First principle calculations and superconductivity.

- Who are band theorists and why have we had such a success in last decades?

- How do we deal with the *conventional* (electron-phonon) superconductivity?

- How do we predict anything (if at all)?

- How do we deal with an *unconventional* (spin-fluctuation) superconductivity?

- What do we know so far about the pairing state of the new Fe-based superconductors (review of the experiment)?

Who are we and why have we had such a success in last decades?

Post-cuprate Materials	Key concept	Band theorists	Many-body theorists
C_{60}	High-energy intramolecular modes	+	+
$ZrZn_2$	Sample inhomogeneity	+	-
$MgCNi_3$	Anharm. phonons suppressed by spin fluctuations	+	-
MgB_2	Two gaps	+	-
Sr_2RuO_4	p-wave		+?
Hcp Fe under pressure	Unconventional, magnetism-driven	+?	
CaC_6	C and intercalant phonons	+	-
Fe-based	$S_{+/-}$	+?	-

- *Not that we are smarter (we are not)*
- *Not that we have much better tools (any tool is as good as the hand that holds it)*
- *Our secret is that we start from a material, and work out a theory to fit our material, while they start from a theory and work on a material to fit their theory. They have intuition for models – we have intuition for materials.*

Вредные советы

1. *Learn many-body first, and numerology second.*
2. *It is easy to run a modern code. It is difficult to run it right, and much more difficult to interpret.*
3. *Equally important information can be gained from successes as from failure (approximations are largely controllable!)*

First principle calculations and superconductivity.

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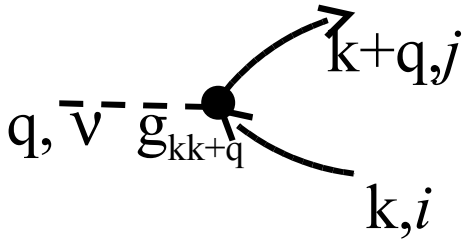
Superconductivity: First principles calculations

Within the Migdal-Eliashberg theory, all electronic properties are determined by the electron-phonon vertex $g_{kk'}(\omega_\nu)$, that defines the scattering amplitude of an electron with the momentum **k** into a state with the momentum **k'** (possibly in a different band) by a phonon with the wave vector **k-k'** and energy ω_ν, belonging to a phonon branch ν.

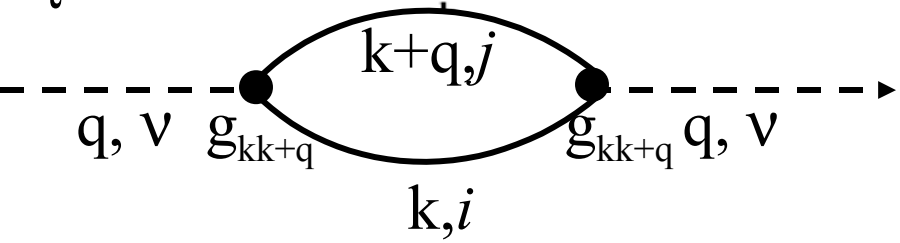
$g_{\mathbf{k},\mathbf{k}+\mathbf{q},\nu} =$



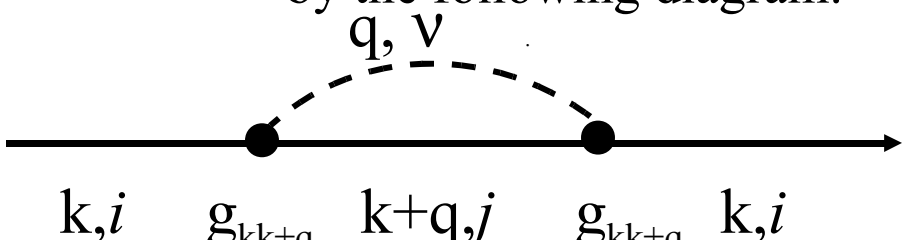
$$g_{\mathbf{k},\mathbf{k}+\mathbf{q},\nu} = \langle \mathbf{k} | \mathrm{d}V / \mathrm{d}Q_{\mathbf{q},\nu} | \mathbf{q} \rangle$$

Summation over all possible electron scatterings for a given phonon gives us a probability of the phonon to decay into an electron-hole pair, that is, phonon lifetime:

$\tau^{-1} =$ $$\gamma_{\mathbf{q},\nu} = 2\pi\omega_{\mathbf{q},\nu} \sum |g_{\mathbf{k},\mathbf{k}+\mathbf{q},\nu}|^2 \delta(\varepsilon_{\mathbf{k}} - E_F)\, \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \hbar\omega_{\mathbf{q},\nu}).$$

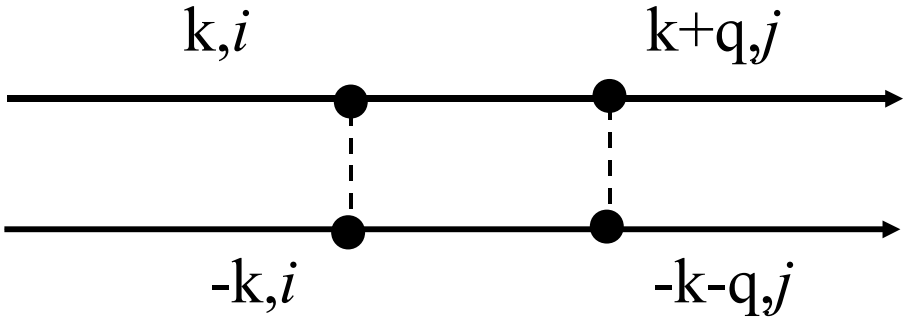


Electron self energy is defined by the following diagram:

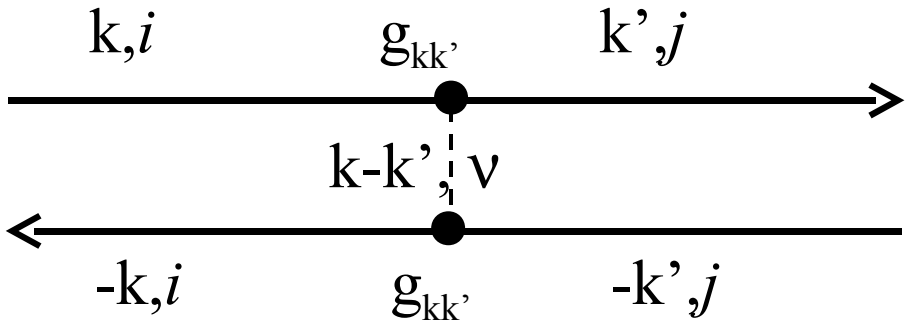


Superconductivity: First principles calculations

while the pairing amplitude is related to the following graph:



All these diagrams can be related to a basic quantity, scattering amplitude of a pair of electrons in the states **k** and -**k** into two other states, **k'** and -**k'** by all available phonons:



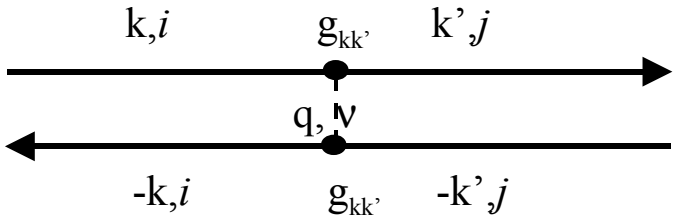
Ladder sequence of these diagrams gives the pairing amplitude. Integration over **q** gives the electron self-energy.

This basic quantity is called the Eliashberg function, $\alpha^2 F_{\mathbf{kk'}}(\omega)$, and is, explicitly

Superconductivity: First principles calculations

This basic quantity is called the Eliashberg function, $\alpha^2 F_{\mathbf{kk'}}(\omega)$, and is, explicitly

$$\alpha^2 F_{\mathbf{kk'}}(\omega) = N^{-1} \sum_{\nu} \left| g_{\mathbf{kk'},\nu} \right|^2 \delta(\omega - \omega_{\mathbf{kk'},\nu})$$



while its isotropic average is

$$\alpha^2 F(\omega) = \frac{1}{2} \sum_{\mathbf{q},\nu} \omega_{\mathbf{q},\nu} \lambda_{\mathbf{q},\nu} \delta(\omega - \omega_{\mathbf{q},\nu}) \quad \text{where} \quad \lambda_{\mathbf{q},\nu} = \gamma_{\mathbf{q},\nu} / \pi N(E_F) \omega^2_{\mathbf{q},\nu}$$

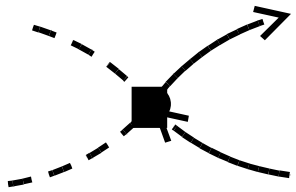
Connecting the right hand legs of this diagram gives electron self energy.

Important note: The full Eliashberg theory can be formulated in real space, so that instead of phonons enter the ionic displacement correlators. A corollary of that fact is the absence of the isotope effect on λ independent of complexity of crystal structure or even periodicity.

Superconductivity: First principles calculations

So far we have made the following assumptions:

1. Migdal theorem (ions are slow compared to electrons – similar to Born-Oppenheimer adiabatic approximation)
2. Harmonicity (relatively easy to remove)
3. Linearity (no two-phonon vertices)



Now we need to find the phonon spectra and the one-electron states

We will do it using the so-called Density Functional Theory

(the following several slides are taken from a Richard Martin lecture, www.ipam.ucla.edu/publications/matut/matut_5904.ppt)

The Fundamental Hamiltonian

Interacting electrons in an external potential

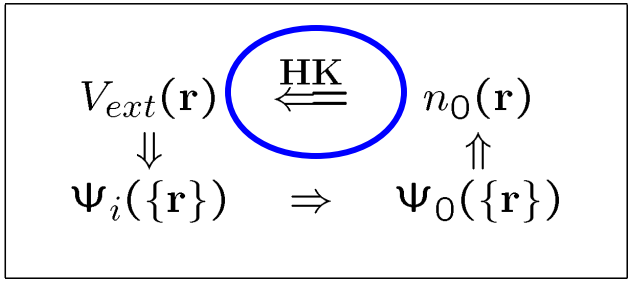
$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_{i,I}\frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$-\sum_I \frac{\hbar^2}{2M_I}\nabla_I^2 + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}$$

- Only one small term: The kinetic energy of the nuclei
- If we omit this term, the nuclei are a fixed external potential acting on the electrons
- The final term is essential for charge neutrality – but is a classical term that is added to the electronic part

The basis of most modern calculations
Density Functional Theory (DFT)

- Hohenberg-Kohn (1964)



- All properties of the many-body system are determined by the ground state density $n_0(r)$

- Each property is a functional of the ground state density $n_0(r)$ which is written as f

The Kohn-Sham Ansatz

- Kohn-Sham (1965) – Replace original many-body problem with an independent electron problem – that can be solved!
- The ground state density is required to be the same as the exact density

$$n_0(\mathbf{r}) = \sum_{\sigma} \sum_{i=1} |\psi_i^{\sigma}(\mathbf{r})|^2,$$

$$\begin{array}{ccccccc} V_{ext}(\mathbf{r}) & \overset{HK}{\Longleftarrow} & n_0(\mathbf{r}) & \overset{KS}{\Longleftrightarrow} & n_0(\mathbf{r}) & \overset{HK_0}{\Longrightarrow} & V_{KS}(\mathbf{r}) \\ \Downarrow & & \Uparrow & & \Uparrow & & \Downarrow \\ \Psi_i(\{\mathbf{r}\}) & \Rightarrow & \Psi_0(\{\mathbf{r}\}) & & \psi_{i=1,N_e}(\mathbf{r}) & \Leftarrow & \psi_i(\mathbf{r}) \end{array}$$

- Only the ground state density and energy are required to be the same as in the original many-body system

The Kohn-Sham Ansatz II

- From Hohenberg-Kohn the ground state energy is a functional of the density E[n], minimum at n = n0
- From Kohn-Sham

$$n_0(\mathbf{r}) = \sum_{\sigma} \sum_{i=1} |\psi_i^{\sigma}(\mathbf{r})|^2,$$

$$E_{KS} = \frac{1}{2} \sum_{\sigma} \sum_{i=1} |\nabla \psi_i^{\sigma}|^2 + \int d\mathbf{r} V_{ext}(\mathbf{r}) n(\mathbf{r}) + E_{Hartree}[n] + E_{II} + E_{xc}[n].$$

Equations for independent particles - **soluble**

Exchange-Correlation Functional – Exact theory but **unknown** functional!

