Superconducting glue: are there limits on T_c?

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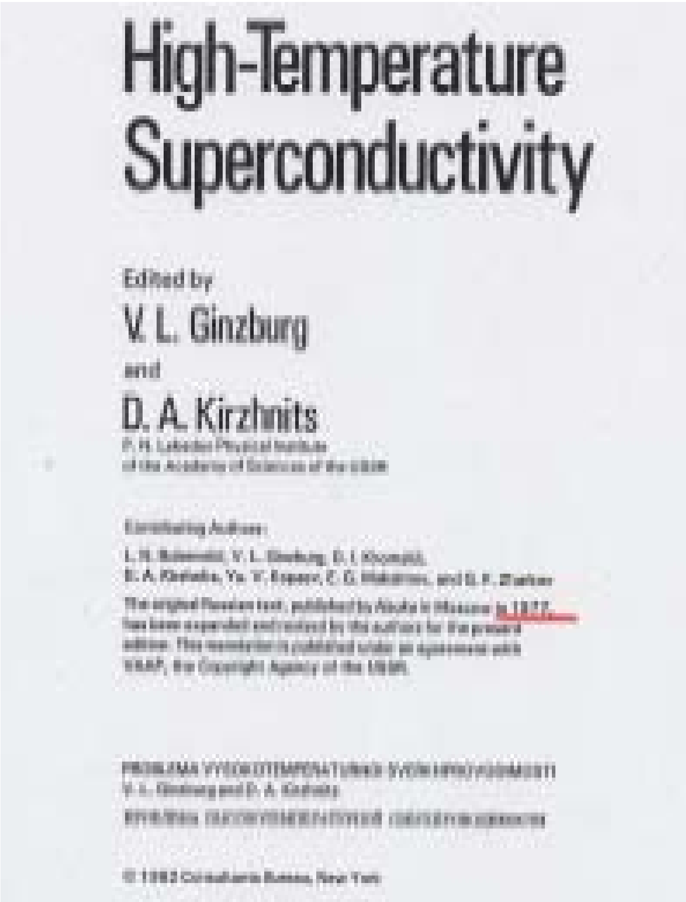


High-Temperature Superconductivity

Edited by

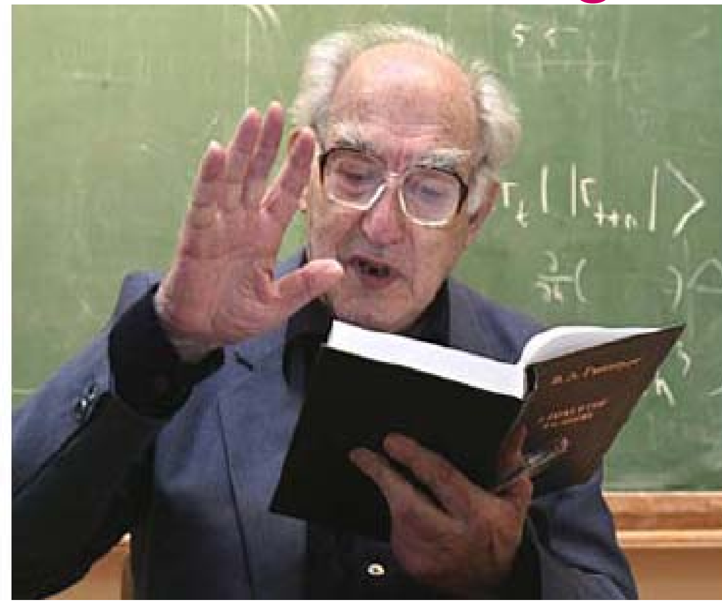
V. L. Ginzburg

and

D. A. Kirzhnits

P. N. Lebedev Physical Institute of the Academy of Sciences of the USSR

'Nauka' Publishing, Moscow, 1977



$T_c \leqslant 30 \div 40$ K (фононный механизм сверхпроводимости). (1.12)

Следует, правда, отметить, что оценка (1.12) базируется на рассмотрении металлов с более или менее известными параметрами и не может непосредственно применяться ко всем гипотетическим случаям. Так, для металли-

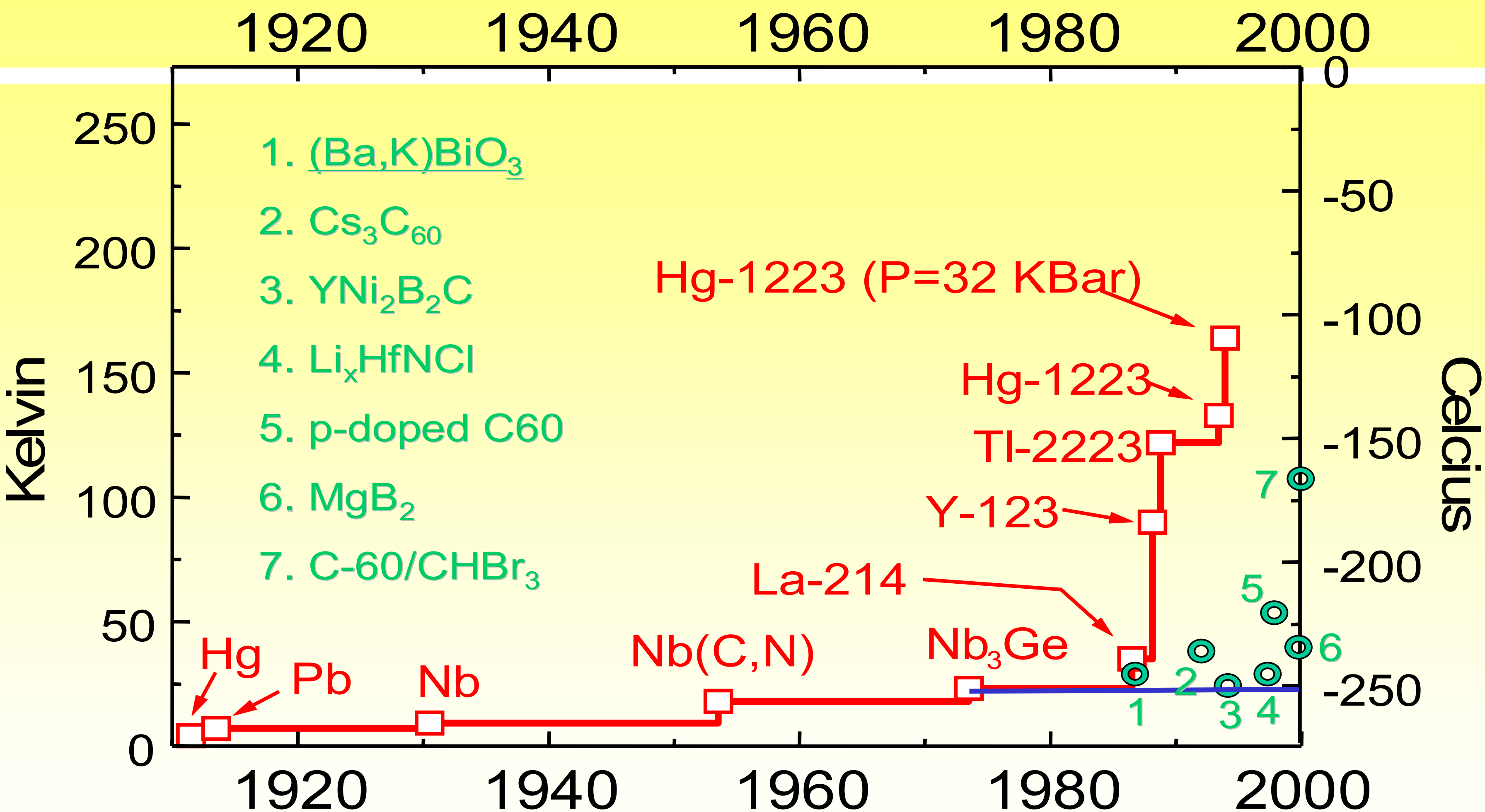
we have to point out, however, that the above estimate is based on a standard metal and can not be applied to all hypothetical situations

Outline

1. Introduction.
2. Electron-phonon interaction.
3. Causality and stability.
4. Restrictions from Eliashberg equations.
5. Phonon instability.
6. Nonphonon mechanisms.
7. Conclusions.

Briefly:

1. Pnictides
2. ***Quasiparticle renormalization effects in the optical properties of iron pnictides*** (with A.V. Boris)



1920
1940
1960
1980
2000
Kelvin
250
200
150
100
50
0
Celcius
0
-50
-100
-150
-200
-250
1. (Ba,K)BiO$_3$
2. Cs$_3$C$_{60}$
3. YNi$_2$B$_2$C
4. Li$_x$HfNCl
5. p-doped C60
6. MgB$_2$
7. C-60/CHBr$_3$
Hg-1223 (P=32 KBar)
Hg-1223
Tl-2223
Y-123
La-214
Nb$_3$Ge
Nb(C,N)
Nb
Pb
Hg
1
2
3
4
5
6
7

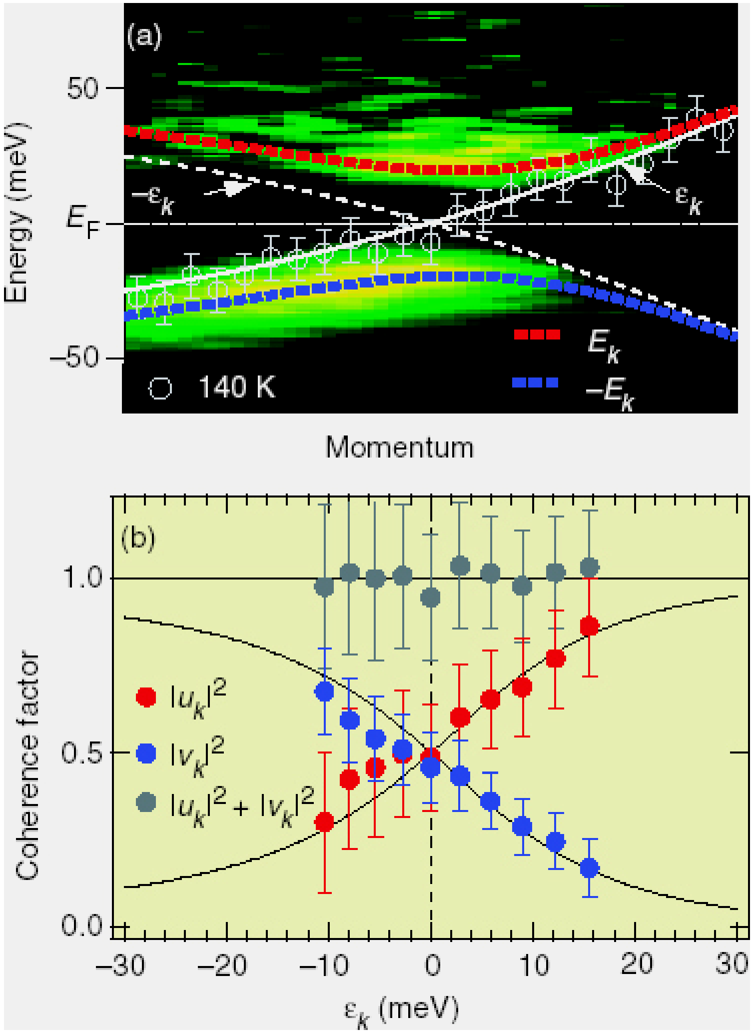
BCS type behavior

- M.Matsui *et al.* PRL,**90**,217002(2003)

$$G(\mathbf{k},\omega)=\frac{u_{\mathbf{k}}^2}{\omega-E(\mathbf{k})+i\delta}+\frac{v_{\mathbf{k}}^2}{\omega-E(\mathbf{k})-i\delta}$$

$$u_{\mathbf{k}}^2=\frac{1}{2}\left(1+\frac{\varepsilon_{\mathbf{k}}}{E(\mathbf{k})}\right)$$

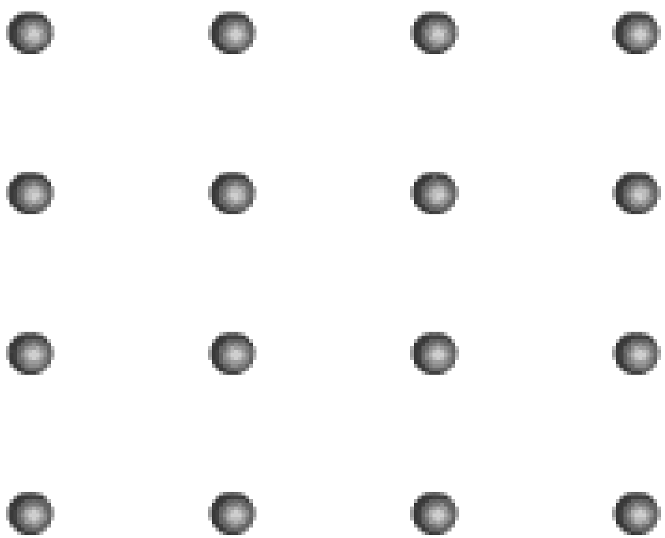
$$v_{\mathbf{k}}^2=\frac{1}{2}\left(1-\frac{\varepsilon_{\mathbf{k}}}{E(\mathbf{k})}\right)$$



Electrons join to form Cooper Pairs

usually

Regular Superconductors



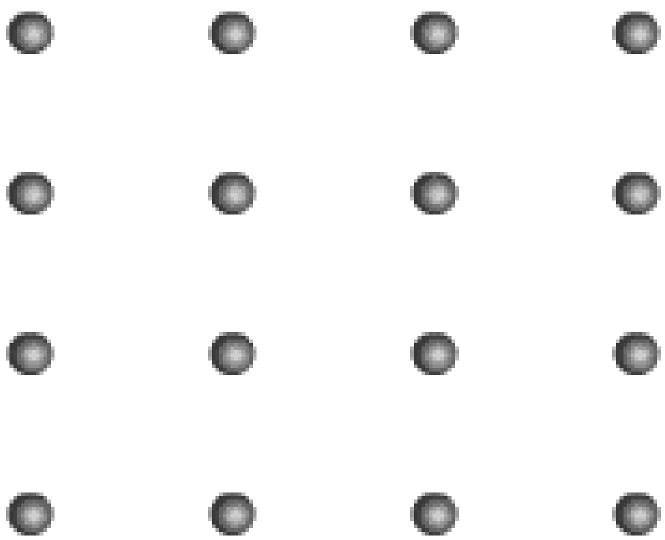
High-Temperature Superconductors

- A Magnetic Attraction ?
- Spin attraction ?
- The lattice after all ?
- Something else ?

Electrons join to form Cooper Pairs

usually

Regular Superconductors



High-Temperature Superconductors

- A Magnetic Attraction ?
- Spin attraction ?
- The lattice after all ?
-

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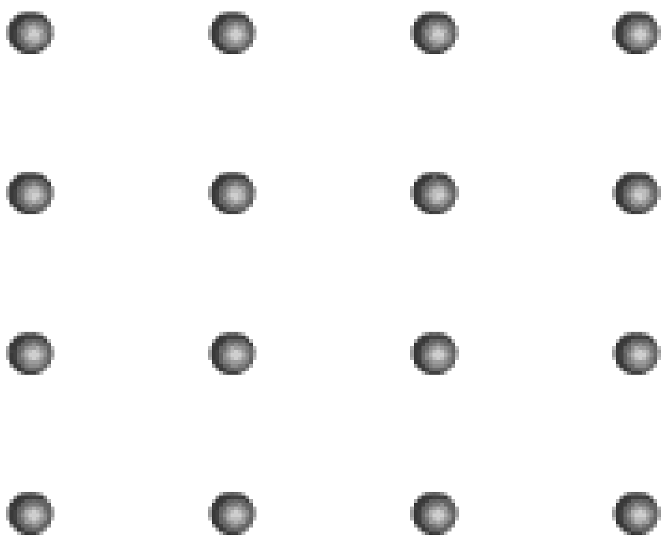
Regular Superconductors



High-Temperature Superconductors

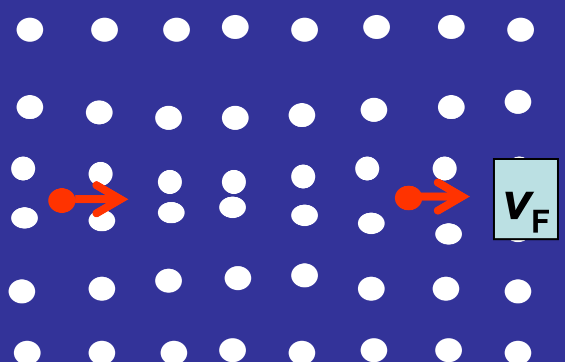
- A Magnetic Attraction ?
- Spin attraction ?
- The lattice after all ?
- Excitons (Little,Ginzburg)

Phonon mediated superconductivity

attraction: ● = N(0)V

Coulomb repulsion:

$$\mu^* = \frac{\mu}{1 + \mu \log(\varepsilon_F / \Omega_D)}$$



● 📭 ❍* > 0, then pairing

BCS model: ● << 1 and constant for ◆ < ⌖$_D$

Eliashberg formalism: l general and ●☎◆➂ (strong coupling effects)

How can two electron attract ?

