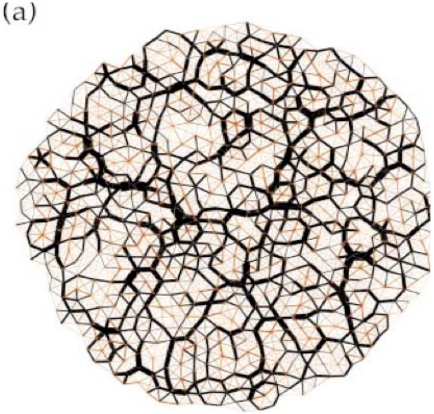
PHYSICAL REVIEW B **66**, 174205 (2002)

Continuum limit of amorphous elastic bodies: A finite-size study of low-frequency harmonic vibrations

A. Tanguy,* J. P. Wittmer, F. Leonforte, and J.-L. Barrat
Département de Physique des Matériaux, Université Claude Bernard & CNRS, 69622 Villeurbanne Cedex, France
(Received 11 April 2002; revised manuscript received 27 June 2002; published 27 November 2002)

The approach of the elastic continuum limit in small amorphous bodies formed by weakly polydisperse Lennard-Jones beads is investigated in a systematic finite-size study. We show that classical continuum elasticity breaks down when the wavelength of the solicitation is smaller than a characteristic length of approximately 30 molecular sizes. Due to this surprisingly large effect ensembles containing up to $N=40\,000$ particles have been required in two dimensions to yield a convincing match with the classical continuum predictions for the eigenfrequency spectrum of disk-shaped aggregates and periodic bulk systems. The existence of an effective length scale ξ is confirmed by the analysis of the (non-Gaussian) noisy part of the low frequency vibrational eigenmodes. Moreover, we relate it to the *nonaffine* part of the displacement fields under imposed elongation and shear. Similar correlations (vortices) are indeed observed on distances up to $\xi \approx 30$ particle sizes.

(a)



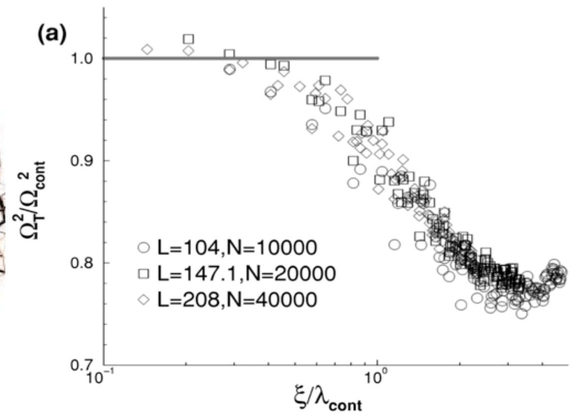


FIG. 1. (Color) Representation of the network of quenched stresses in two small quenched Lennard-Jones particle systems in two dimensions: (a) a disk-shaped aggregate of diameter $2R \approx 32a$ containing $N=732$ particles (protocol I) on the left and (b) a periodic bulk system with $L=32.9a$ and $N=1000$ (protocol III) on the right-hand side. The line scale is proportional to the tension transmitted along the links between beads. The black lines indicate repulsive forces (negative tensions), while the red links represent tensile forces between the verticies. Both shown networks are very similar despite different symmetries and quench protocols. They are strongly inhomogeneous and resemble the pattern seen in granular materials. Zones of weak attractive links appear to be embedded within the strong skeleton of repulsive forces.

24 October 2007 @ ESRF

2008-2017 Upgrade Meeting

HRRS CDR's discussion

The scientific case for 0.1 meV

The “Dynamical Matrix”

GAS/FLUIDS | **LIQUIDS** | **GLASSES** | **XALS**

Short wavelength limit of acoustic excitations

Phonon spectrum

Hydrodynamic ←→ viscoelastic merging

Coarse graining vs elasticity: microscopic relaxation

Extreme conditions

Extreme conditions

CM and electron density

Other than LA modes (transverse, optic)

Low dimentional systems: nanostuctures, surfaces and interfaces

V-DOS and collective properties: the Boson Peak

Vibrations vs Relaxations

ESRF UP

- INELX
- PHIXS
- NR-HE
- NR-NSM