- **The new paradigm – find useful, approximate functionals**

The Kohn-Sham Equations

$$n_0(\mathbf{r}) = \sum_{\sigma} \sum_{i=1} |\psi_i^{\sigma}(\mathbf{r})|^2,$$

- $$E_{KS} = \frac{1}{2} \sum_{\sigma} \sum_{i=1} |\nabla \psi_i^{\sigma}|^2 + \int d\mathbf{r} V_{ext}(\mathbf{r}) n(\mathbf{r}) + E_{Hartree}[n] + E_{II} + E_{xc}[n].$$

$$\frac{\delta E_{KS}}{\delta \psi_i^{\sigma *}(\mathbf{r})} = 0, \qquad (1)$$

Constraint – required Exclusion principle for independent particles

$$\langle \psi_i^{\sigma} | \psi_j^{\sigma'} \rangle = \delta_{i,j} \delta_{\sigma,\sigma'}. \qquad (2)$$

Assuming a f

$$(-\frac{1}{2}\nabla^2 + V_{KS}^{\sigma}(\mathbf{r}), -\varepsilon_i^{\sigma})\psi_i^{\sigma}(\mathbf{r}) = 0 \qquad (3)$$

- Minimizing e

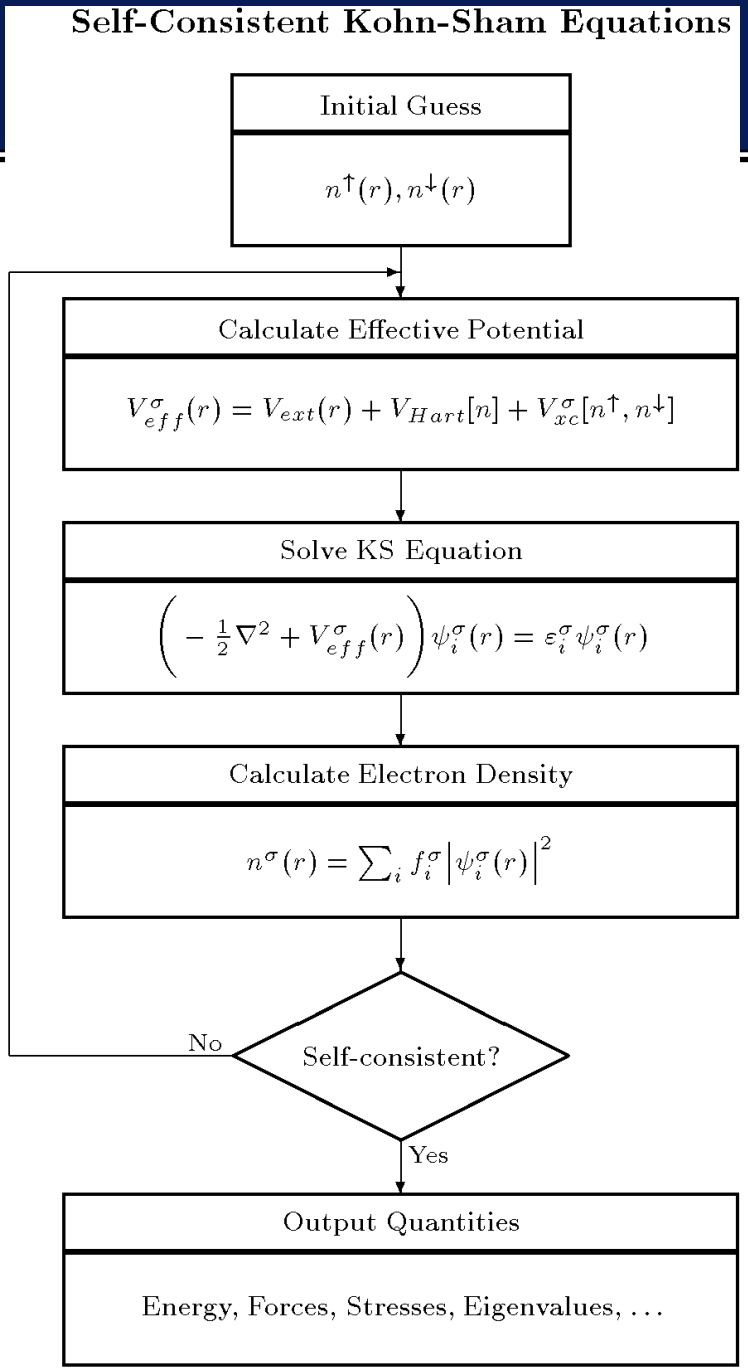
$$\begin{aligned} V_{KS}^{\sigma}(\mathbf{r}) &= V_{ext}(\mathbf{r}) + \frac{\delta E_{Hartree}}{\delta n(\mathbf{r},\sigma)} + \frac{\delta E_{xc}}{\delta n(\mathbf{r},\sigma)} \\ &= V_{ext}(\mathbf{r}) + V_{Hartree}(\mathbf{r}) + V_{xc}^{\sigma}(\mathbf{r}) \qquad (4) \end{aligned}$$

Eigenvalues are approximation to the energies to add or subtract electrons –electron bands

More later

Solving Kohn-Sham Equations

- Structure, types of atoms
- Guess for input
- Solve KS Eqs.
- New Density and Potential
- Self-consistent?
- Output:
  - Total energy, force, stress, ...
  - Eigenvalues



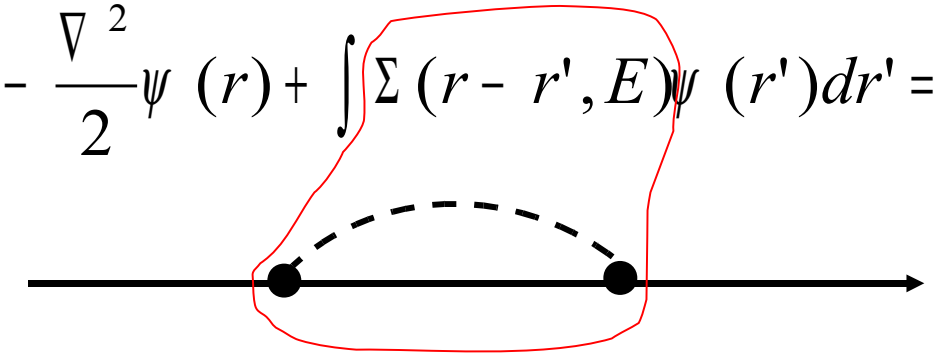
Now we have a set of one-particle energies and one-particle wave functions.

Can we use them for one-electron excitation energies?

Compare Kohn-Sham Equations and Dyson Equation:

$$-\frac{\nabla^2}{2}\psi(r) + V[n](r)\psi(r) = E\psi(r)$$

$$-\frac{\nabla^2}{2}\psi(r) + \int \Sigma(r - r', E)\psi(r')dr' = E\psi(r)$$



As long as the Coulomb interaction is well screened (not true in insulators) and/or there is no strong energy dependence in the interaction (not true in strongly correlated materials), KS eigenvalues represent real electrons.

Linear response technique – not your usual linear response

The standard linear response is based on the Rayleigh-Schrodinger perturbation theory: the new wave functions are expanded in terms of the old wave functions. Disadvantage: a very large number of unoccupied states need to be computed. Workaround: Sternheimer perturbation theory. One way to look at this theory:

$$\psi_v = \sum_i A_{vi}\phi_i; \quad \delta\psi_v = \sum_i \delta A_{vi}\phi_i; \quad or \quad \delta\psi_v = \sum_i A_{vi}\delta\phi_i$$

When ions shifts, atomic orbitals also shift and deform.

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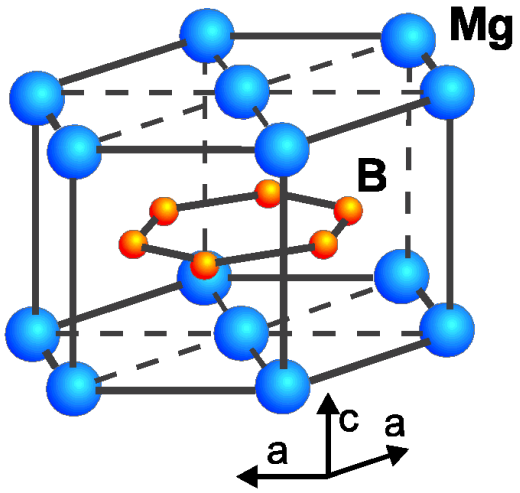
Recent applications: superconductivity in doped graphenes