1. Repulsive Coulomb interaction:

$$V_C(\mathbf{q},\omega)=\frac{4\pi e^2}{q^2+\chi_{TF}^2}$$

2. Screening by other electrons and ions

$$V(\mathbf{q},\omega)=\frac{4\pi e^2}{q^2\varepsilon_{tot}(\mathbf{q},\omega)}=\frac{4\pi e^2}{q^2}[1+\frac{4\pi e^2}{q^2}\chi_{tot}(\mathbf{q},\omega)]$$

$$\tilde{V}_C(\mathbf{q},\omega)=\frac{4\pi e^2}{q^2+\chi_{TF}^2}$$

"Overscreening" by phonons

$$V(\mathbf{q},\omega)=\tilde{V}_C(\mathbf{q},\omega)+V_{ph}(\mathbf{q},\omega)=\frac{4\pi e^2}{q^2+\chi_{TF}^2}(1+\frac{\omega_q^2}{\omega^2-\omega_q^2})$$

T_c problem

$$T_c = 1.14\omega_{av} \exp[-\frac{1}{N(0)V}]$$

$$V = < V(\mathbf{k}-\mathbf{k}', \omega = 0) >_{FS} = -\int d^3q \frac{4\pi e^2}{q^2 \varepsilon_{tot}(\mathbf{q}, \omega = 0)};$$

$$V(\mathbf{q}, \omega) = \tilde{V}_C(\mathbf{q}, \omega) + V_{ph}(\mathbf{q}, \omega)$$

$$T_c = 1.14\omega_D \exp(-\frac{1}{\lambda - \mu^*})$$

$$\lambda = N(0)\int d^3\mathbf{q}\, V_{ph}(\mathbf{q},0) \qquad \mu^* = \frac{\mu}{1+\mu \ln \frac{\varepsilon_F}{\omega_D}}$$

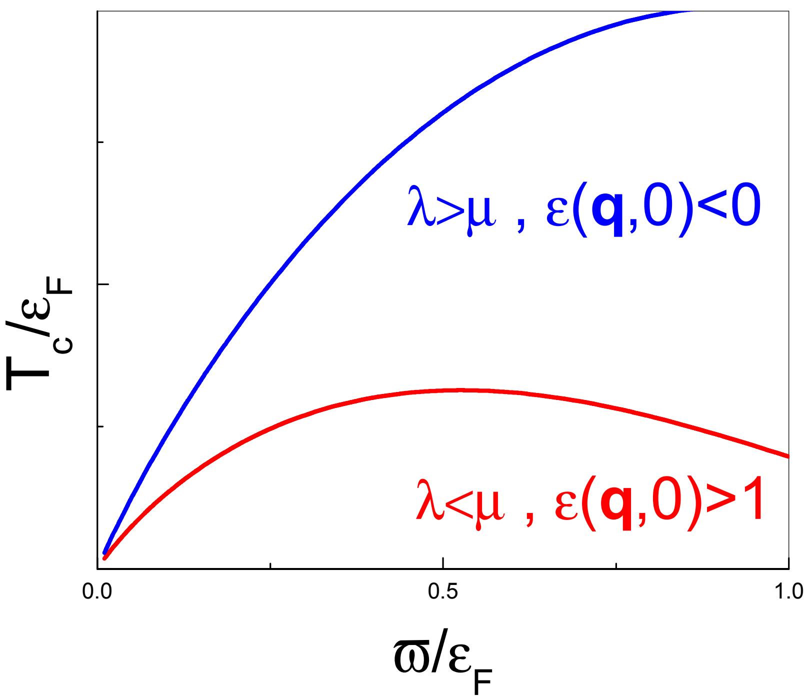
$$\mu = N(0)\int d^3\mathbf{q}\, \tilde{V}_C(\mathbf{q},0)$$

$$\varepsilon_{tot}(\mathbf{q},0) \geq 1$$

$$\lambda \leq \mu$$

$$T_c \approx 1.14\varpi \exp[-\frac{1+\lambda}{\lambda - \frac{\mu}{1+\mu \log(\varepsilon_F / \varpi)}}];$$

$$T_c \approx 1.14\varpi \exp\left[-\frac{1+\lambda}{\lambda - \frac{\mu}{1+\mu\log(\varepsilon_F/\varpi)}}\right];$$



COMMENTS ON THE MAXIMUM SUPERCONDUCTING TRANSITION TEMPERATURE

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Bell Laboratories, Murray Hill, New Jersey, 07974

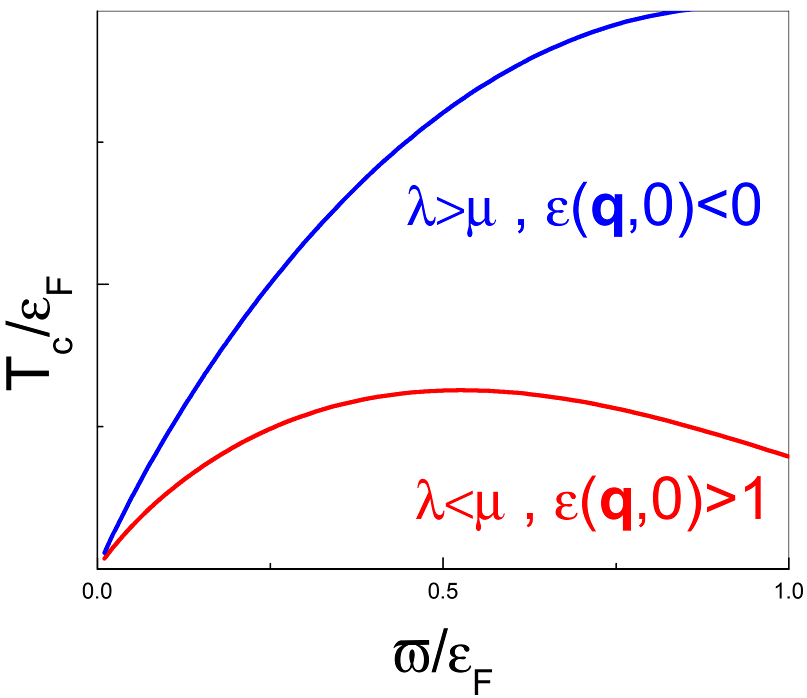
Superconductivity in d- and f-Band Metals, AIP Conf. Proc., p.17 (1972)

SUMMARY

So our comments on the maximum superconducting transition temperature are:
(1) Reasonable theoretical estimates of T_c can be made.
(2) Oversimplified models imply that resonant boson frequencies, ω_0, should be as large as possible and this is not true.
(3) Two square-well (2SW) models (like McMillan's model) should give reasonable estimates of T_c and T_c^{max}.
(4) Assuming no umklapps and using a 2SW model and a stability condition we find, ω_0 (optimum) $\sim e^{-4}E_F$ and for $E_F \sim 7$ eV, $T_c \sim 10^oK$. Phonon frequencies are not too far from the optimum value.
(5) Umklapps lead to large electron-phonon couplings, hence we want symmetric structures. There is a tendency to form bonds and to have instabilities.
(6) We present a simple model which exhibits the dependence of λ on ω_{ph} and a lattice instability for large coupling constant.
(7) The only system which might have a high T_c would involve high ω_0 and umklapp scattering. We can see no physical method of realizing this.

!!!

$$T_c \approx 1.14\varpi \exp\left[-\frac{1+\lambda}{\lambda - \frac{\mu}{1+\mu\log(\varepsilon_F/\varpi)}}\right];$$



$$T_c^{\max} \approx \varepsilon_F \exp(-\frac{3}{\lambda}); \qquad \lambda^{opt} = \mu = \frac{1}{2};$$

↑

Stoner instability

$\varepsilon_F \approx 7\ eV$

$$T_c^{\max} \approx \varepsilon_F \exp(-\frac{3}{\lambda});$$

$$\lambda^{opt} = \mu = \frac{1}{2};$$

↑

Stoner instability

$\varepsilon_F \approx 7\ eV$

$$T_c^{\max} \approx 10K$$

We need $\varepsilon(\mathbf{q},0) \leq 0)$!

Response functions

$$A = R \times I$$

Response functions

$A = R \times I$

causality requirements

↓

Kramers-Kronig relations

$$R(\mathbf{q},\omega) = R(\mathbf{q},\infty) + \frac{1}{\pi}\int_0^\infty \frac{dE^2}{E^2-\omega^2-i\delta}\,\mathrm{Im}\,R(\mathbf{q},E)$$

Response functions

A = R x I

causality requirements

↓

Kramers-Kronig relations

$$R(\mathbf{q},\omega) = R(\mathbf{q},\infty) + \frac{1}{\pi}\int_0^\infty \frac{dE^2}{E^2-\omega^2-i\delta}\,\mathrm{Im}\,R(\mathbf{q},E)$$

static case

$$R(\mathbf{q},0) = R(\mathbf{q},\infty) + \frac{1}{\pi}\int_0^\infty \frac{dE^2}{E^2}\,\mathrm{Im}\,R(\mathbf{q},E)$$

Electromagnetic response functions

$$\delta\mathbf{D}(\mathbf{q},\omega) = \underline{\varepsilon(\mathbf{q},\omega)}\,\delta\mathbf{E}(\mathbf{q},\omega)$$

or

$$\delta\mathbf{E}(\mathbf{q},\omega) = \underline{\varepsilon^{-1}(\mathbf{q},\omega)}\,\delta\mathbf{D}(\mathbf{q},\omega)$$

$$div\,\delta\mathbf{D} = 4\pi\delta\rho_{ext}, \qquad div\,\delta\mathbf{E} = 4\pi\delta\rho_{tot},$$

$$1/\varepsilon(\mathbf{q},0) = 1 + \frac{1}{\pi}\int_0^\infty \frac{dE^2}{E^2}\,\mathrm{Im}\,1/\varepsilon(\mathbf{q},E)$$ arbitrary ***q***

$$\varepsilon(\mathbf{q}=0,0) = 1 + \frac{1}{\pi}\int_0^\infty \frac{dE^2}{E^2}\,\mathrm{Im}\,\varepsilon(\mathbf{q}=0,E)$$ ***q*→*0***

$$1/\varepsilon(\mathbf{q},0) = 1 + \frac{1}{\pi}\int_0^\infty \frac{dE^2}{E^2}\,\mathrm{Im}\,1/\varepsilon(\mathbf{q},E)$$ arbitrary ***q***

$$\varepsilon(\mathbf{q}=0,0) = 1 + \frac{1}{\pi}\int_0^\infty \frac{dE^2}{E^2}\,\mathrm{Im}\,\varepsilon(\mathbf{q}=0,E)$$ ***q*→*0***

requirements of **stability**

$\mathrm{Im}\,\varepsilon(\mathbf{q},\omega) \geq 0,$ or $\mathrm{Im}\,1/\varepsilon(\mathbf{q},\omega) \leq 0,$ for all ***q***,ω

$$1/\varepsilon(\mathbf{q},0) = 1 + \frac{1}{\pi}\int_0^\infty \frac{dE^2}{E^2}\,\mathrm{Im}\,1/\varepsilon(\mathbf{q},E)$$ arbitrary ***q***

$$\varepsilon(\mathbf{q}=0,0) = 1 + \frac{1}{\pi}\int_0^\infty \frac{dE^2}{E^2}\,\mathrm{Im}\,\varepsilon(\mathbf{q}=0,E)$$ ***q→0***

requirements of **stability**

$\mathrm{Im}\,\varepsilon(\mathbf{q},\omega) \geq 0,$ or $\mathrm{Im}\,1/\varepsilon(\mathbf{q},\omega) \leq 0,$ for all ***q***,ω

$$1/\varepsilon(\mathbf{q},0) \leq 1 \quad (\varepsilon(\mathbf{q},0) \geq 1,\ \varepsilon(\mathbf{q},0) \leq 0)$$

$$\varepsilon(\mathbf{0},0) \geq 1$$

Rev. Mod. Phys., **53**, 81(1981)

Local field effects

- Lorentz-Lorenz formula

$$\varepsilon(\omega) = 1 + 4\pi n\alpha(\omega)/(1 - 4\pi/3\, n\alpha(\omega)) \qquad \alpha > 0$$

- General expression

local field corrections

$$\varepsilon(\mathbf{q},\omega) = 1 - \frac{(4\pi/q^2)\Pi_{eff}(\mathbf{q},\omega)}{1 + (4\pi/q^2)G(\mathbf{q})\Pi_{eff}(\mathbf{q},\omega)} \qquad \Pi_{eff} < 0$$

Wigner crystal

- Dielectric function

$$\frac{1}{\varepsilon(\mathbf{q},\omega)} = 1 - \frac{\omega_{\mathrm{pl}}^2}{q^2} \sum_{\lambda} \frac{\left(\mathbf{q}\mathbf{e}_{\mathbf{q}\lambda}\right)^2}{\omega^2(\mathbf{q},\lambda) - \omega^2}$$

$$\sum_{\lambda} \left(\mathbf{n}\mathbf{e}_{\mathbf{q}\lambda}\right)^2 = 1$$

$$\frac{1}{\varepsilon(\mathbf{q},0)} = \sum_{\lambda} \left\{ \left(\mathbf{n}\mathbf{e}_{\mathbf{q}\lambda}\right)^2 \left[1 - \frac{\omega_{\mathrm{pl}}^2}{\omega^2(\mathbf{q},\lambda)} \right] \right\} \leq 0$$

$$\sum_{\lambda} \omega^2(\mathbf{q},\lambda) = \omega_{\mathrm{pl}}^2$$

sum rule

$$\varepsilon(\mathbf{q},0) < 0$$

- Negative for all $\mathbf{q}$

Dielectric functions for real systems

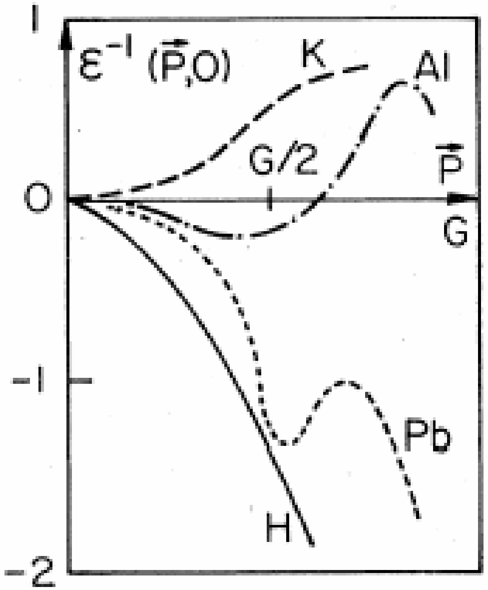


FIG. 2. Static dielectric function for normal metals (K, Al, Pb, and metallic H) vs wave vector in (1, 0, 0) direction (G—reciprocal lattice vector).

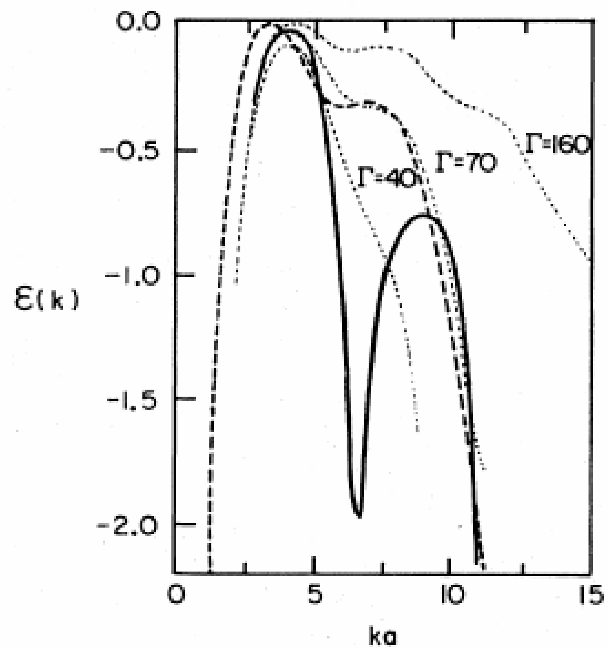


FIG. 1. Statistical dielectric function for classical charged fluids vs wave number. Dotted curves: classical one-component plasma, for three values of plasma parameter Γ; dashed curve: symmetric molten salt; full curve: molten

normal metals : *K, Al, Pb*

hypothetical metallic *H*

classical charge fluid

PHYSICAL REVIEW B 74, 094520 (2006)

Two bounds on the maximum phonon-mediated superconducting transition temperature

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(Received 2 June 2006; published 29 September 2006)

The argument of Cohen and Anderson postulates that stability requires the static dielectric function of a material to be positive, which leads to an upper bound on T_c of approximately 10 K. This bound and stability requirement are subsequently dismissed in the paper because of the neglect of local fields and umklapp processes, and further work[4] has clarified that stability only requires a positive static dielectric function at long wavelengths.

[4] O. V. Dolgov, D. A. Kirzhnits, and E. G. Maksimov, Rev. Mod. Phys. 53, 81 (1981).

Parameters, which determine Tc

$$T_c \approx \omega_{\ln} \exp[-\frac{1+\lambda}{\lambda-\mu^*}]$$

- large energies of intermediate bosons (phonons, excitons, spin-fluctuations, *etc*.)

$$\omega_{\ln} \approx \sqrt{\frac{1}{M}}$$

- large coupling constants

$$\lambda = 2\int d\Omega \alpha^2(\Omega) F(\Omega) \frac{1}{\Omega}$$

$$\alpha^2_{\mathbf{k}\lambda}(\Omega)F(\Omega) = \frac{1}{N(0)} \sum_{\mathbf{k}',\lambda',\nu} \left| g^{\lambda,\lambda',\nu}_{\mathbf{k}',\mathbf{k}} \right|^2 \delta(\omega_{\mathbf{k}'-\mathbf{k},\nu} - \Omega)\delta(\varepsilon_{\mathbf{k}'\lambda'}),$$

$\alpha^2 F(\omega)$ from tunneling conductance

- planar junctions $Bi_2Sr_2CaCu_2O_8 - GaAs$ (and Au)
- break-junctions from $Bi_2Sr_2CaCu_2O_8$

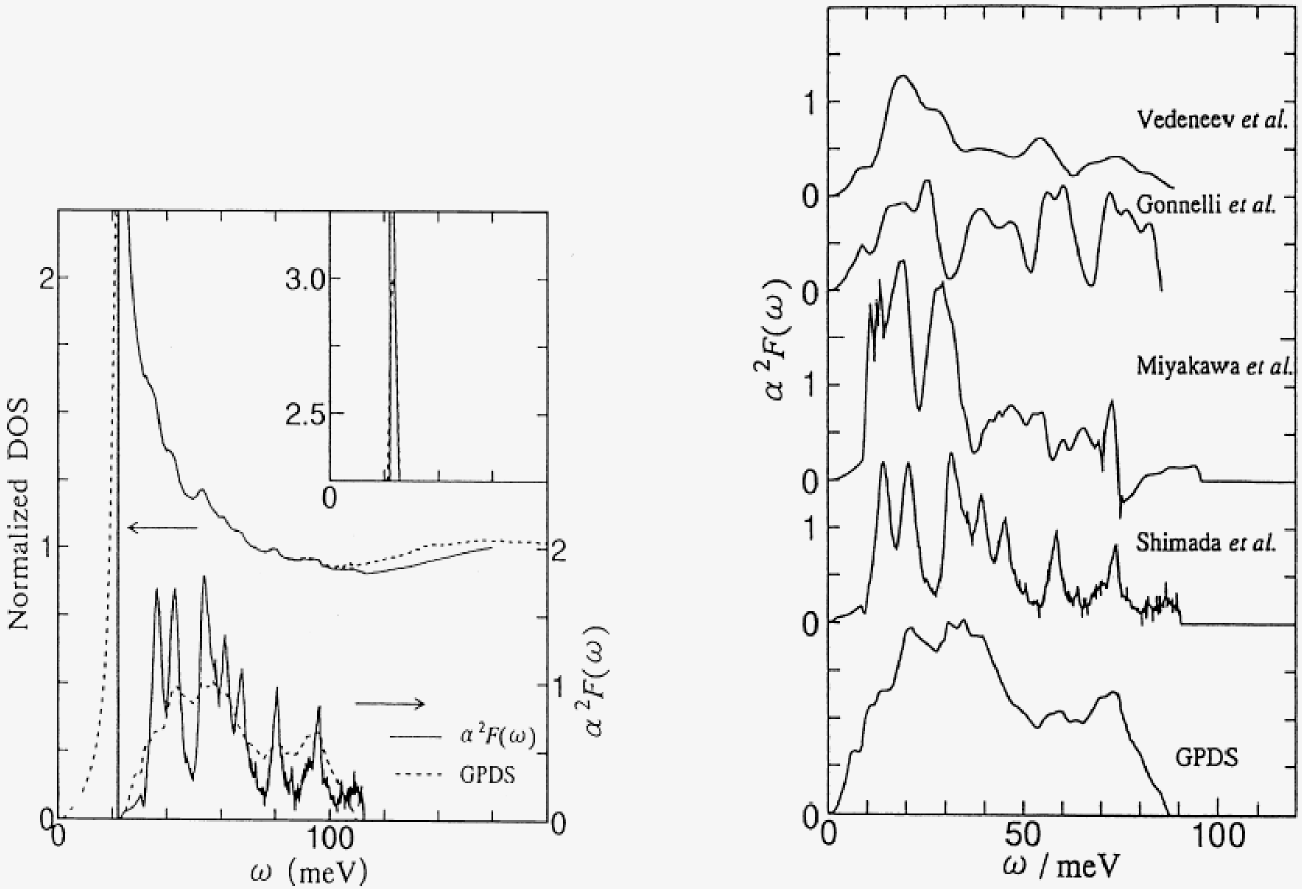


Fig. 58. The spectral function $\alpha^2F(\omega)$ and the calculated density of states at 0 K (upper solid line) obtained from the conductance measurements on the Bi(2212)–Au planar tunneling junction; from [42].

BCS, McMillan, Eliashberg

$$\Delta(i\omega_n)Z(i\omega_n) = \pi T \sum_{m=-\infty}^{+\infty} [\lambda\ (m-n) - \mu]\, \Delta(i\omega_m)/\,|\omega_m|$$

$$\omega_n Z(i\omega_n) = \omega_n + \pi T \sum_{m=-\infty}^{+\infty} \lambda\ (m-n) \qquad \text{sign}(\omega_m)$$

$$T_c \approx 1.14\omega_{ph} \exp\left[\frac{-1}{\lambda - \mu^*}\right]$$

1) $Z(0) = 1 + \lambda$ - mass renormalization

2) frequency dependence of 👎

$$\lambda \to \frac{\lambda}{1+\lambda}$$

1.14→1/1.2

Mass renormalization *increases* DOS;
why does it reduce the coupling?

Strong coupling

BCS $$1 = T_c \lambda \int_{-\theta_D}^{\theta_D} d\xi \sum_{n=-\infty}^{\infty} \frac{1}{(2n+1)^2 (\pi T_c)^2 + \xi^2};$$

$$2\pi T_c \ll \theta_D$$ or λ<<1

$$1 = \lambda \left[\ln\left(\theta_D / 2\pi T_c\right) - \ln\left(e^{-\gamma}/4\right) \right]$$

$$T_c \approx 1.13\, \theta_D \exp(-1/\lambda);$$

$$2\pi T_c \gg \theta_D$$ or λ>>1

$$1 \approx \lambda \frac{2\theta_D}{\pi^2 T_c}$$

$$T_c \approx \lambda \frac{2\theta_D}{\pi^2}$$

Strong coupling

BCS $$1 = T_c \lambda \int_{-\theta_D}^{\theta_D} d\xi \sum_{n=-\infty}^{\infty} \frac{1}{(2n+1)^2 (\pi T_c)^2 + \xi^2};$$

$$2\pi T_c \ll \theta_D$$ or λ<<1

Z $$1 = \lambda \left[\ln\left(\theta_D / 2\pi T_c\right) - \ln\left(e^{-\gamma}/4\right)\right]$$

$$T_c \approx 1.13\,\theta_D \exp(-1/\lambda);$$

$$2\pi T_c \gg \theta_D$$ or λ>>1

$$1 \approx \lambda \frac{2\theta_D}{\pi^2 T_c}$$

$$T_c \approx \lambda \frac{2\theta_D}{\pi^2}$$

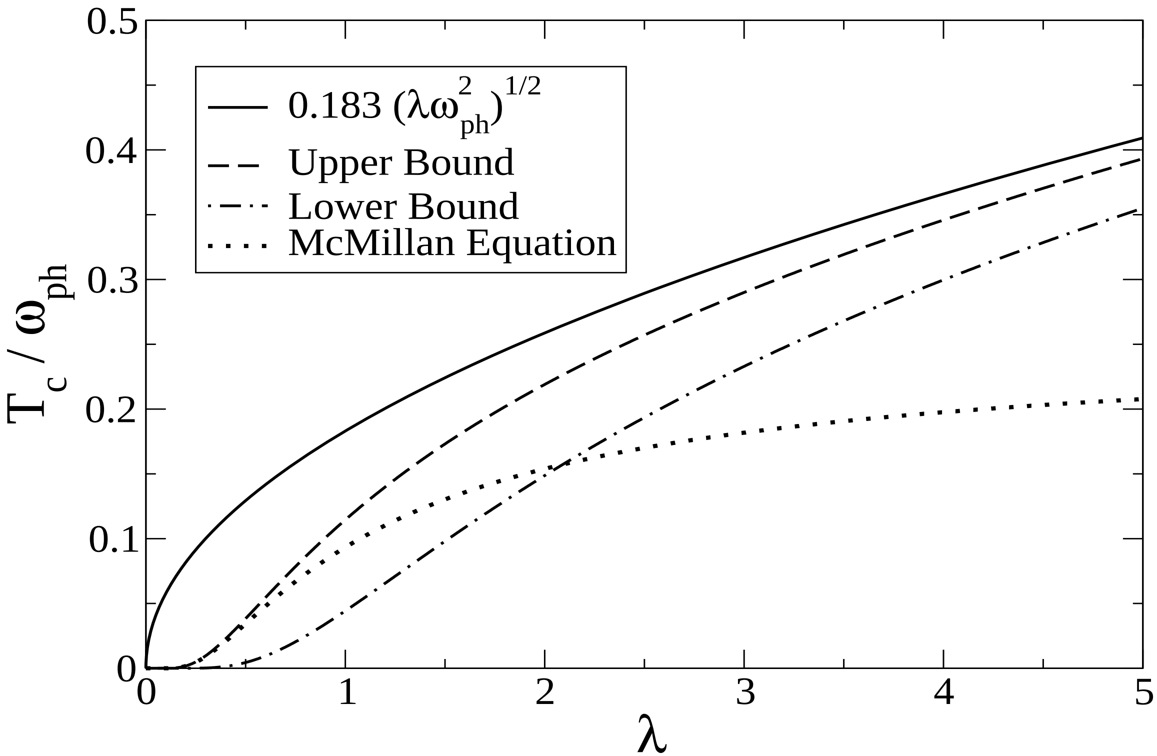
(λ crossed out, replaced by √λ)

Superstrong coupling (λ>>1)

$$0 \le T_c \le 0.183\underline{\sqrt{\lambda\langle\omega^2\rangle}}.$$

$$\tilde{\lambda}\langle\tilde{\omega}^2\rangle = \sum_i \frac{\tilde{\eta}_i}{M_i}.$$

$$\tilde{\eta}_i(E) = \sum \left| \langle \ldots \frac{\partial V_{SCF}}{\ldots} \ldots \rangle \right|^2 \delta(E - E \ldots)$$



Metallic Hydrogen

E.G.Maksimov,D.Savrasov

SSC.**119**,569 (2001)

$$\Omega_{pl} = \sqrt{\frac{4\pi e^2 n}{M}}. \qquad (9)$$

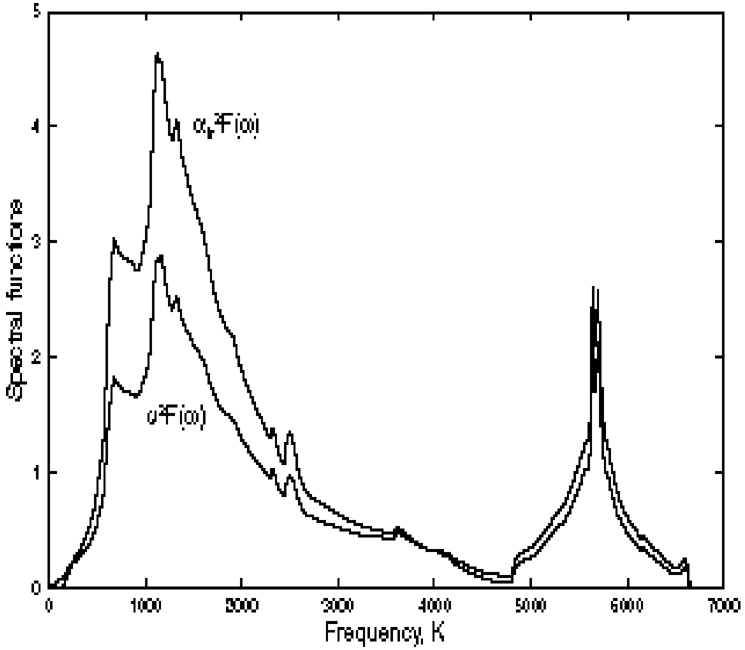
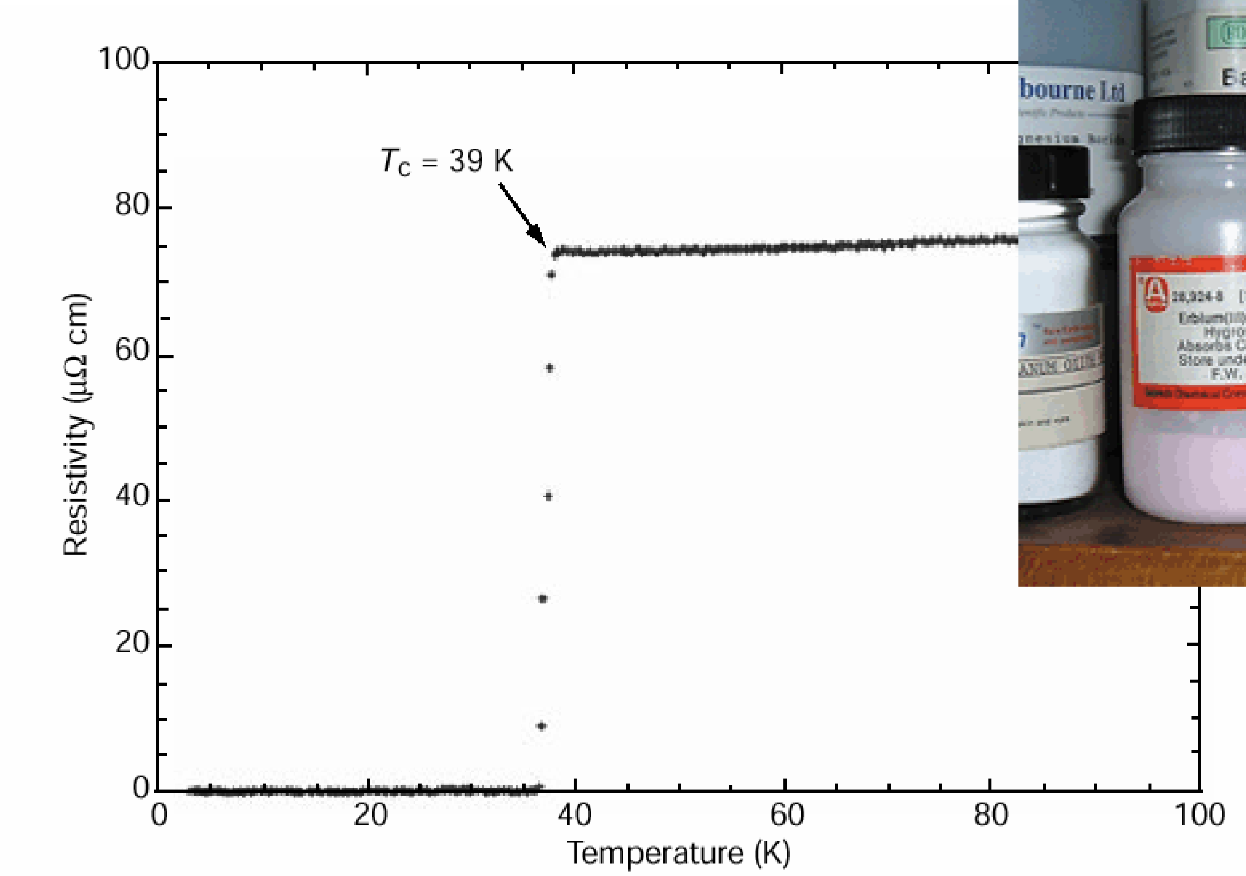


Fig. 2. Calculated spectral and transport spectral function of electron–phonon interaction of metallic hydrogen in FCC lattice for $r_s = 1$.

λ=7.33,

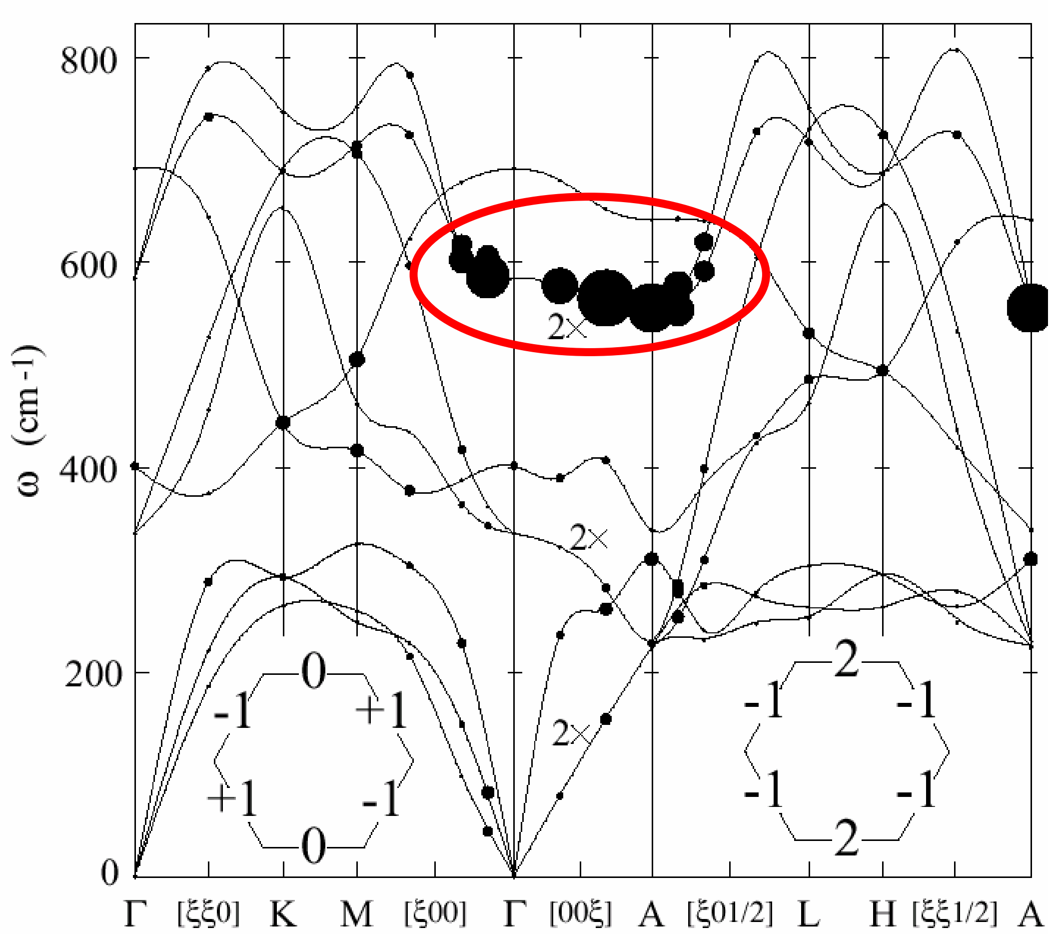
Tc= 600 K !

Superconductivity at 39K in MgB_2



Akimitsu *et al.* Nature (London) **410**, 63 (2001)

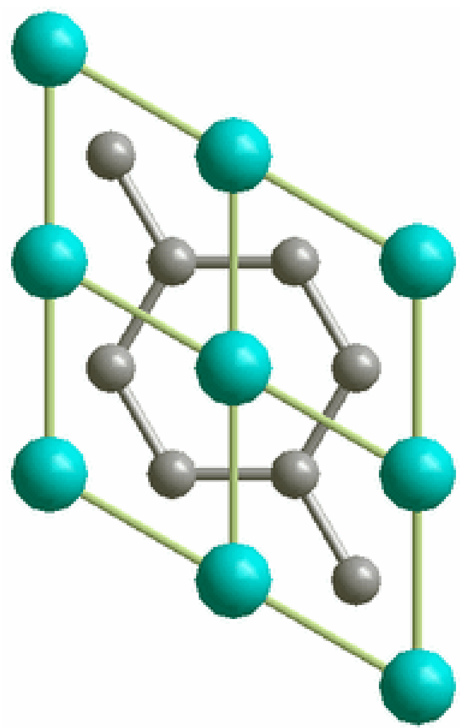
Something unusual is going on

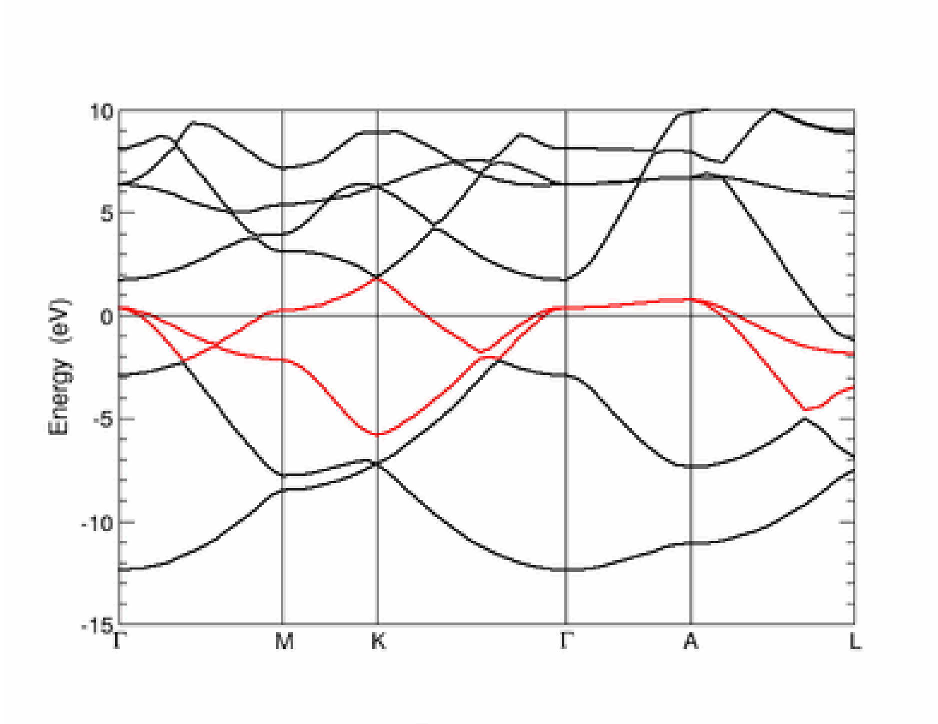


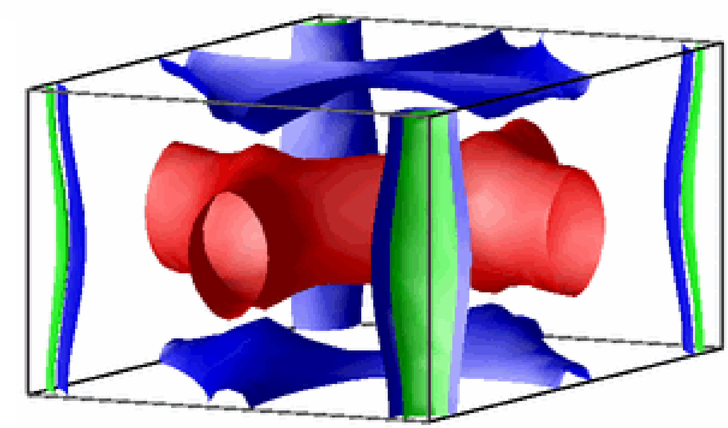
The quasi-2D ♦ bands couple to the optical B-B bond-stretching modes which are softened by the e-ph coupling and are strongly anharmonic.