MgB2



Graphite:
ABABAB

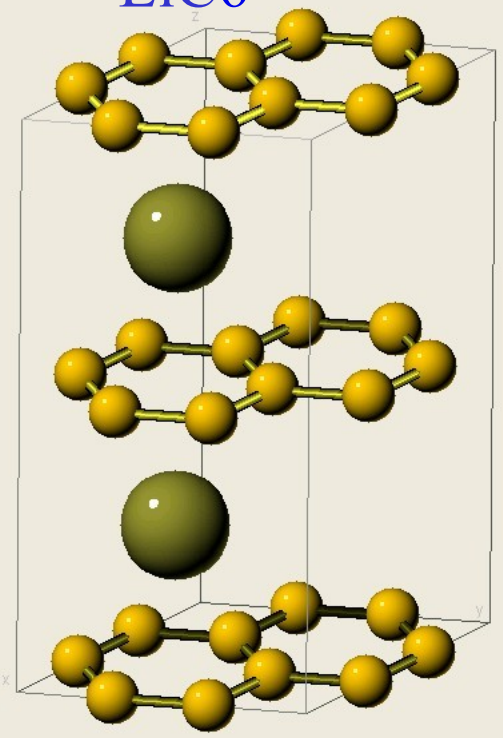
LiC_6:
AαAαAαA

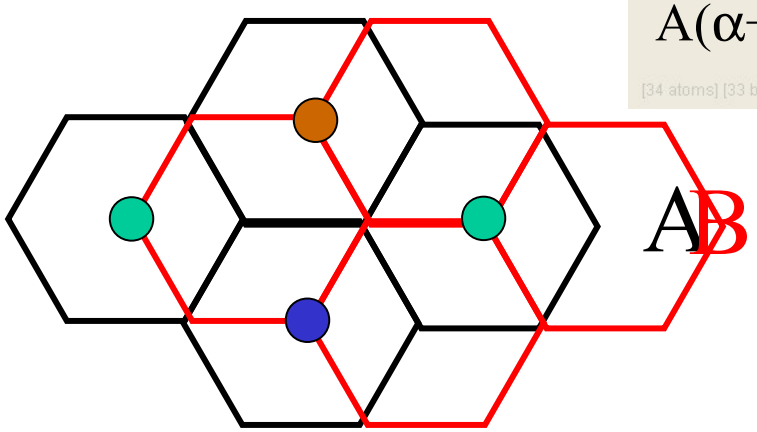
YbC_6:
AαAβAαA

CaC_6:
AαAβAγA

MgB_2:
A(α+β+γ)A

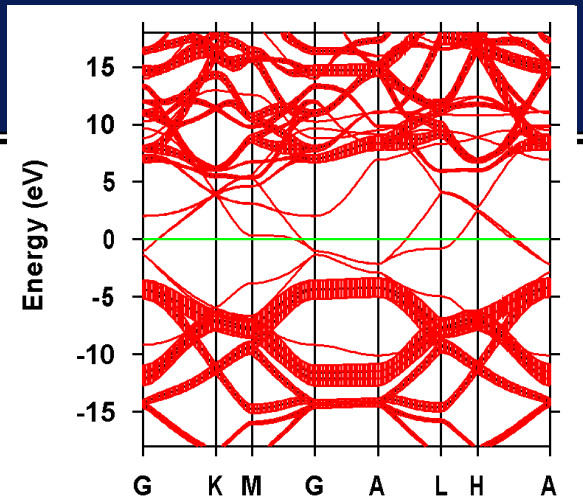
LiC6





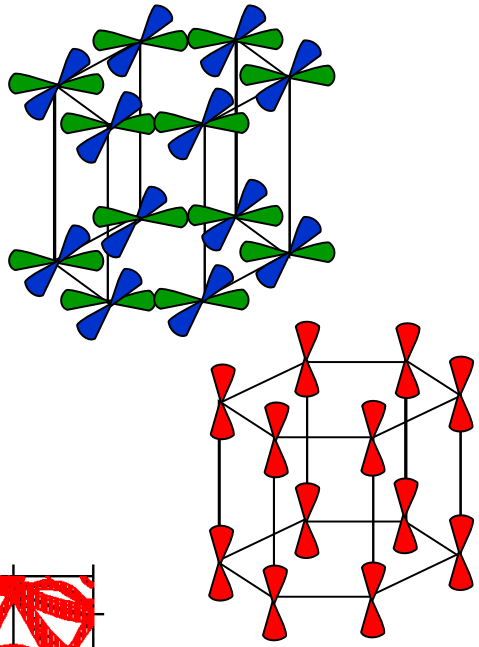
α β γ

Intercalated graphene: electronic structure

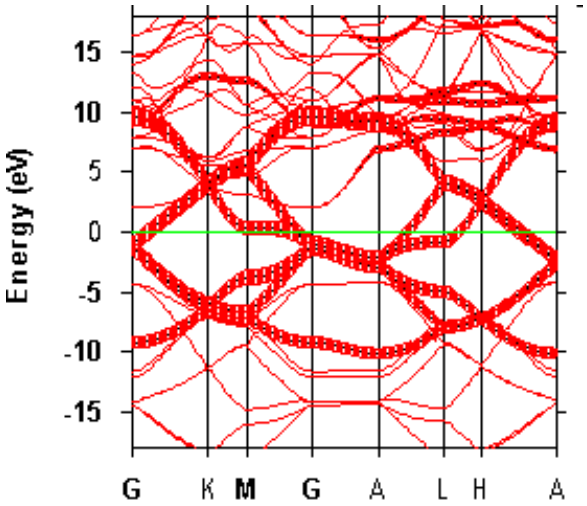


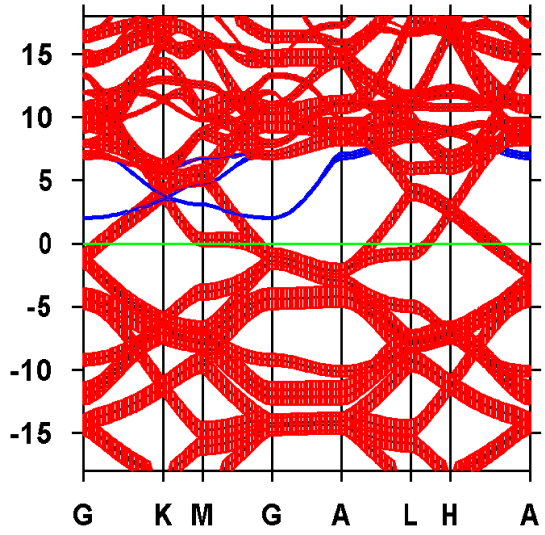
Formation of the electronic structure

- C px,y



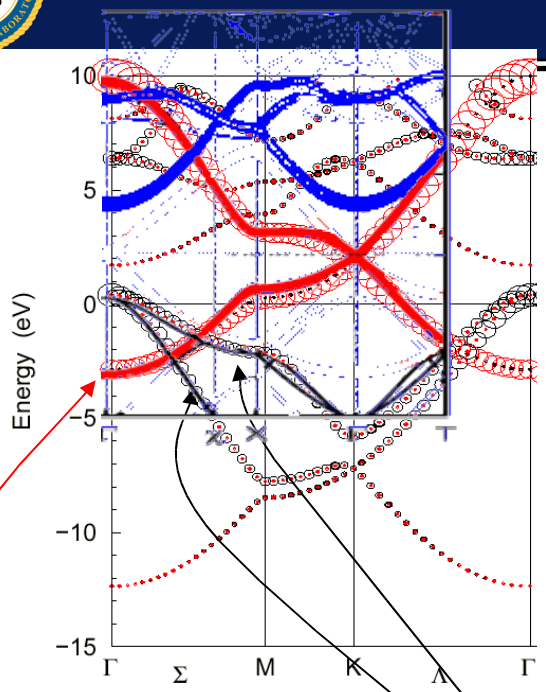
- C pz



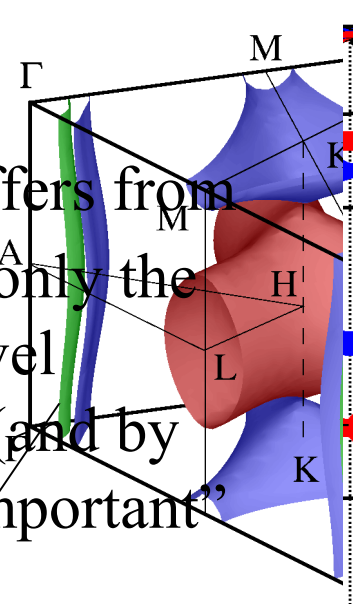


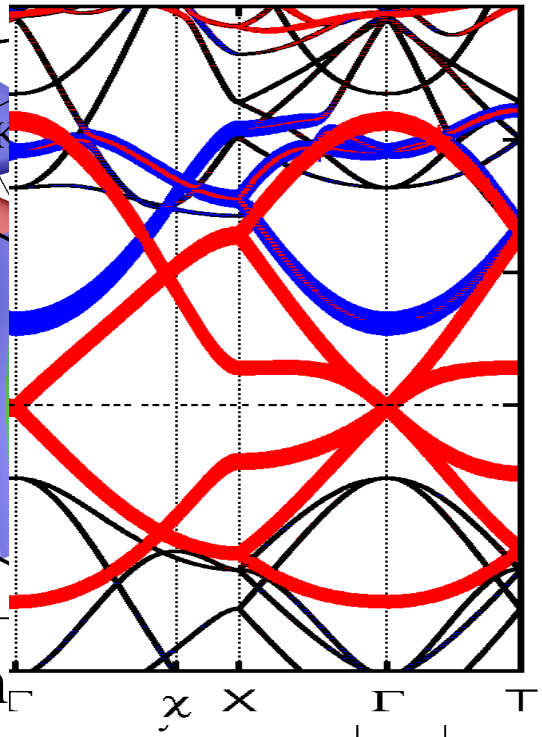
- intercalant orbitals (s, d, f…)
- “nearly-free-electron” states

MgB_2: σ-band + π-band

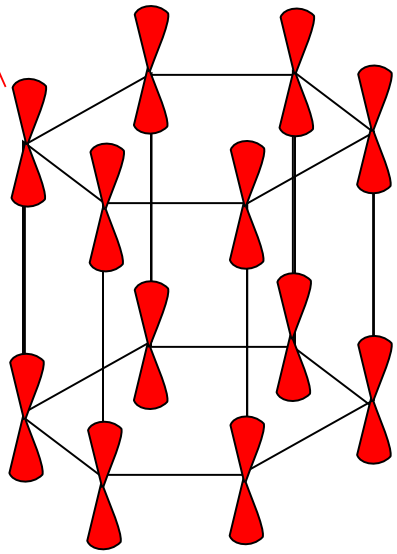


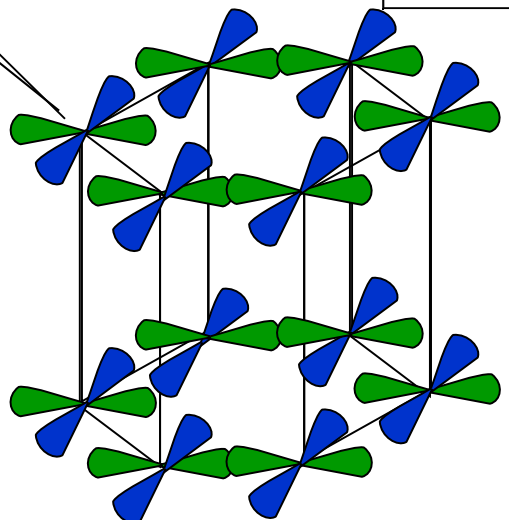
MgB_2 differs from graphite only the Fermi level position (and by the "unimportant" ζ-band)