Kong, OVD, Jepsen, Andersen PRB 64, 020501(R) (2001)

Coupling of the E_{2g} phonon mode to the electronic structure







Journal of Superconductivity and Novel Magnetism, Vol. 19, Nos. 3–5. Julv 2006 (C 2006)

Electron–Phonon-Induced Superconductivity

Marvin L. Cohen[1,2]

Published online: 12 December 2006

Some background regarding the evolution of calculations, predictions, and approaches to understand and increase T_c for phonon-mediated superconductivity is presented. This is followed by a description of a successful "after the fact" theoretical study of MgB_2 and a description of current thinking about the relationship between phonon renormalization and T_c. It is then argued that in the search for high T_cs the evolution has gone from searching for high density of states materials to high electron–phonon couplings described by λ. Finally, it is suggested that the focus on finding large λ can be supplemented by a search for large electronic spring constants η. This is expected to be particularly relevant for the highest T_c materials in this class of superconductors.

KEY WORDS: Superconductivity; electron-phonon interactions; superconducting transition temperature maximizing.

Journal of Superconductivity and Novel Magnetism, Vol. 19, Nos. 3−5, July 2006

Journal of Superconductivity and Novel Magnetism, Vol. 19, Nos. 3−5, July 2006

Design for a Room-Temperature Superconductor

W. E. Pickett[1]

Published online: 19 December 2006

The vision of "room-temperature superconductivity" has appeared intermittently but prominently in the literature since 1964, when W. A. Little and V. L. Ginzburg began working on the *problem of high-temperature superconductivity* around the same time. Since that time the prospects for room-temperature superconductivity have varied from gloom (around 1980) to glee (the years immediately after the discovery of HTS), to wait-and-see (the current feeling). Recent discoveries have clarified old issues, making it possible to construct the blueprint for a viable room-temperature superconductor.

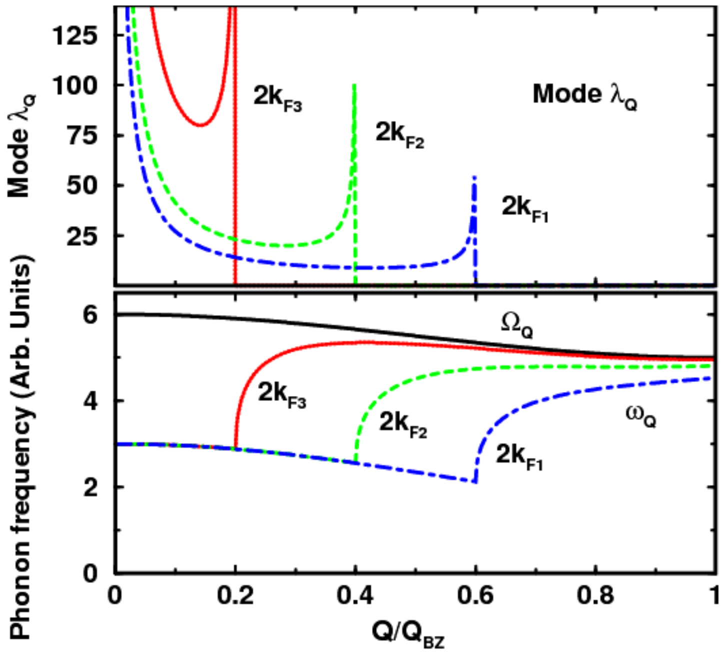
W.E. Pickett: Tc=430K !!!

λ=22.5

Problems:

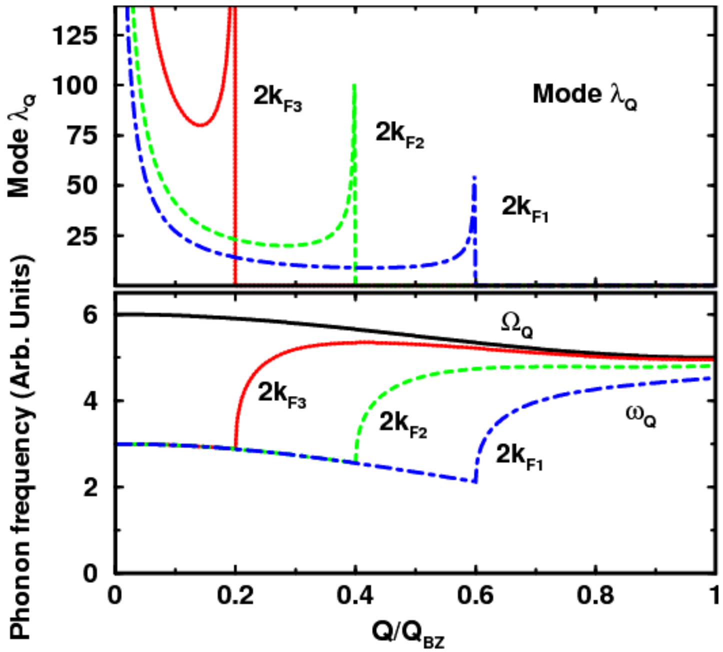
- lattice stability ?
- pair-breaking effect by low-energy phonons (*Dolgov&Golubov, PRB*, ***77***, *214526(2008)*)

This extension from MgB_2 is not yet optimum, because MgB_2 uses only 2/9 of its branches. Optimally, every branch would be drafted into service in strong coupling, giving another factor of 4.5, or a total enhancement of ~30–35. The strongly coupled modes in MgB_2 have mode-λ_Q's of mean value 20–25 (calculations so far have not been precise enough to pin this down). Let us not be pessimistic, and therefore use $\bar{\lambda}_Q = 25$; this value is consistent with the value of λ from the strongly coupled modes divided by 3%, i.e. $0.7/0.03 \sim 23$. Then with 90% participation of the phonons $\lambda = 25 \times 0.90 = 22.5$. Using the Allen–Dynes equation [33] to account properly for the strong-coupling limit that is being approached, and using the MgB_2 frequency of 60 meV, one obtains $T_c = 430$ K. The strong coupling limit [34] of the ratio $2\Delta/k_B T_c$ is 13, so we can estimate the gap of such a superconductor to be $2\Delta \sim 12 k_B T_c \sim 0.4$ eV. This will be an interesting superconductor indeed.



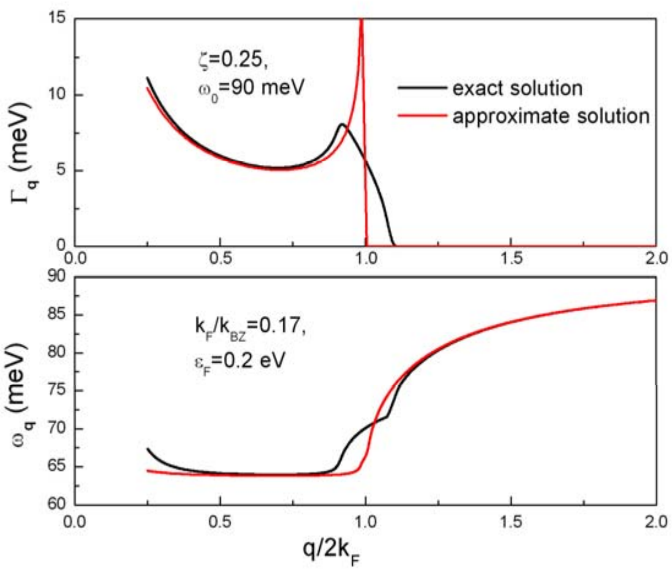
$$\lambda_{\mathbf{Q}} = \frac{1}{MN(0)\omega_{\mathbf{Q}}^2} \sum_{\mathbf{k}} | g_{\mathbf{k},\mathbf{k}+\mathbf{Q}} |^2 \delta(\varepsilon_{\mathbf{k}}) \delta(\varepsilon_{\mathbf{k}+\mathbf{Q}})$$

W.E. Pickett



$$\lambda_{\mathbf{Q}} = \frac{1}{MN(0)\omega_{\mathbf{Q}}^2} \sum_{\mathbf{k}} |g_{\mathbf{k},\mathbf{k+Q}}|^2 \delta(\varepsilon_{\mathbf{k}})\delta(\varepsilon_{\mathbf{k+Q}})$$

W.E. Pickett



$$\lambda_{\mathbf{Q}} = \frac{1}{MN(0)} \sum_{\mathbf{k}} |g_{\mathbf{k},\mathbf{k+Q}}|^2 \frac{\delta(\varepsilon_{\mathbf{k}})\delta(\varepsilon_{\mathbf{k+Q}})}{\omega_{\mathbf{Q}}^2 + \Gamma_{\mathbf{Q}}^2}$$

O.V.D., O.K. Andersen, I.I. Mazin
PRB (2008)

Phys. Rev. B **74**,094520 (2006)

Two Bounds on the Maximum Phonon-Mediated Superconducting Transition Temperature

Jonathan E. Moussa* and Marvin L. Cohen
Department of Physics, University of California at Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

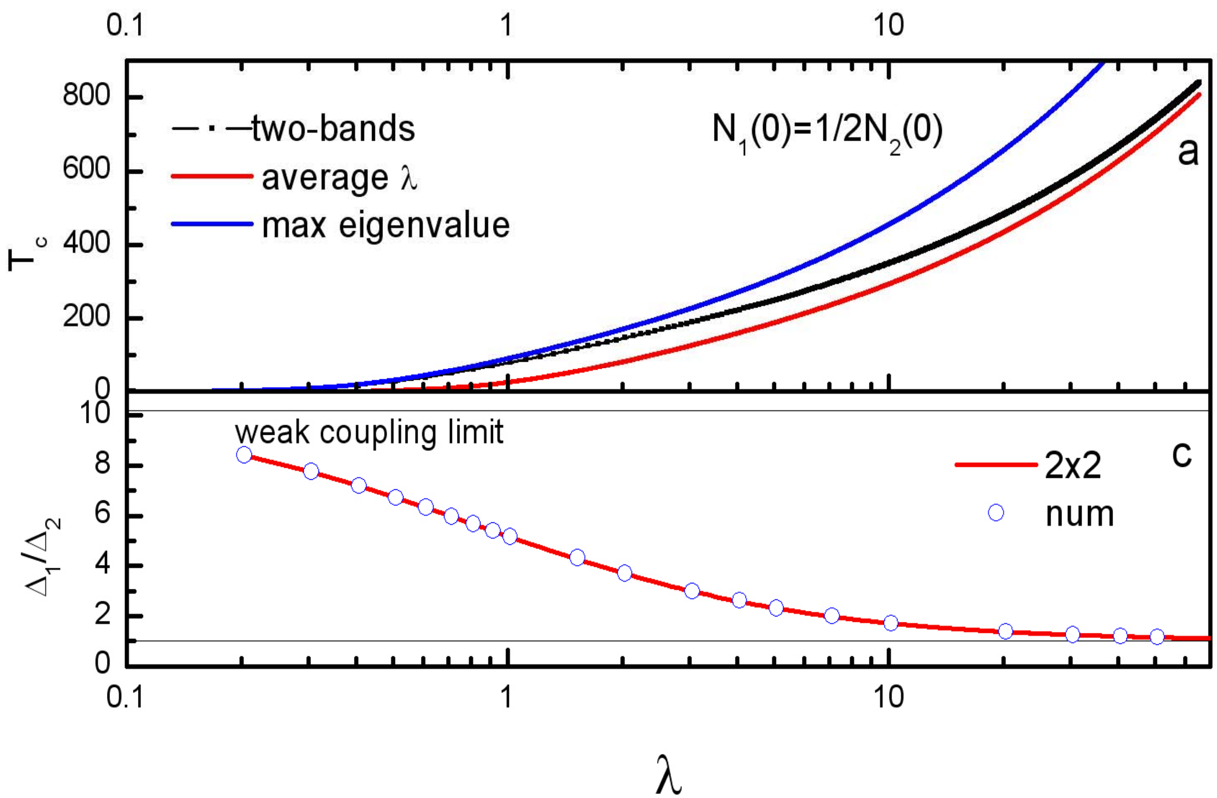
(Dated: July 31, 2006)

Two simple bounds on the T_c of conventional, phonon-mediated superconductors are derived within the framework of Eliashberg theory in the strong coupling regime. The first bound is set by the total electron-phonon coupling available within a material given the hypothetical ability to arbitrarily dope the material. This bound is studied by deriving a generalization of the McMillan-Hopfield parameter, $\tilde{\eta}(E)$, which measures the strength of electron-phonon coupling including anisotropy effects and rigid-band doping of the Fermi level to E. The second bound is set by the softening of phonons to instability due to strong electron-phonon coupling with electrons at the Fermi level. We apply these bounds to some covalent superconductors including MgB_2, where T_c reaches the first bound, and boron-doped diamond, which is far from its bounds.

Hypothetical *BC* (boron-doped diamond)

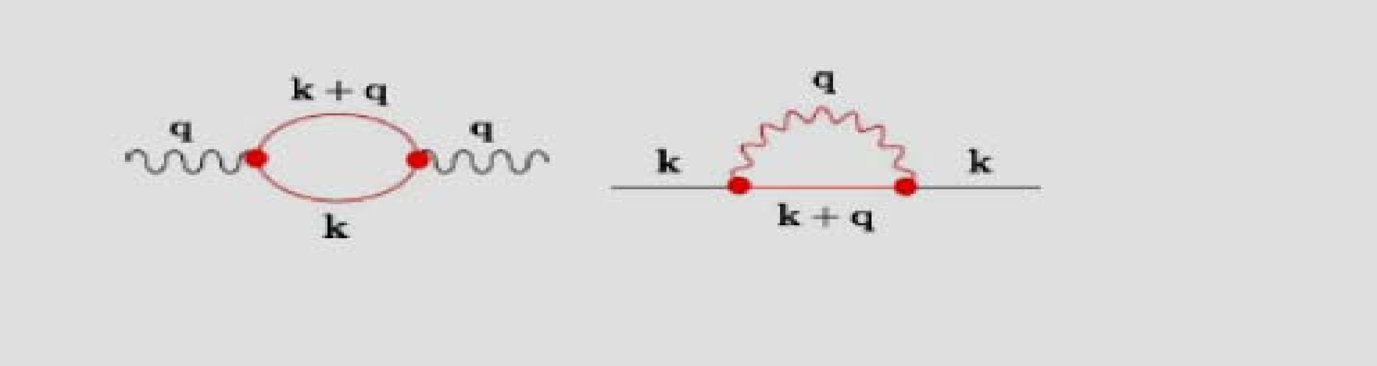
λ=3.6, T_c=140 – 160 K

Anisotropy vanishes for strong coupling



OVD, A.A. Golubov, PRB, **77**, 214526 (2008)

Phonon instability

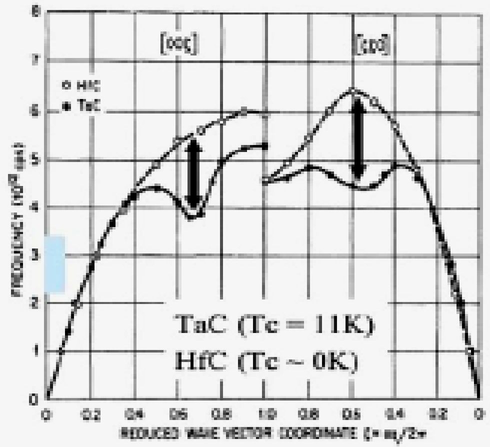


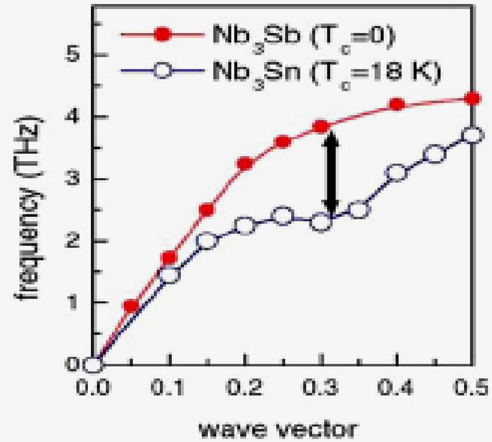
$$\omega_{\mathbf{q}}^2 = \omega_{bare}^2 - 2\sum_{\mathbf{k}} \frac{|g|^2}{M} \frac{n_{\mathbf{k}} - n_{\mathbf{k+q}}}{\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k}}}$$

$$\Sigma(\mathbf{k},\omega) = \sum_{\mathbf{q}} \delta(\varepsilon_{\mathbf{k+q}}) \frac{|g|^2}{2M} \int d\xi \left[\frac{\theta(\xi)}{\omega - \xi - \omega_{\mathbf{q}} + i\delta} + \frac{\theta(-\xi)}{\omega - \xi + \omega_{\mathbf{q}} - i\delta} \right]$$

$$\lambda_A = \frac{N(0)\,|\,g\,|^2}{M\omega_{bare}^2}; \lambda = \frac{N(0)\,|\,g\,|^2}{M\omega_{\mathbf{q}}^2}$$

$$\lambda = \lambda_A \Big/ 1 - 2\lambda_A$$

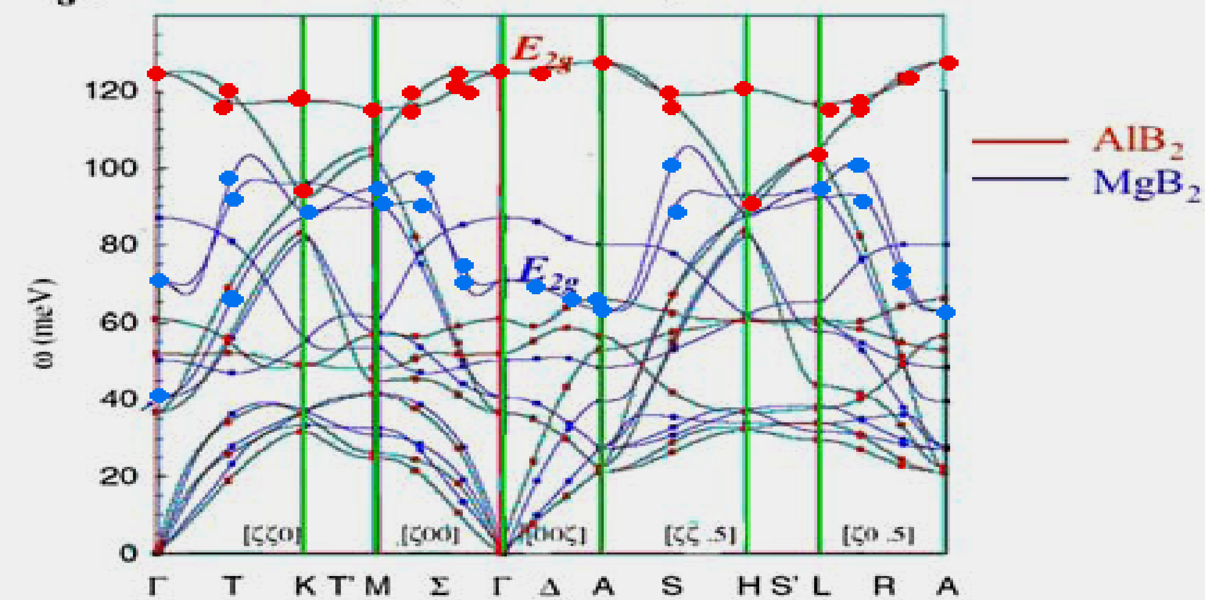




H. G. Smith and W. Glaser, PRL 25, 1611 (1970).

L. Pinstchovius et al., PRL 54, 1260 (1985)
L. Pinstchovius et al. PRB 28, 5866 (1983)
L. Pintschovius, phys. stat. sol. (b) 242, 30 (2005)