Bondin





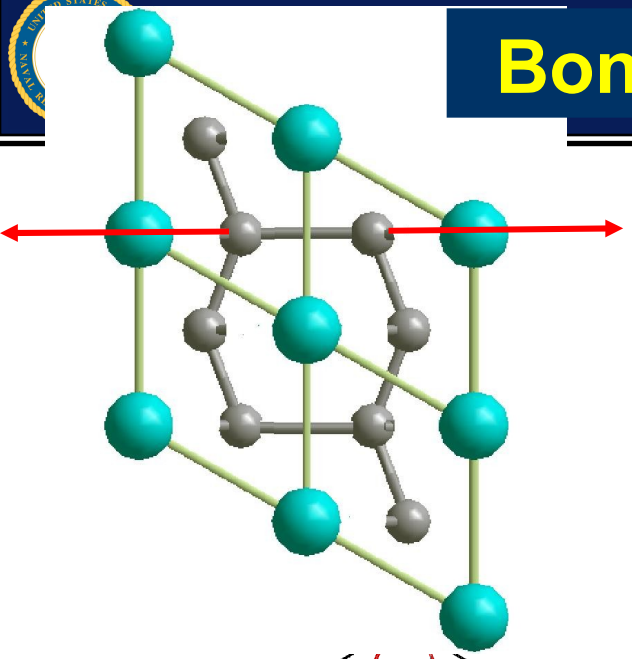
Graphite

Bonding p_z (π)

Antibonding p_z (π)

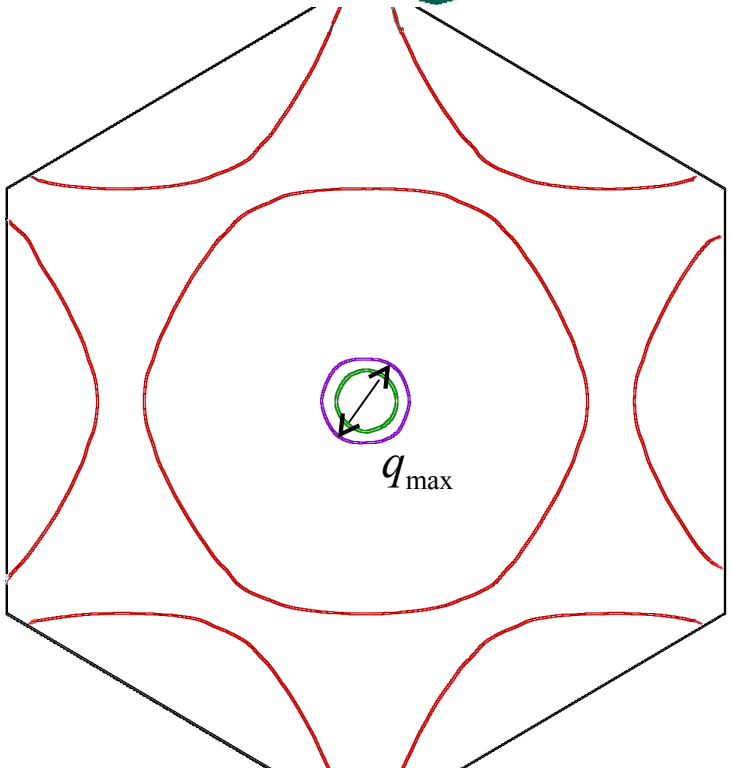
No Mg states at E_F

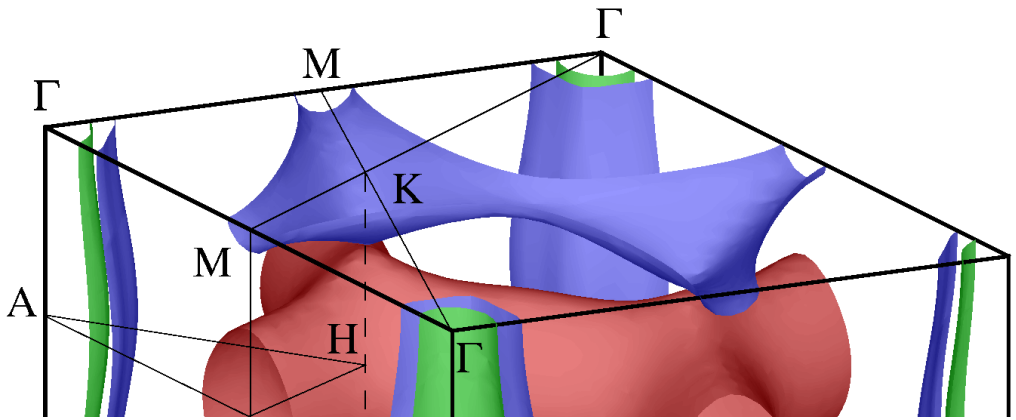
Bond-stretching E_{2g} mode: main player

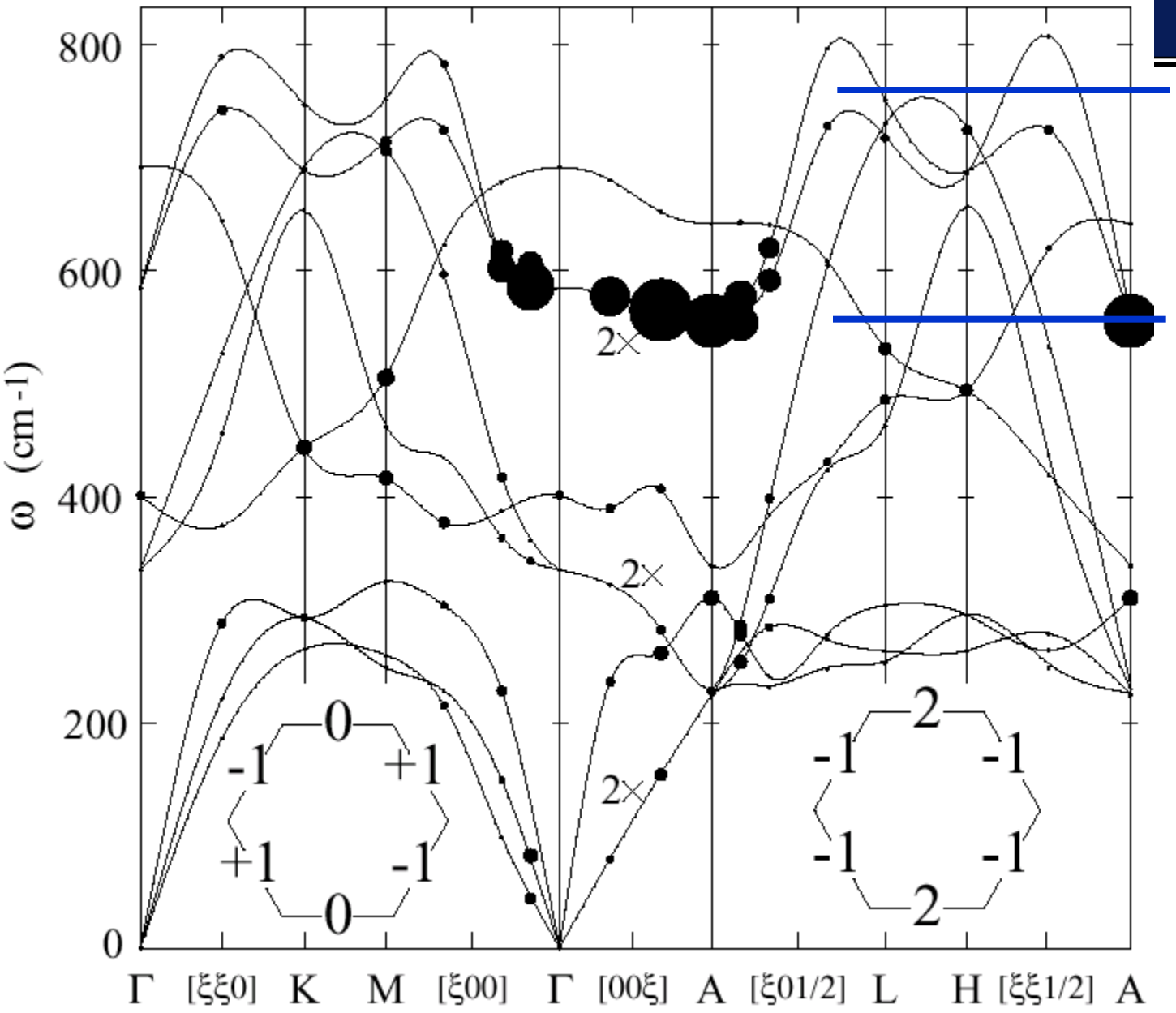


2D Kohn anomaly:

If a phonon interacts primarily with the $p\sigma$ bands, one should expect substantial softening ($\Delta\omega/\omega \sim \lambda$) and broadening ($\gamma/\omega \sim \pi N\omega\lambda \sim 0.1\lambda$) for $q < q\text{max}$







e-ph interaction induced softening

Linear-response calculations of phonons and e-ph coupling (Stuttgart group). Similar results: Amy Liu et al, Heid et al

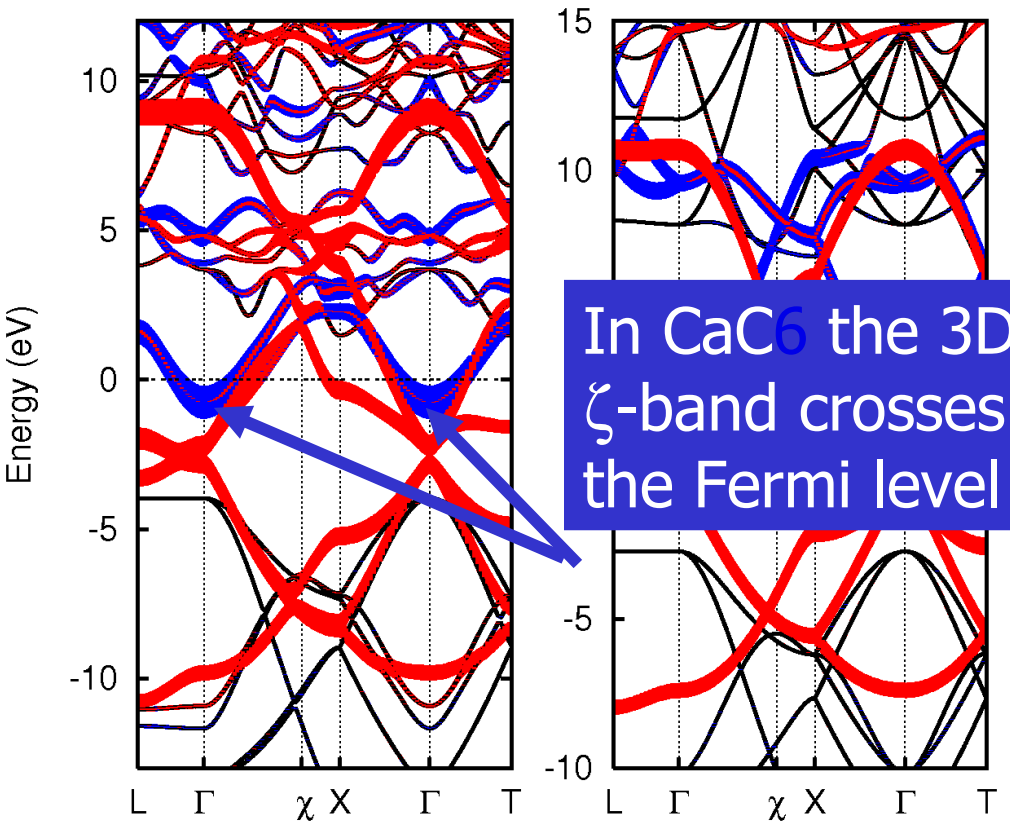
It seems like the π band plays no positive role in electron-phonon coupling. It was suggested at an early (Pickett) that if it were not there at all, T_c would have been the same or even higher:

However, this very untrue, and I will come back to that after discussing CaC_6, where it is another band that "takes a lead" in superconductivity.