E_{2g} phonon in MgB_2 and AlB_2



K. P. Bohnen, R. Heid, and B. Renker, PRL 86, 5771 (2001).

Excitonic mechanisms

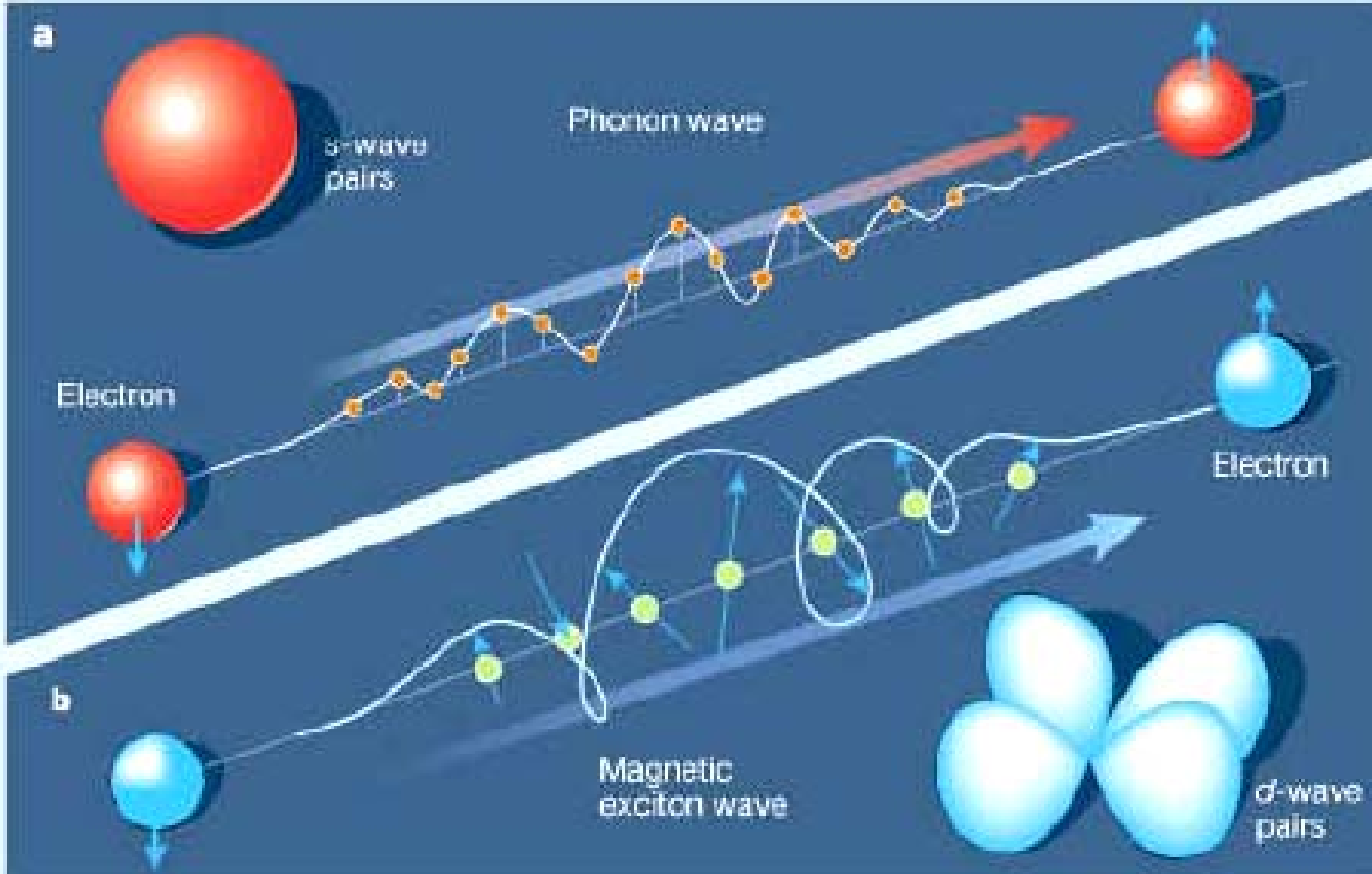
- Negative Electronic Dielectric Function

$$\varepsilon_{el}(\mathbf{q},0) < 0$$

- Problems with the stability of phonons

$$\omega_{ph}{}^2(\mathbf{q}) = \frac{\Omega^2_{pl}}{\varepsilon_{el}(\mathbf{q},0)} \leq 0; \qquad \Omega^2_{pl} = \frac{4\pi Z_i{}^2 e^2 N_i}{M_i}$$

Interaction via spin-waves

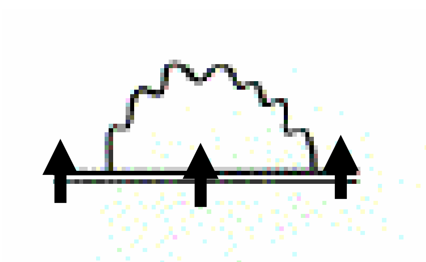


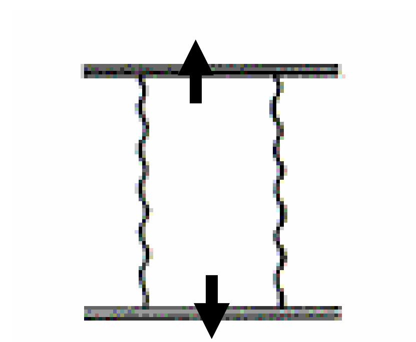
Spin fluctuations

• How exactly are spin fluctuations different from phonons?

• Phonon induced superconductivity is much better understood than spin-fluctuation induced (despite comparable history – *Berk-Schrieffer ‘66, Fay-Appel ’77-80*)

• Opposite effect of ●$_{SF}$ on Z and on 👎 (in singlet pairing):





Spin fluctuations *increase* the mass but *decrease* the net pairing strength

Spin resonance B.Keimer(2002)

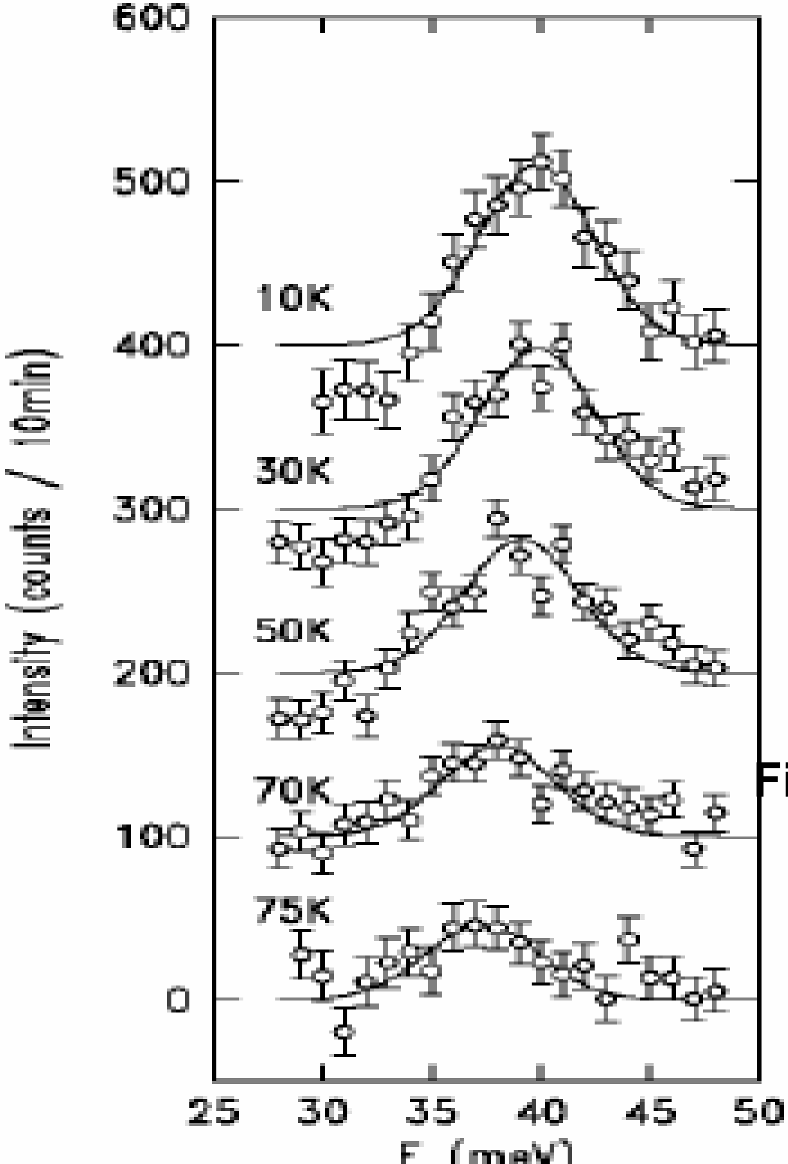
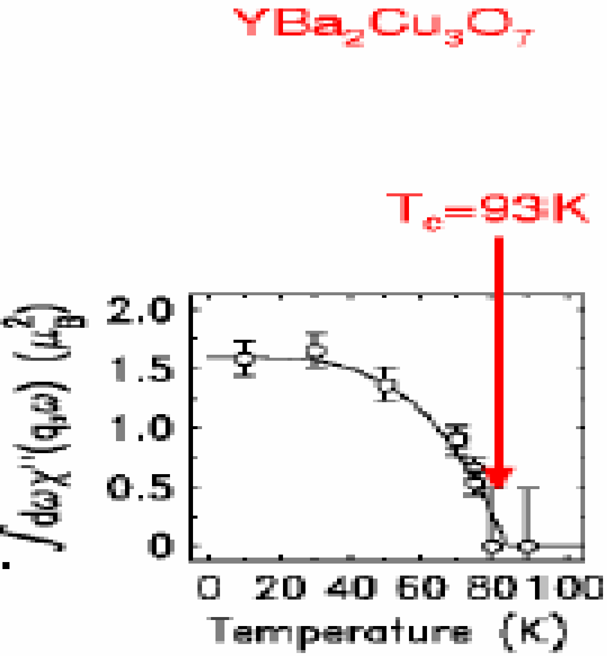
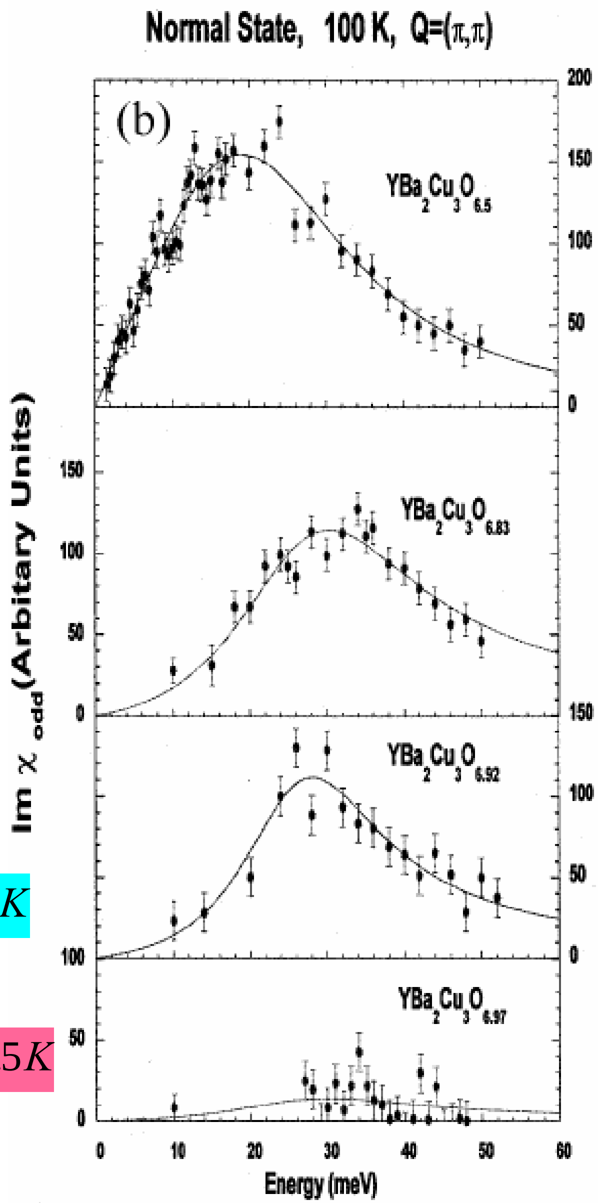


Fig.



Magnetic neutron scattering and NMR against SFI

⇓

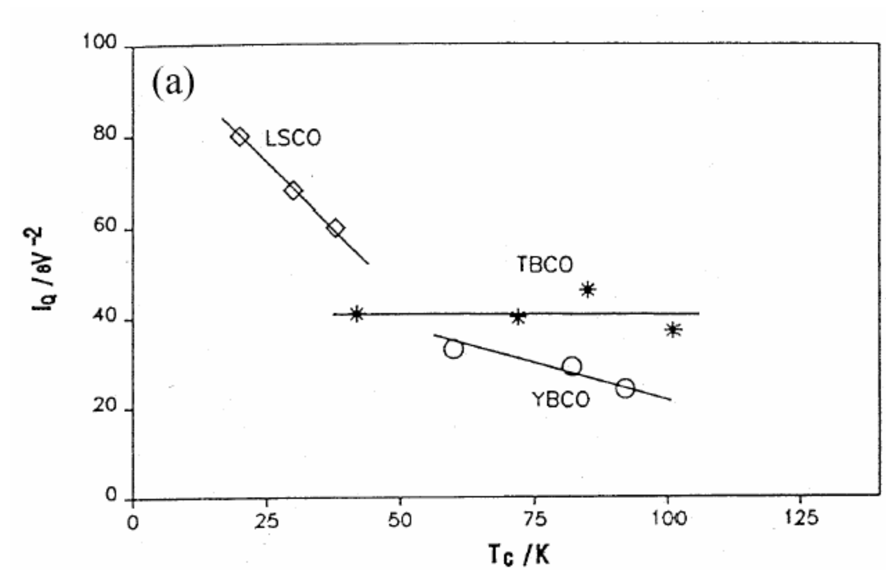


$T_c = 91K$

$T_c = 92.5K$

⇓

$$I_Q = \lim_{\omega \to 0} (\mathrm{Im}\,\chi(\mathbf{Q},\omega)/\omega)$$



$$\lambda_{sf}^{pair} \sim g_{sfi}^2 \int d\omega \frac{\mathrm{Im}\,\chi(\mathbf{Q},\omega)}{\omega}$$

- big change of $\chi(\mathbf{Q},\omega)$ but small change of T_c !