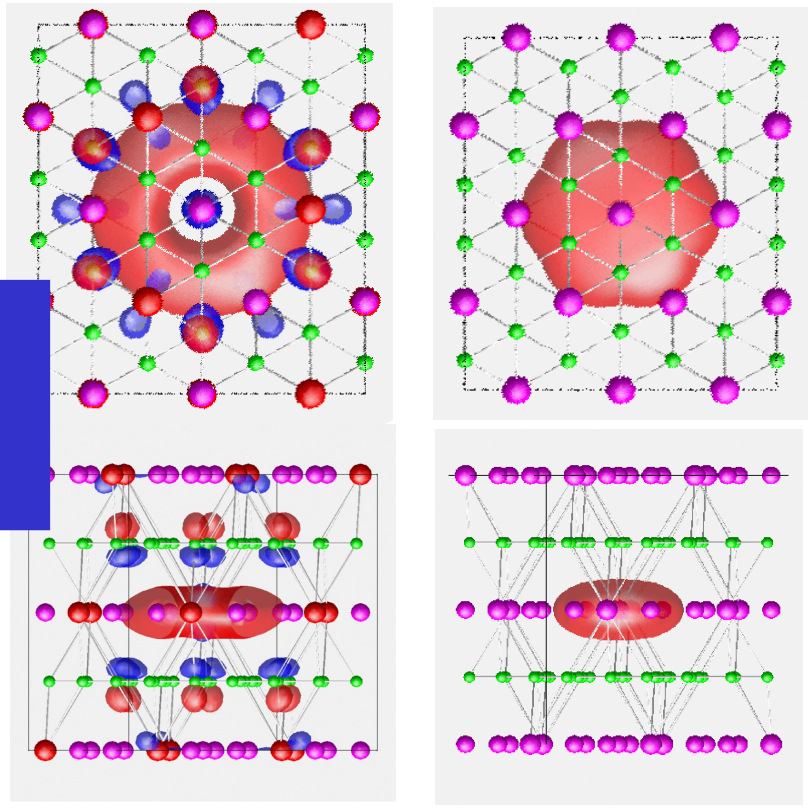
$$\lambda_{ij} = \begin{pmatrix} [0.95\text{-}1.0] & [0.16\text{-}0.17] \\ [0.21\text{-}0.23] & [0.3\text{-}0.45] \end{pmatrix}$$

$\lambda_{eff} \sim 1\text{-}1.05$; $\lambda_{av} = 0.87\text{-}0.9$

3D band: free electrons or intercalant states?



In CaC6 the 3D ζ-band crosses the Fermi level

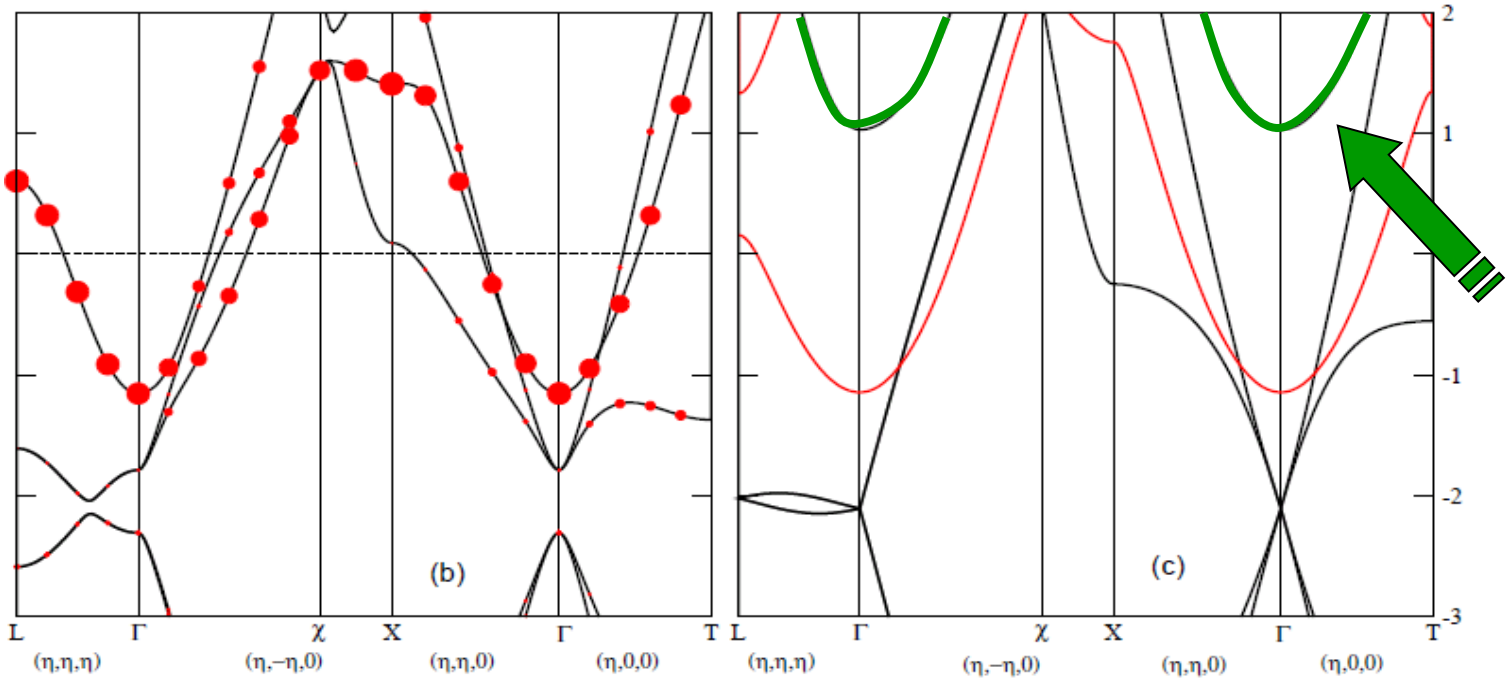


CaC_6 C_6 CaC_6 C_6

carbon *p(z)* vs Ca/empty *s*

- ζ-band: free electrons or intercalant's electrons?
- Both! (cf. bands in the Ca metal).

CaC_6: π-band + ζ-band



CaC_6 fcc Ca + C_6

- Ca states

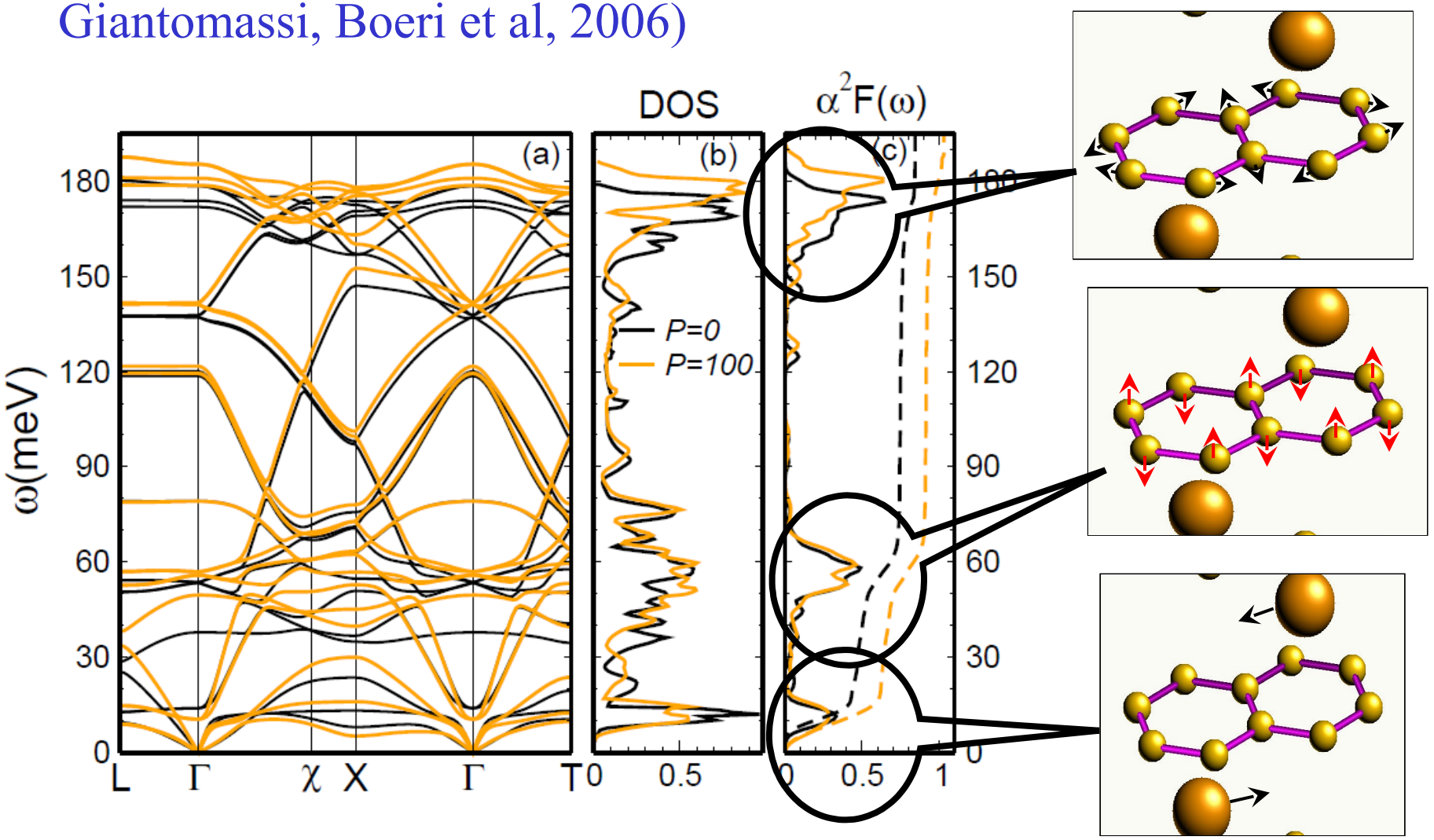
Cf. MgB_2 -- σ-band + π-band.

Is it possible to create a material with all three types of carriers?

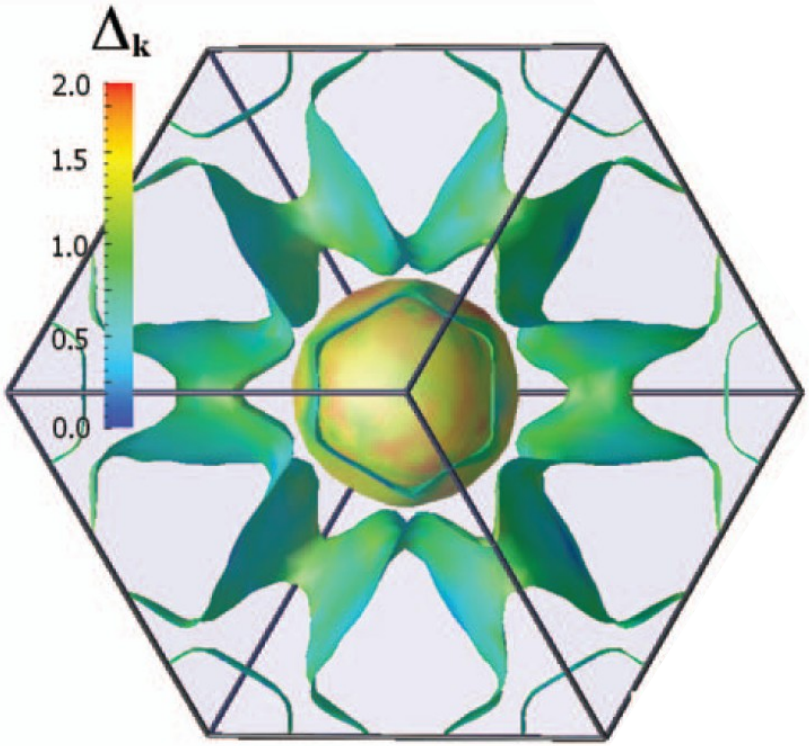
XXX -- σ-band + π-band + ζ-band?

Full DFT calculations

Pseudopotential calculations (Calandra & Mauri, 2005, Giantomassi, Boeri et al, 2006)



CaC_6: π-band + ζ-band



Massida, Gross et al

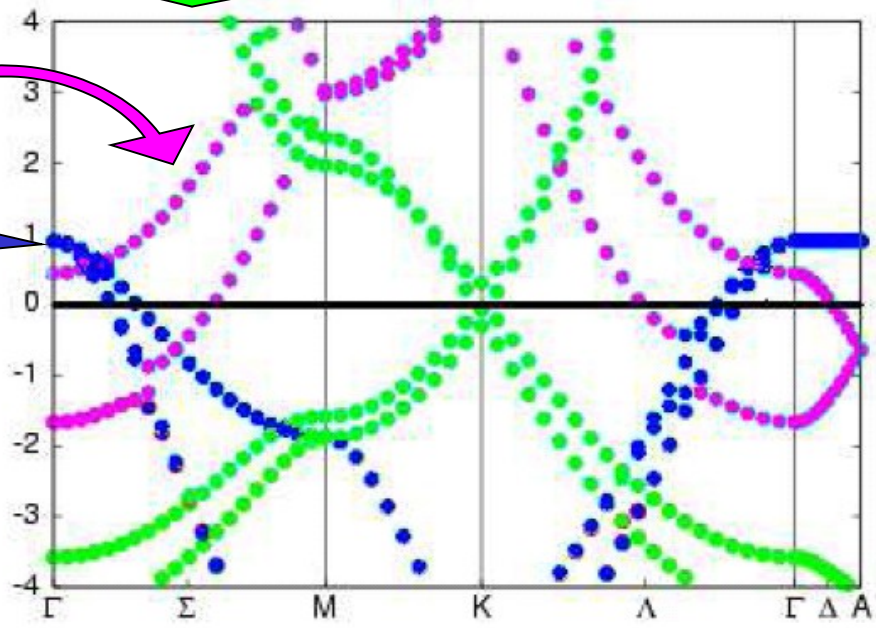
Note that most of the coupling comes the free-electron like spherical FS (the ζ-band).

$MgB_2+CaC_6=?$

CaC_6: π-band + ζ-band

MgB_2: σ-band + π-band

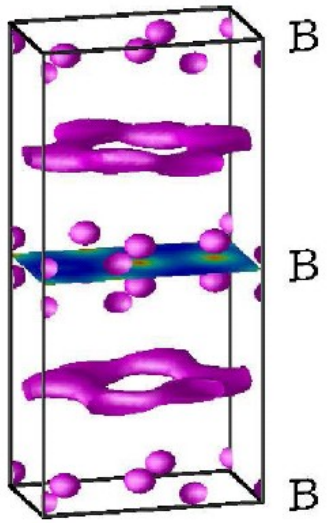
Li_2B_2: σ-band + ζ-band!



Theoretically predicted by Kolmogorov and Curtarolo in 2005 (metastable at ambient pressure, stabilized by moderate pressure)

Where have all the π-electrons gone??

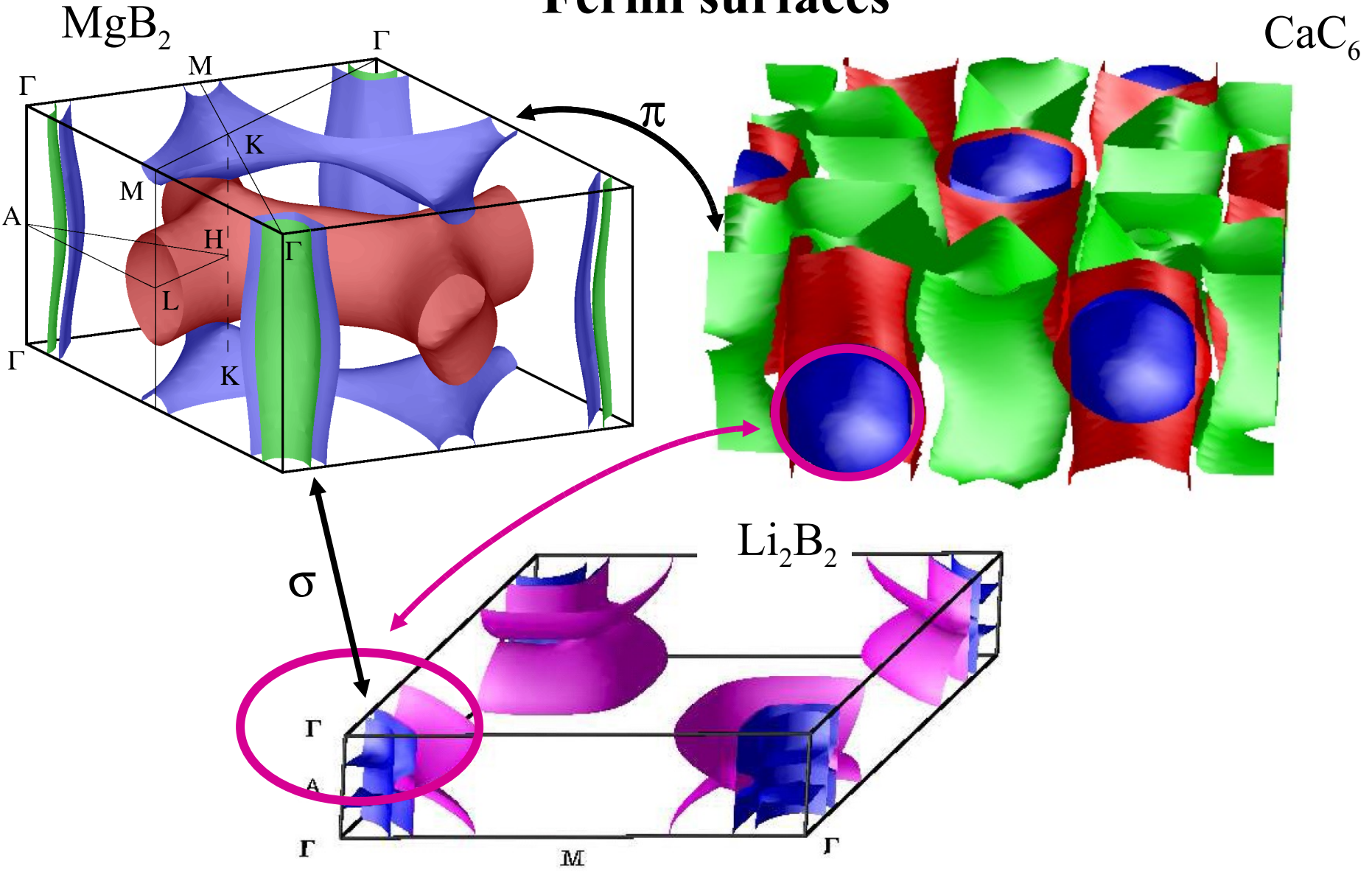
In terms of the π-band **Li_2B_2** is an exact analogue of the *undoped* graphite



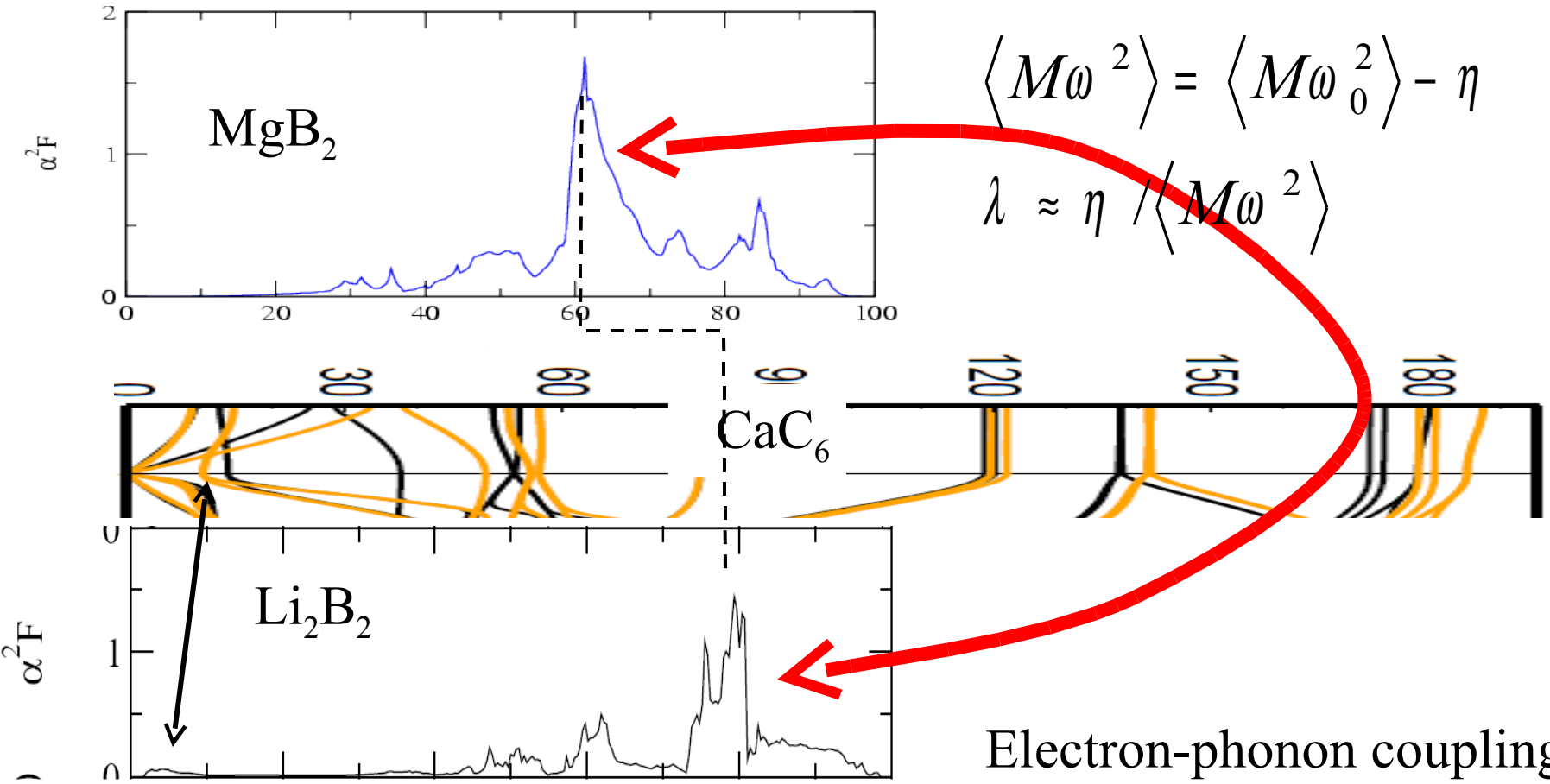
Better to see once than to be told about thrice