Spin fluctuations

$$\tilde{\lambda}_{\mathrm{sp}} = 2\sum_{\mathbf{q}}\int_0^T \frac{\mathrm{d}\omega}{\omega}\, g_{\mathrm{sp}}^2\, \mathrm{Im}\,\chi(\mathbf{q},\omega)\,.$$

$$n_{\mathrm{s}} \sim \sum_{\mathbf{q}}\int_0^\infty \mathrm{d}\omega\, \mathrm{Im}\,\chi(\mathbf{q},\omega)\,.$$

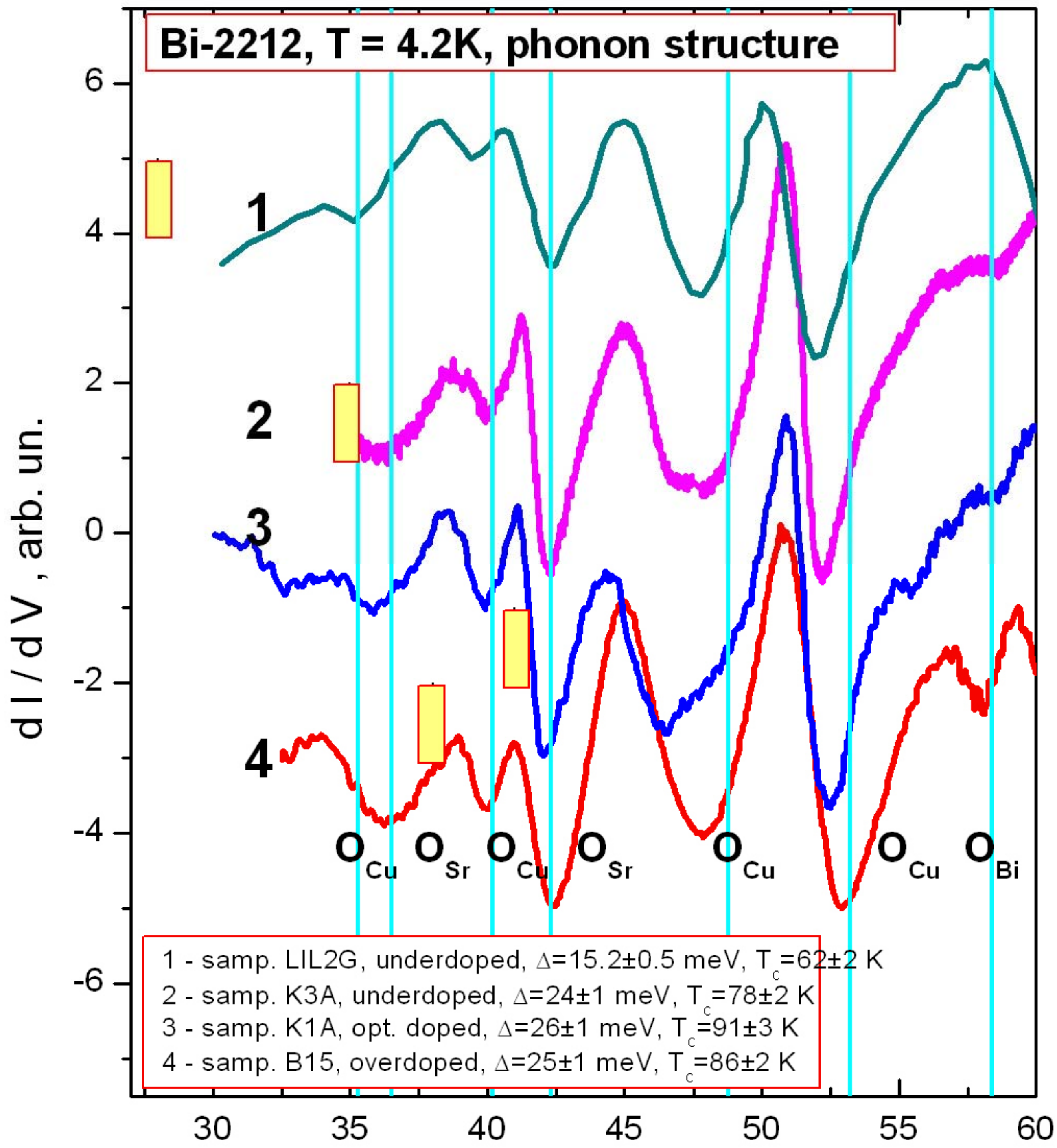
$$\tilde{n}_{\mathrm{s}} \sim \sum_{\mathbf{q}}\int_0^T \mathrm{d}\omega\, \mathrm{Im}\,\chi(\mathbf{q},\omega)\,.$$

$$n_{\mathrm{s}} \sim 1.$$

$$\tilde{\lambda}_{\mathrm{sp}} = \lambda_{\mathrm{sp}}\frac{\tilde{n}_{\mathrm{s}}}{n_{\mathrm{s}}}\,,$$

$$\tilde{n}_s \approx 3.2\%$$

$$\lambda_{sp} \approx \frac{t}{ZU} \approx 0.1$$



Bi-2212, T = 4.2K, phonon structure
d I / d V , arb. un.
6
4
2
0
-2
-4
-6
30
35
40
45
50
55
60
1
2
3
4
O Cu
O Sr
O Cu
O Sr
O Cu
O Cu
O Bi
1 - samp. LIL2G, underdoped, Δ=15.2±0.5 meV, T c=62±2 K
2 - samp. K3A, underdoped, Δ=24±1 meV, T c=78±2 K
3 - samp. K1A, opt. doped, Δ=26±1 meV, T c=91±3 K
4 - samp. B15, overdoped, Δ=25±1 meV, T c=86±2 K

d-wave

Non-phonon

$$Z(i\omega_n)\Delta(\mathbf{k},i\omega_n)=\pi T_c\sum_{n'}^{\Omega_{\mathrm{n.ph}}}\sum_{\mathbf{q}}V_{\mathrm{n.ph}}(\mathbf{k},\mathbf{q},\omega_n,\omega_{n'})\frac{\Delta(\mathbf{q},i\omega_{n'})}{|\omega_{n'}|}$$

$$Z(i\omega_n)\approx 1+\Gamma_{ep}/\omega_n.$$

$$\Gamma_{ep}\approx 2\pi\lambda_{ep}T$$

d-wave

Non-phonon

$$Z(i\omega_n)\Delta(\mathbf{k}, i\omega_n) = \pi T_c \sum_{n'}^{\Omega_{\text{n.ph}}} \sum_{\mathbf{q}} V_{\text{n.ph}}(\mathbf{k}, \mathbf{q}, \omega_n, \omega_{n'}) \frac{\Delta(\mathbf{q}, i\omega_{n'})}{|\omega_{n'}|}$$

$$Z(\omega) \approx 1 + i\Gamma_{ep} / \omega \, .$$

✍$_{ep}$ ◆ 2 γ✞$_{ep}$ T

Damping due to phonons

T_c ◆ $T_{c0}\, e^{-}$✍✞$_{ep}$.

d-wave

Non-phonon

$$Z(i\omega_n)\Delta(\mathbf{k},i\omega_n) = \pi T_c \sum_{n'}^{\Omega_{\mathrm{n.ph}}} \sum_{\mathbf{q}} V_{\mathrm{n.ph}}(\mathbf{k},\mathbf{q},\omega_n,\omega_{n'}) \frac{\Delta(\mathbf{q},i\omega_{n'})}{|\omega_{n'}|}$$

$$Z(\omega) \approx 1 + i\Gamma_{ep}/\omega .$$

$$\Gamma_{ep} \approx 2\pi\lambda_{ep} T$$

Damping due to phonons

$$T_c \approx T_{c0}\, e^{-\lambda_{ep}} .$$

For λ_{ph}~1-2, and T_c~160 K

bare $T_{c0} \approx (400 - 1100)$ K !!!

d-wave

Non-phonon

$$Z(i\omega_n)\Delta(\mathbf{k},i\omega_n) = \pi T_c \sum_{n'}^{\Omega_{\mathrm{n.ph}}} \sum_{\mathbf{q}} V_{\mathrm{n.ph}}(\mathbf{k},\mathbf{q},\omega_n,\omega_{n'}) \frac{\Delta(\mathbf{q},i\omega_{n'})}{|\omega_{n'}|}$$

$$Z(\omega) \approx 1 + i\Gamma_{ep}/\omega .$$

$$\Gamma_{ep} \approx 2\pi\lambda_{ep} T$$

Damping due to phonons

$$T_c \approx T_{c0}\, e^{-\lambda_{ep}} .$$

For λ_{ph}~1-2, and T_c~160 K

bare $T_{c0} \approx (400 - 1100)$ K !!!

Conclusions

- There are NO formal restrictions on T_c.
- There are some problems with phonon instabilities for all mechanisms.
- The ROOM-TEMPERATURE superconductivity is not the myth, but the object for investigations.

LaOFeAs, a not-so-simple superconductor

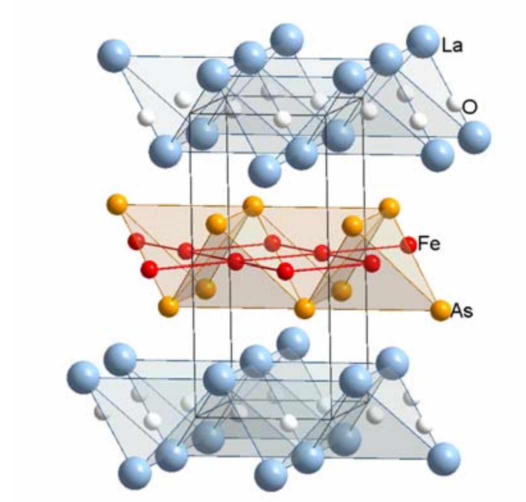
J|A|C|S
COMMUNICATIONS

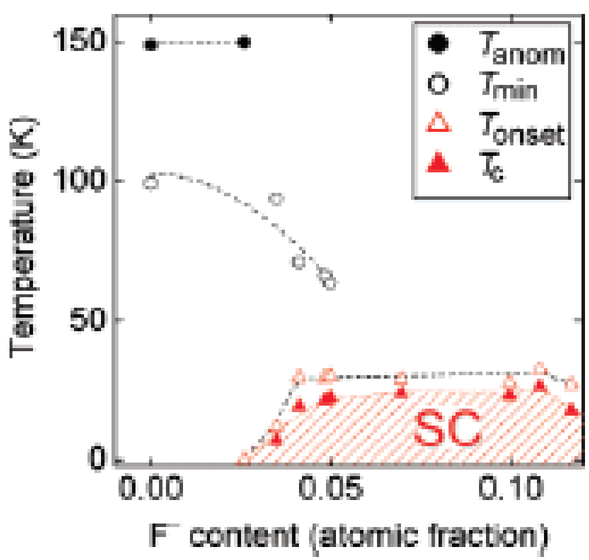
Published on Web 02/23/2008

Iron-Based Layered Superconductor $La[O_{1-x}F_x]FeAs$ ($x = 0.05-0.12$) with $T_c = 26$ K

Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

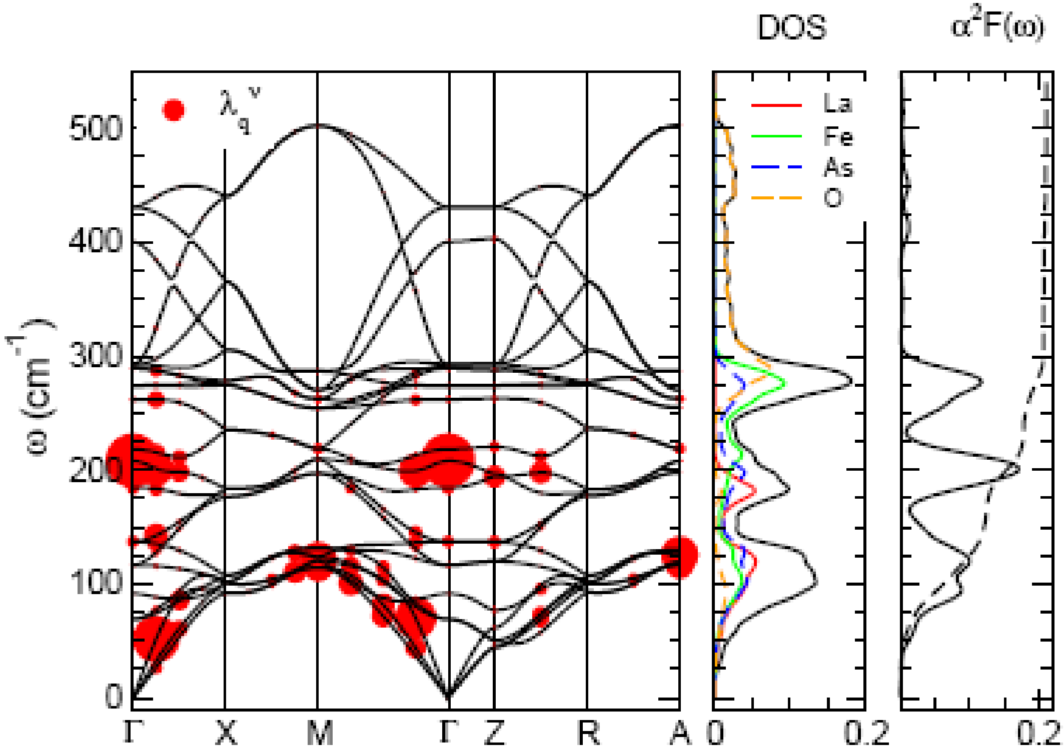
ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan





- 2008: $LaO_{1-x}F_xFeAs$ Tc^{max}=26 K at x=0.11
- Tetragonal layers of La-O + Fe-As
- F replaces O and dopes electrons into the system.
- Replacing La with other Rare-Earths increases Tc up to 55 K (Sm).
- EXP: small coherence length, T-dependent Hall coefficient, no jump in specific heat at Tc, specific heat + point contact: nodes in the gap ?

LaOFeAs, Electron-phonon coupling



$$\lambda = 0.21$$

$$\omega_{\log} = 206K$$

$$T_c^{ME} \leq 0.5K$$

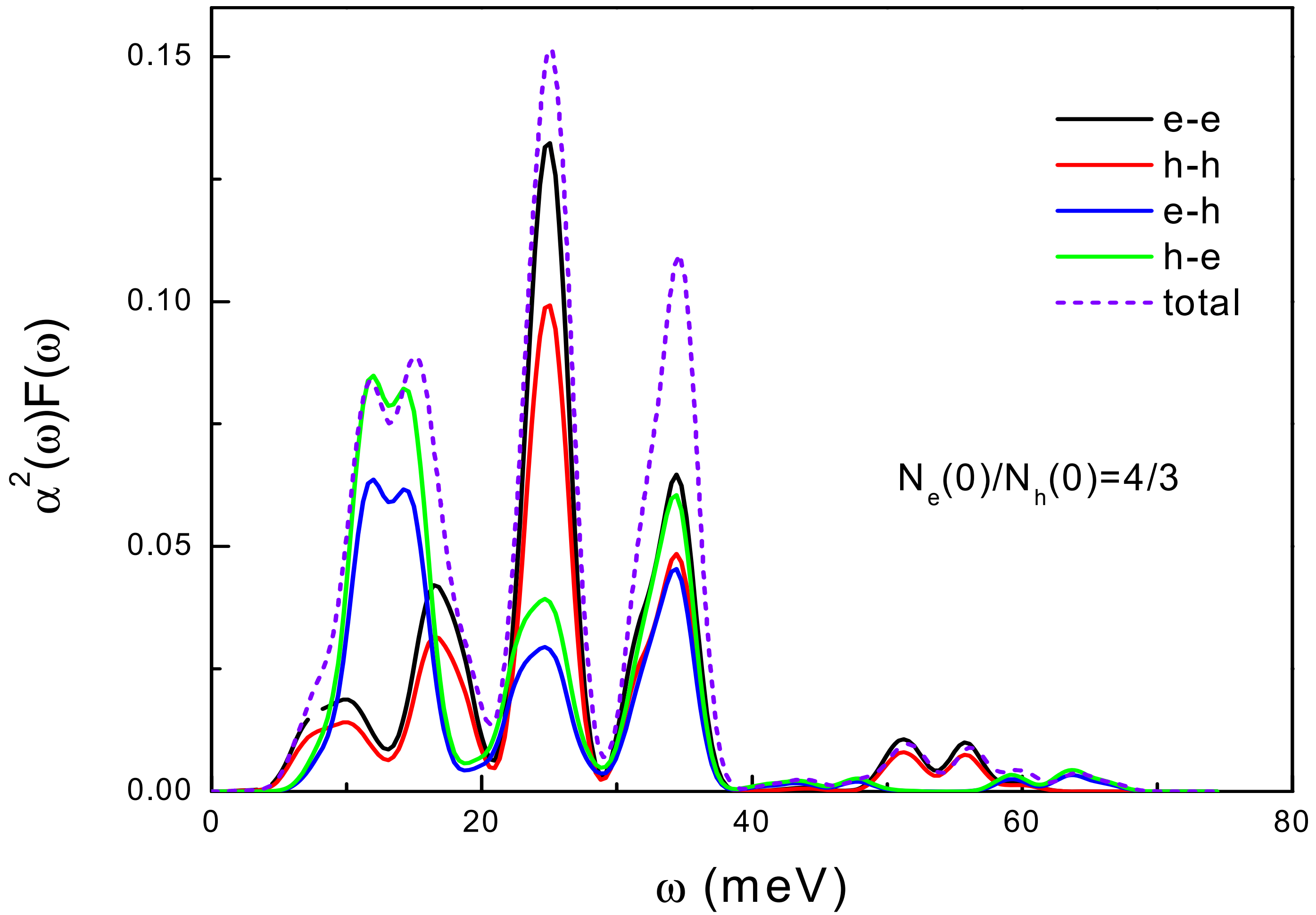
$$N(0) = 2.1 st/eV$$

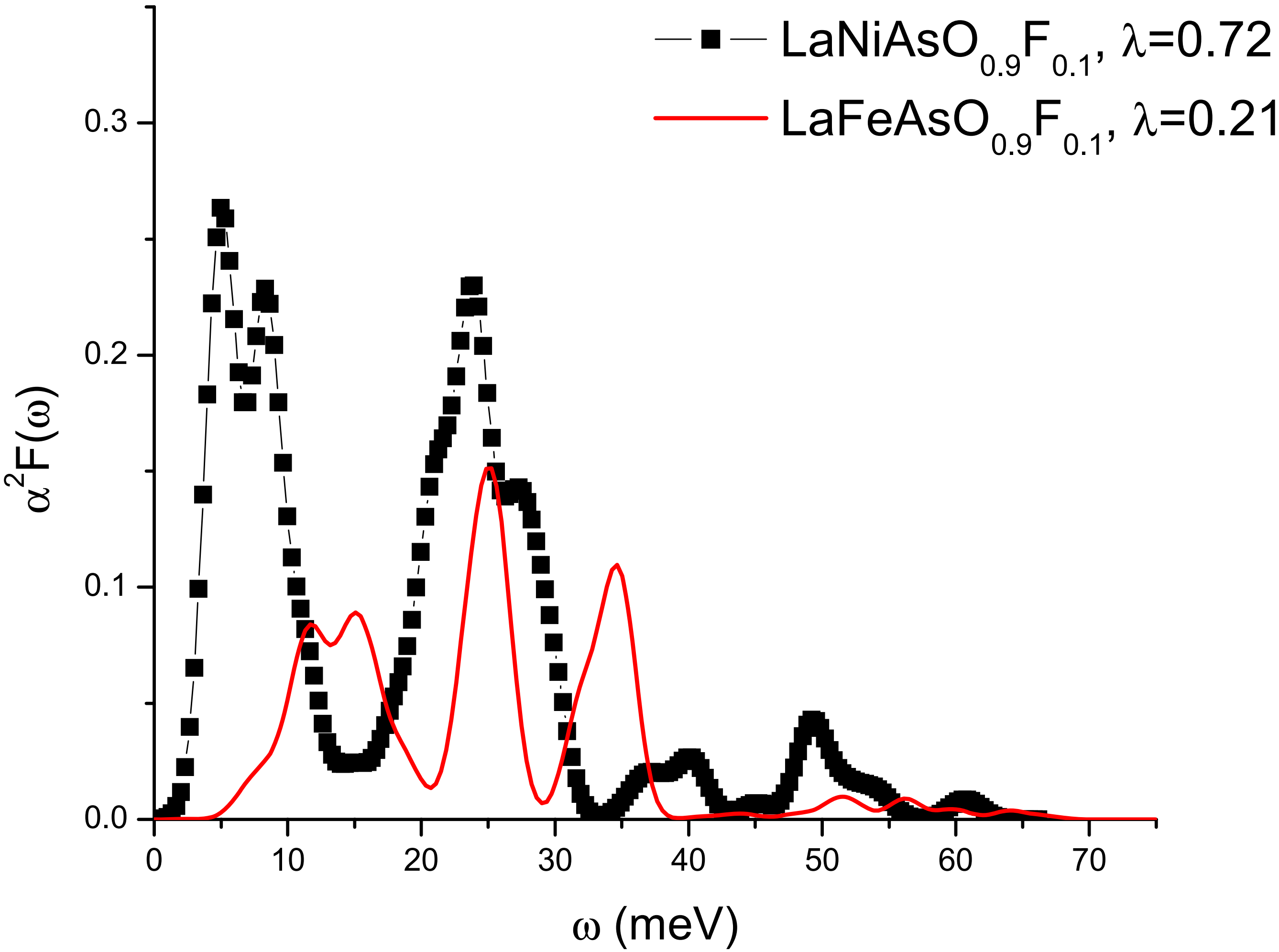
L. Boeri, OVD, A.A. Golubov, PRL, 101, 026403 (2008)