(Russian proverb)

Fermi surfaces



Why do we need that π-band, after all???



$$\langle M\omega^2 \rangle = \langle M\omega_0^2 \rangle - \eta$$

$$\lambda \approx \eta / \langle M\omega^2 \rangle$$

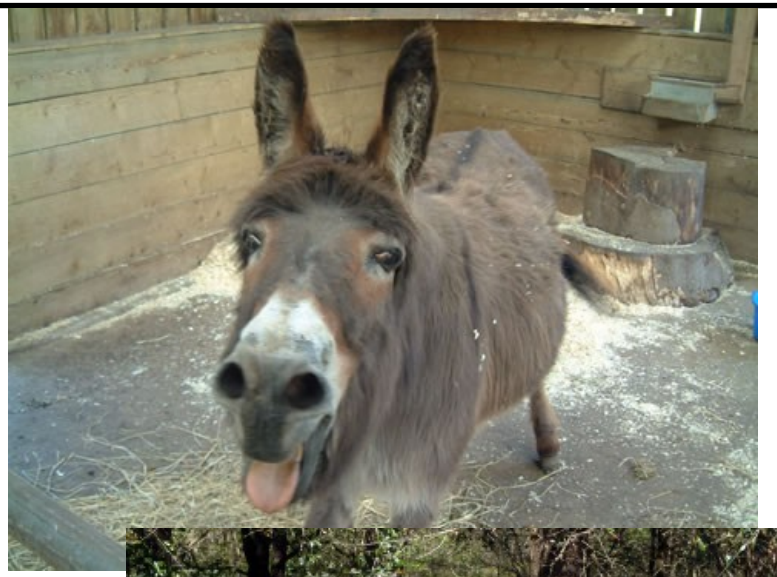
Electron-phonon coupling with π-electrons softens the "working" phonon in MgB_2 from 81 meV to 67: a 50% enhancement of λ!

Calculated T_C~7-8K (including possible multigap effects, up to 15K)

Superconductor husbandry vs. animal husbandry

strength, good temper

endurance, low maintenance



HORSE

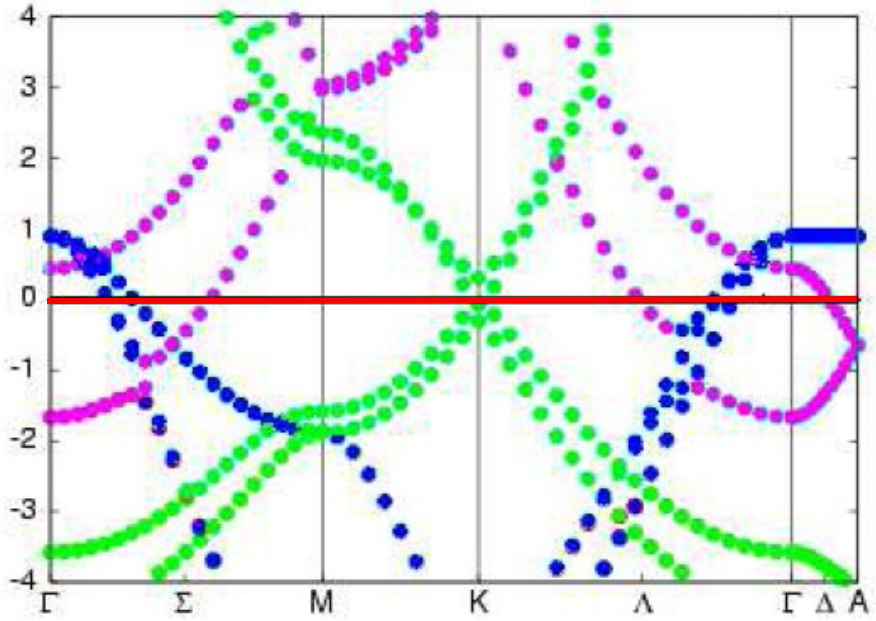
+

=MULE

LACKING: an ordinary, but indispensable common feature of both prototypes:

What you may have thought about cannot be regained.

But the π-band can!



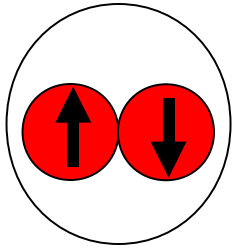
Doping of 0.15 electrons per formula *(e.g.,* Li2B1.85C0.15) raises the Fermi level

...and raises the density of π-states up to a value comparable with that of MgB2.

First principle calculations and superconductivity.

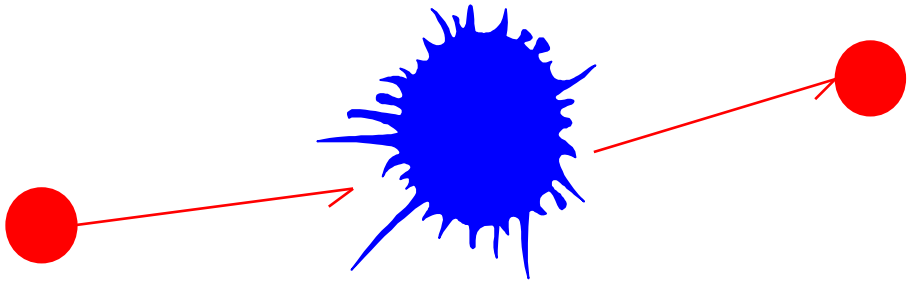
- Who are we and why have we had such a success in last decades?
- How do we deal with the *conventional* (electron-phonon) superconductivity?
- How do we predict anything (if at all)?
- How do we deal with an *unconventional* (spin-fluctuation) superconductivity?
- What do we know so far about the new Fe-based superconductors (review of the experiment)?

Superconductivity and spin fluctuations

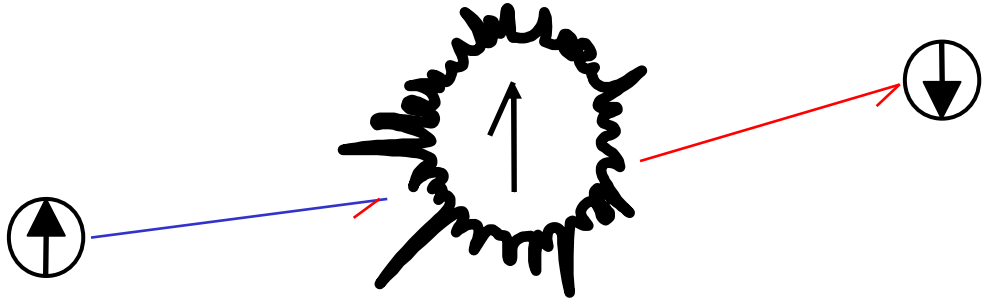


singlet

charge fluctuations (phonons) mediate attraction; spin fluctuations mediate repulsion



2nd electron - charge polarization cloud - 1st electron

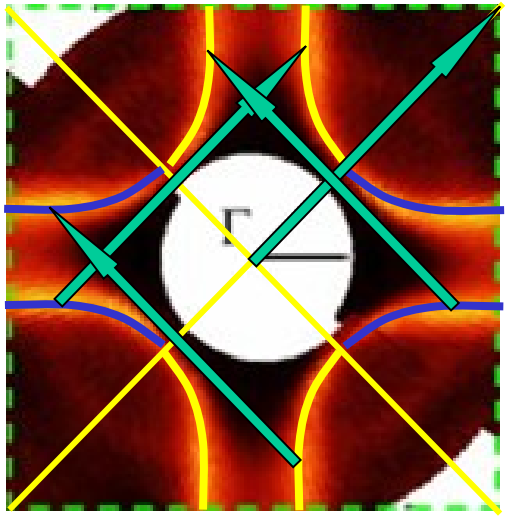


2nd electron - spin polarization cloud - 1st electron

$$\sum_{q\beta} \quad k\alpha \qquad q\beta$$

If $\Delta_{\alpha k}$ and $\Delta_{k\beta}$ have opposite sign, a negative (repulsive) V can still be pairing.

Spin fluctuations model in cuprates



Fermi surface of BSCCO measured by ARPES
(http://en.wikipedia.org/wiki/Fermi_surface)

Superexchange interaction is peaked at Q=(π,π)

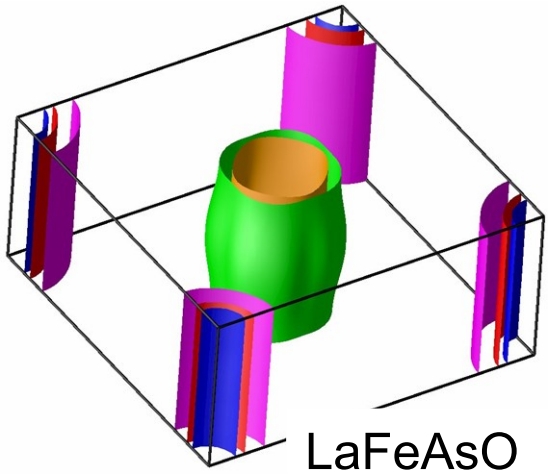
It is perfectly well matching the fermiology of high-Tc cuprates

There are two ingredients in this recipe: (1) Fermiology and (2) momentum dependence of spin fluctuations

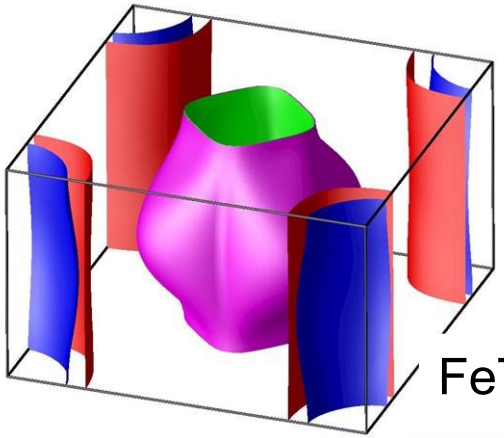
$$\sum_{q\beta} V_{k\alpha,q\beta}\, \Delta_{q\beta}$$

If $\Delta_{k\alpha}$ and $\Delta_{q\beta}$ have opposite signs, a negative (repulsive) V can still be pairing.