- E-ph interaction: λ~0.2 is too small to account for T_c
- Doping can only decrease λ.
- N(0) is large, λ is small because of small e-ph matrix elements.
- The coupling is uniform over phonon modes: the only directed bands sit far from E_F.
- Possible two-gap scenario with large repulsive interband interaction

$$\lambda = \begin{pmatrix} 0.111 & 0.093 \\ 0.124 & 0.083 \end{pmatrix}$$

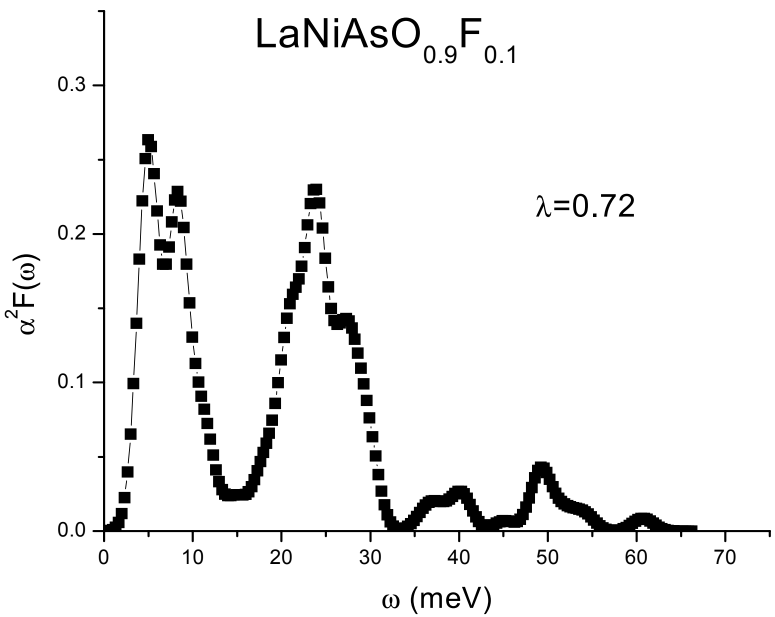
$T_c = 0.8$ K



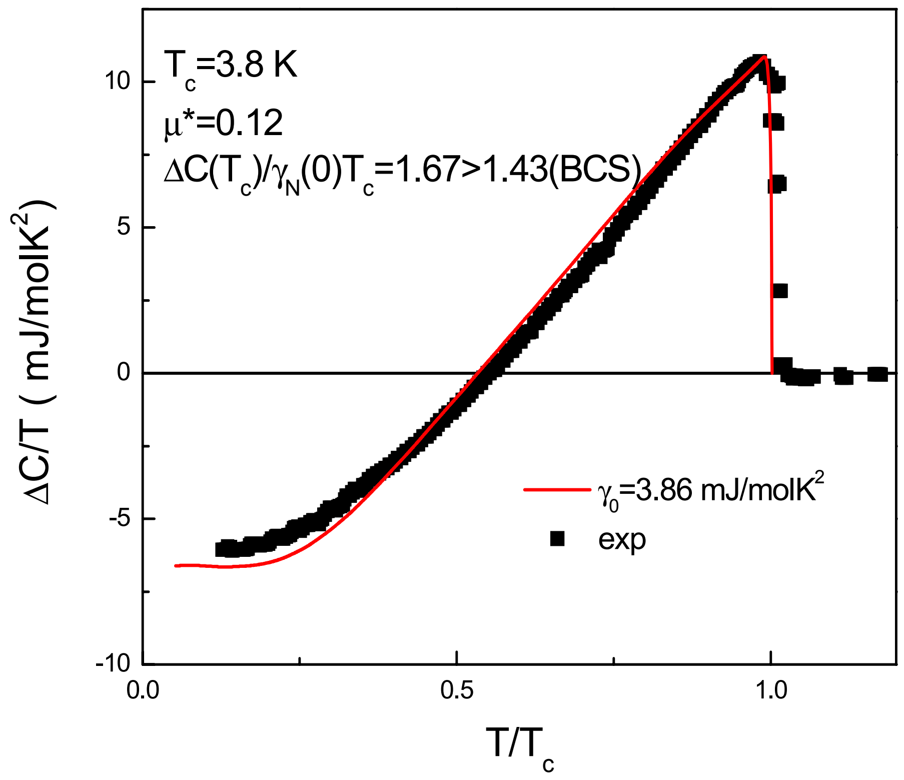


LaNiAsO0.9F0.1, λ=0.72
LaFeAsO0.9F0.1, λ=0.21
α2F(ω)
ω (meV)
0.0
0.1
0.2
0.3
0
10
20
30
40
50
60
70

$LaNiAsO_{0.9}F_{0.1}$

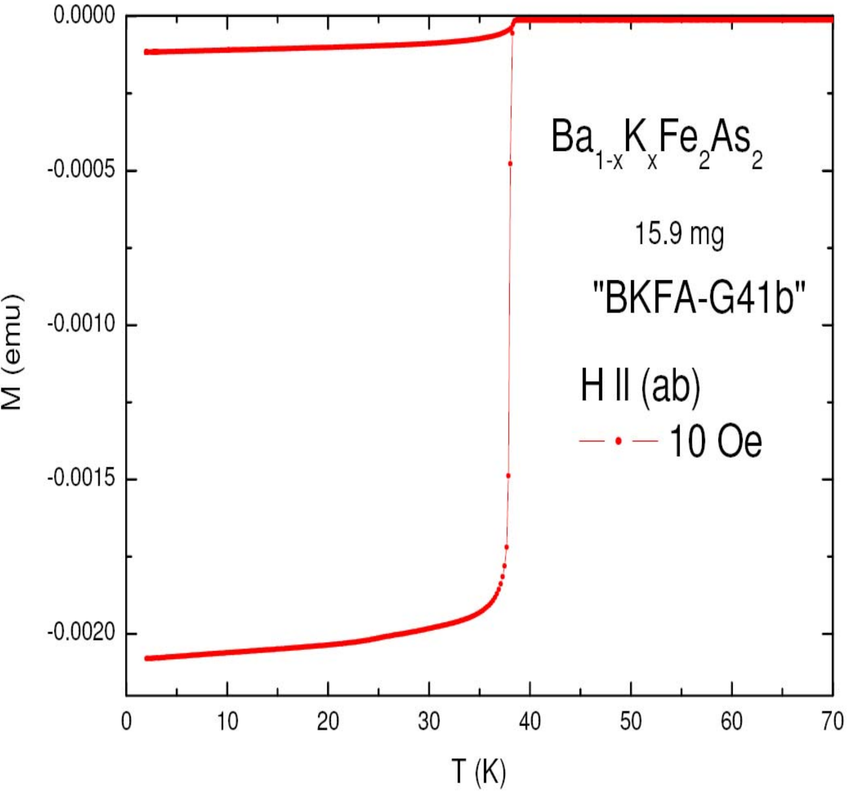


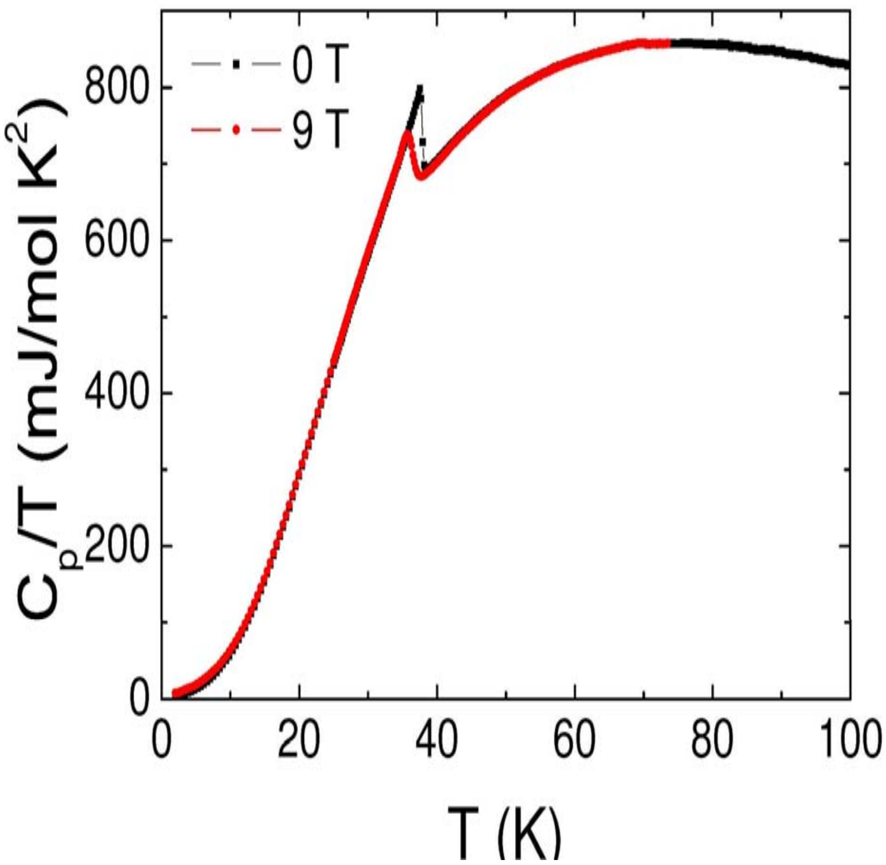
Z. Li et al., Phys. Rev., **B78**, 060504 (R) (2008)



L.Boeri, OVD, A.A. Golubov, the special issue of Physica C (2009)

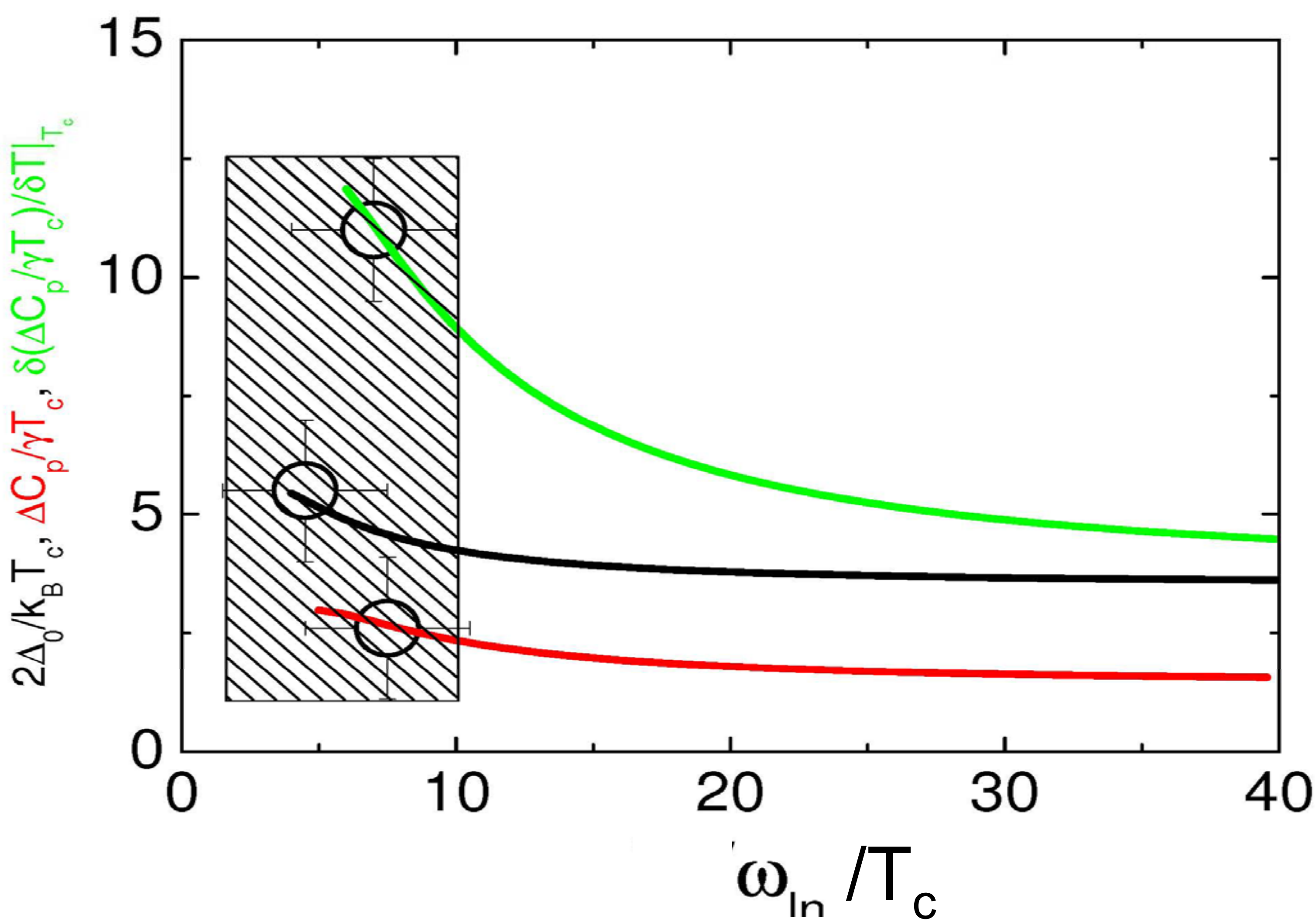
The specific heat of the single crystal $Ba_{1-x}K_xFe_2As_2$

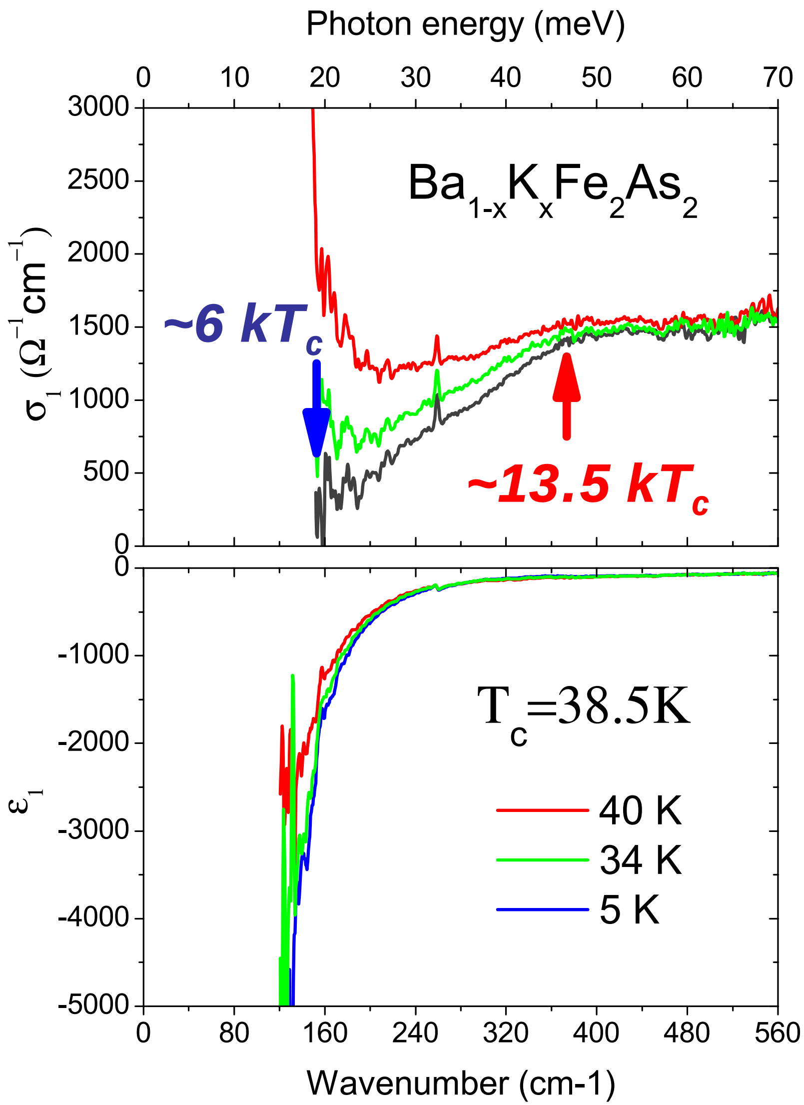


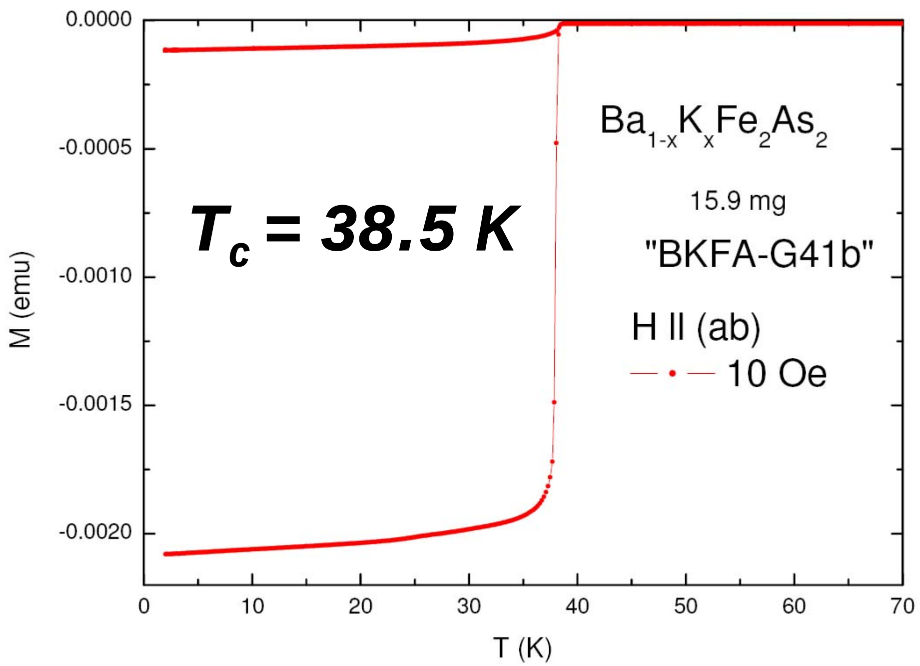


P. Popovich, R. Kremer, A. Boris, OVD

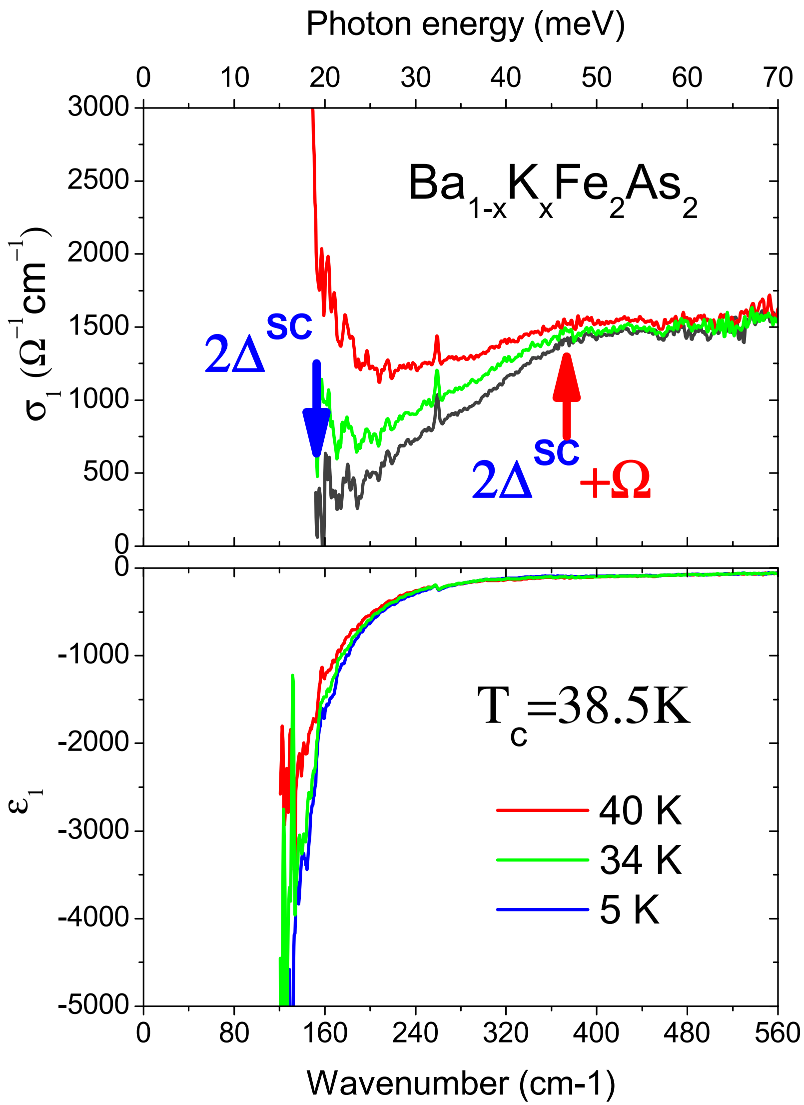
$\blacklozenge_{ln}$~25-40 meV; $\blacklozenge^{ph}_{ln}$~15 meV

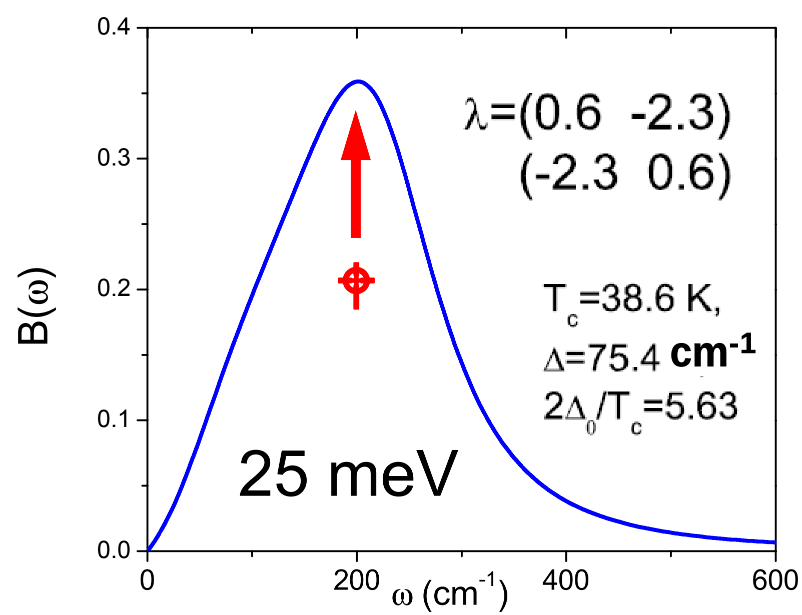


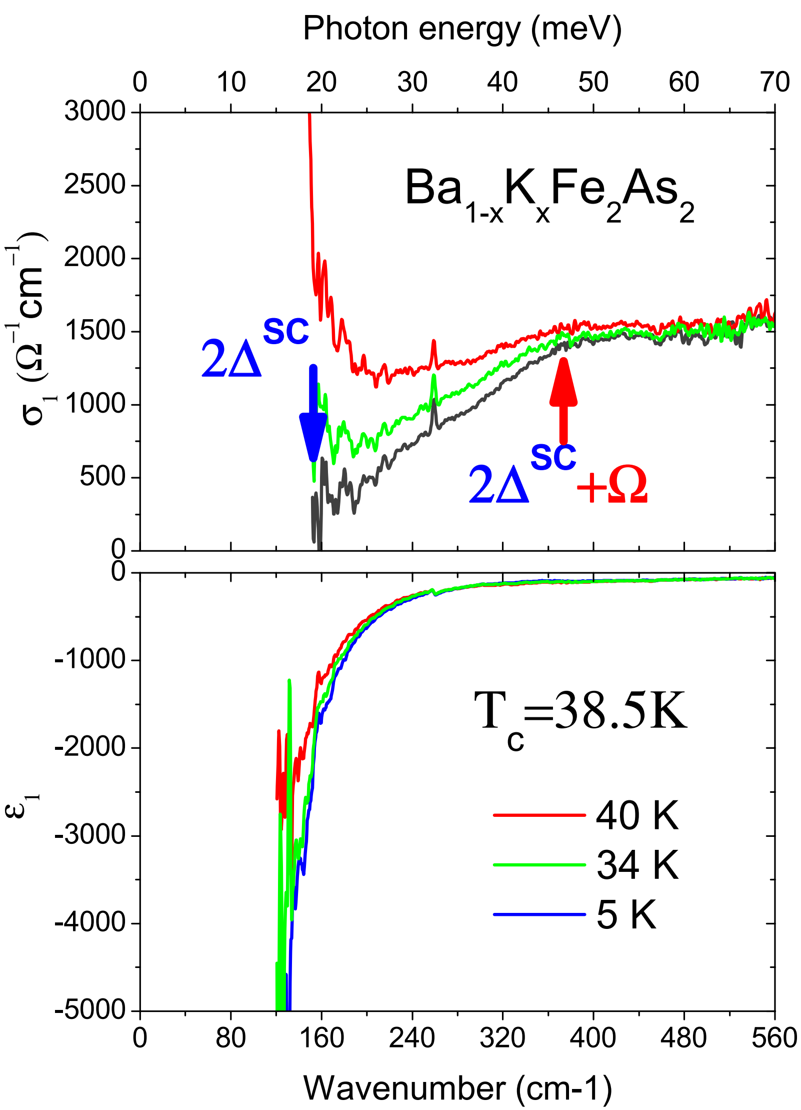

Photon energy (meV)
0 10 20 30 40 50 60 70
3000 2500 2000 1500 1000 500 0
σ_1 (Ω^{-1}cm^{-1})
$Ba_{1-x}K_xFe_2As_2$
~6 kT_c
~13.5 kT_c
0 -1000 -2000 -3000 -4000 -5000
ε_1
T_c=38.5K
40 K
34 K
5 K
0 80 160 240 320 400 480 560
Wavenumber (cm-1)


0.0000 -0.0005 -0.0010 -0.0015 -0.0020
M (emu)
$Ba_{1-x}K_xFe_2As_2$
15.9 mg
"BKFA-G41b"
T_c = 38.5 K
H II (ab)
10 Oe
0 10 20 30 40 50 60 70
T (K)

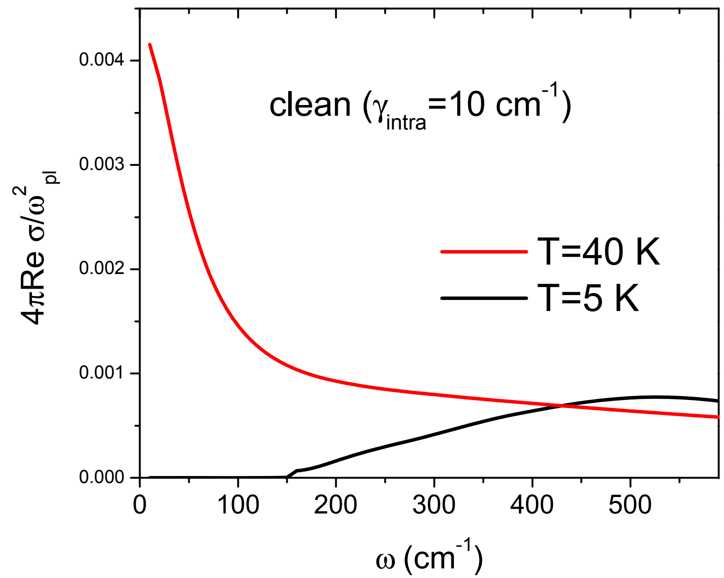
- *single Δ_{SC} =8-9 meV*
- *strong coupling, $2\Delta_{SC}$=5.5-6.5T_c*
- *clean limit, γ ~10 cm^{-1}*
- *s± model with intermediate-boson function:*



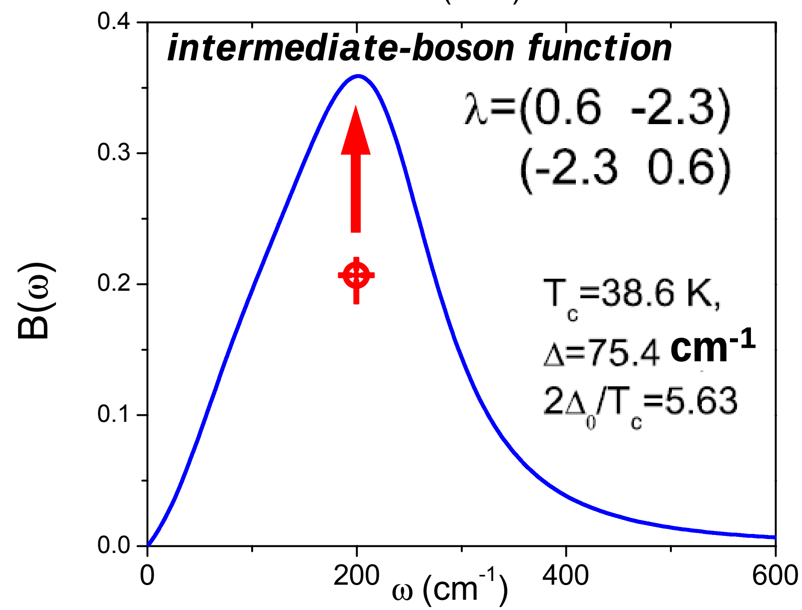




Photon energy (meV)
0
10
20
30
40
50
60
70
3000
2500
2000
1500
1000
500
0
σ_1 (Ω^{-1}cm^{-1})
$Ba_{1-x}K_xFe_2As_2$
$2\Delta^{SC}$
$2\Delta^{SC}+\Omega$
0
-1000
-2000
-3000
-4000
-5000
ε_1
T_c=38.5K
40 K
34 K
5 K
0
80
160
240
320
400
480
560
Wavenumber (cm-1)



0.004
0.003
0.002
0.001
0.000
4πRe σ/ω^2_{pl}
clean (γ_{intra}=10 cm^{-1})
T=40 K
T=5 K
0
100
200
300
400
500
ω (cm^{-1})



intermediate-boson function
λ=(0.6 -2.3)
(-2.3 0.6)
T_c=38.6 K,
Δ=75.4 cm^{-1}
$2\Delta_0/T_c$=5.63
0.4
0.3
0.2
0.1
0.0
B(ω)
0
200
400
600
ω (cm^{-1})

Charge carrier optical self-energy $\Sigma(\omega)$

or

Why I am worry about 1/t(w) representation in Fe pnictides.

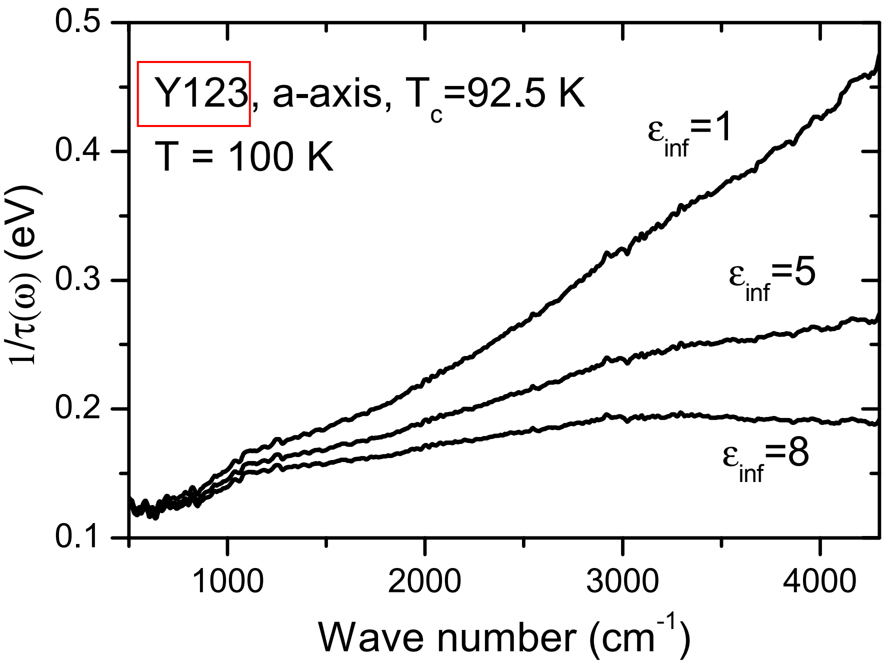
$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

$$\varepsilon(\omega) = 1 + \frac{4\pi i}{\omega}\sigma(\omega)$$

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{4\pi i}{\omega}\sigma^{Drude}(\omega)$$

$$\mathrm{Im}[\Sigma(\omega)] = \frac{1}{\tau(\omega)} = \mathrm{Re}\frac{\omega_{pl}^2}{4\pi\sigma^{Drude}(\omega)} = \frac{\omega_{pl}^2}{\omega}\frac{\varepsilon_2(\omega)}{\varepsilon_2^{\,2}(\omega) + (\varepsilon_\infty - \varepsilon_1(\omega))^2}$$

$$\mathrm{Im}[\Sigma(\omega)] = \frac{1}{\tau(\omega)} = \mathrm{Re}\frac{\omega_{pl}^2}{4\pi\sigma^{Drude}(\omega)} = \frac{\omega_{pl}^2}{\omega}\frac{\varepsilon_2(\omega)}{\varepsilon_2{}^2(\omega) + (\varepsilon_\infty - \varepsilon_1(\omega))^2}$$

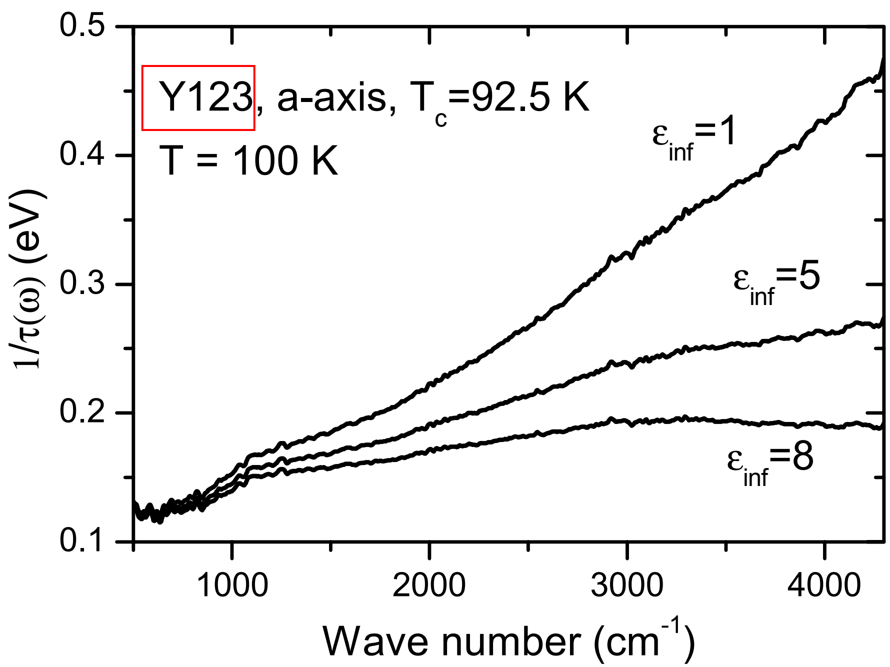


cuprates:

$\varepsilon_\infty \approx$ 5 - 6

lowest inter-band transitions at 1.8 - 2.0 eV

$$\mathrm{Im}[\Sigma(\omega)] = \frac{1}{\tau(\omega)} = \mathrm{Re}\frac{\omega_{pl}^2}{4\pi\sigma^{Drude}(\omega)} = \frac{\omega_{pl}^2}{\omega}\frac{\varepsilon_2(\omega)}{\varepsilon_2{}^2(\omega) + (\varepsilon_\infty - \varepsilon_1(\omega))^2}$$



cuprates:

ε◎ ≈ 5 - 6

lowest inter-band transitions at 1.8 - 2.0 eV

pnictides:

ε◎ ≈ 12 - 15 *!!*

lowest inter-band transitions at 0.2 - 0.5 eV *!!*

An incorrect account of the interband transitions !

Conclusions II

- Pnictides (except $LaNiAsO_{0.9}F_{0.1}$) cannot be described by electron-phonon interaction.
- Optical properties in the N- and SC- states can be described by spin fluctuations.
- The linear frequency dependence of the optical scattering rate $1/\tau(\omega)$ is an artifact of the incorrect account of interband transitions.

Possible connection with other exotic superconductors (S.-L. Drechsler)