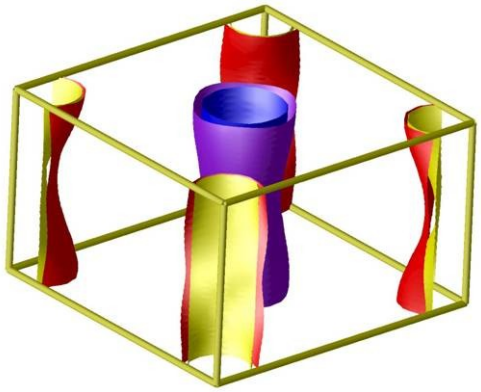
Cooking an $s_{\pm}$ state: ingredient 1 - Fermiology



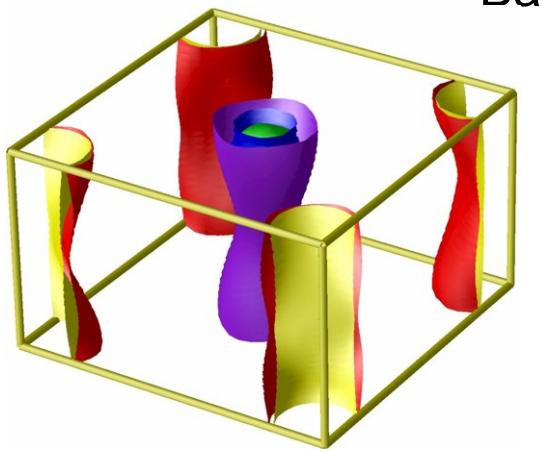
LaFeAsO



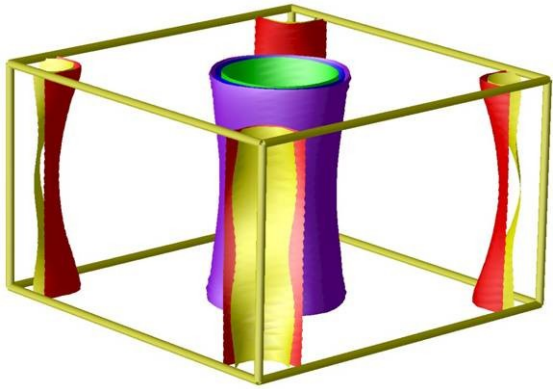
FeTe



$BaFe_2As_2$



Ba122 – 10%e

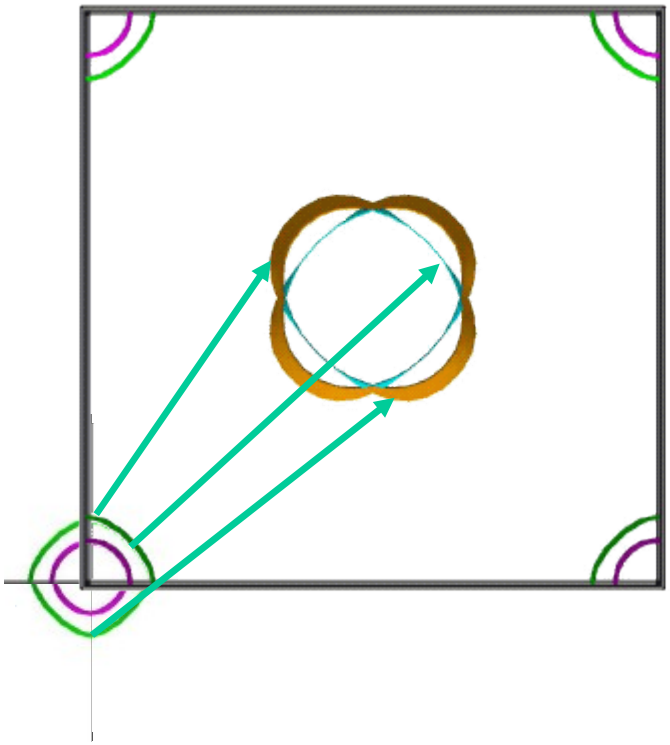


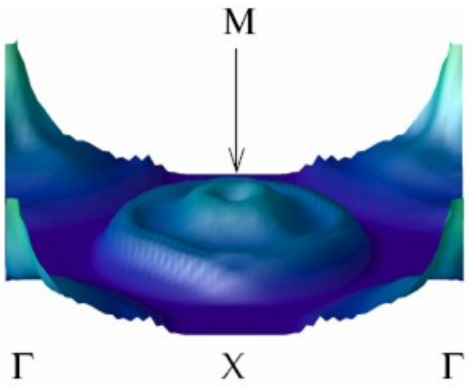
Ba122 – 10%h

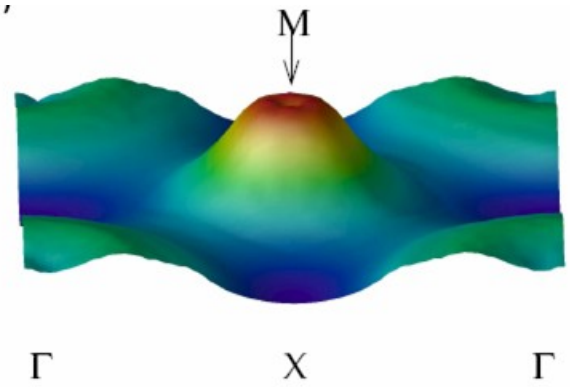
In all actual materials there is some “poor” nesting of the Fermi surfaces .

Cooking an $s_{\pm}$ state: ingredient 2 – spin fluctuation

$$\mathrm{Re}\,\chi_0(\mathbf{q},\omega \to 0) = \sum_{\mathbf{k}} \frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}} \qquad \frac{\mathrm{Im}\,\chi_0(\mathbf{q},\omega)}{\omega}\Big|_{\omega \to 0} = \sum_{\mathbf{k}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - E_F)\delta(\varepsilon_{\mathbf{k}} - E_F)$$







Im $\chi_0(\mathbf{q},\omega)/\omega|_{\omega\to 0}$ Re $\chi_0(\mathbf{q},0)$

fully pairing for the $s_{\pm}$ state (sharp nesting not needed)

FOUND EXPERIMENTALLY!

Origin of spin fluctuations: not important!

$$\chi(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{1 - J(\mathbf{q},\omega)\ \chi_0(\mathbf{q},\omega)}$$

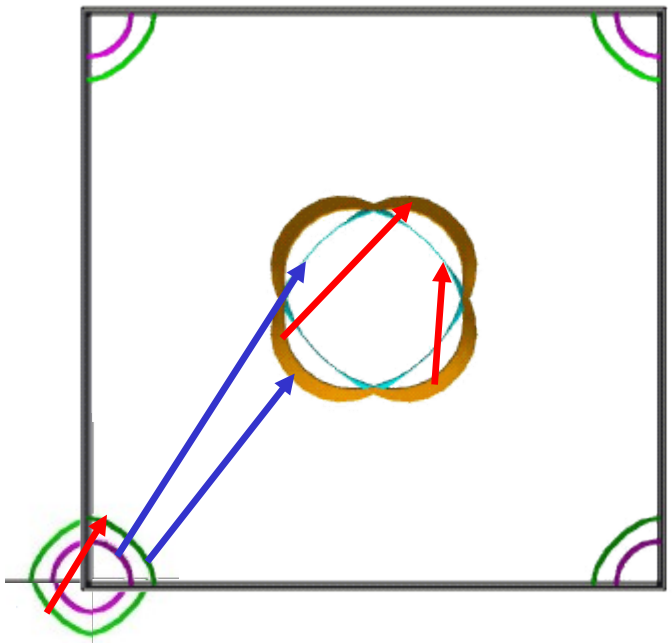
For a Mott-Hubbard system, $J(\mathbf{q},\omega)$ is main factor – magnetic interaction is *local in real space*

For LFAO, we expect the structure to come mainly from non-interacting part, interaction is *local in momentum space*

$$\chi_0(\mathbf{q},\omega) = \sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}+\mathbf{q}}) - f(\varepsilon_{\mathbf{k}})}{(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \omega - i\delta)}$$

IF it were a Mott-Hubbard system, the nearest neighbor superexchange ($\{0,0\}, J_1$) would be pair-breaking, and the 2nd neighbors superexchange ($\{\pi,\pi\}, J_2$) would be pairing.

Some clarification about phonons



these phonons are pairing, positive isotope effect

these phonons are pair-breaking, negative isotope effect.

1. First principles calculations of e-ph coupling give $\lambda_{e\text{-}ph}$~0.2. They *<u>are reliable</u>* for a truly nonmagnetic ground state. *<u>Magnetism</u> provides up to ~50% enhancement.*

L. Boeri, M. Calandra, IIM, arXiv:1004.1943

1. Magnetoelastic coupling in these materials is *spectacularly strong.*

1. Isotope effect in systems with variable T_c is notoriously hard to measure (cf. CaC_6, possibly $MgNiC_3$).

In principle, these phonons can induce nodes

Theory: Summary

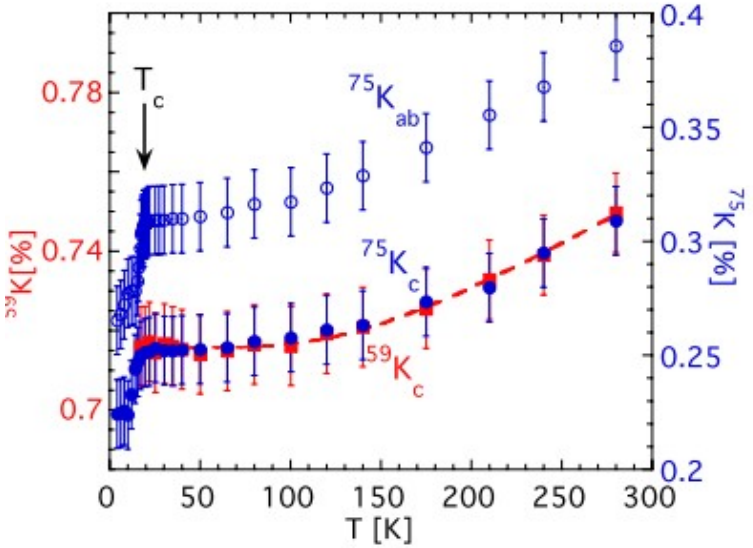
1. First principle calculations predict two disjoint sets of the Fermi surfaces separated by a particular wave vector (experiment concurs)
2. First principle calculations predict spin fluctuations with the same wave vector (experiment concurs)
3. First principle calculations predict weak to moderate e-ph coupling
4. The only state naturally compatible with all the above is $s^{\pm}$

   the **s state.**

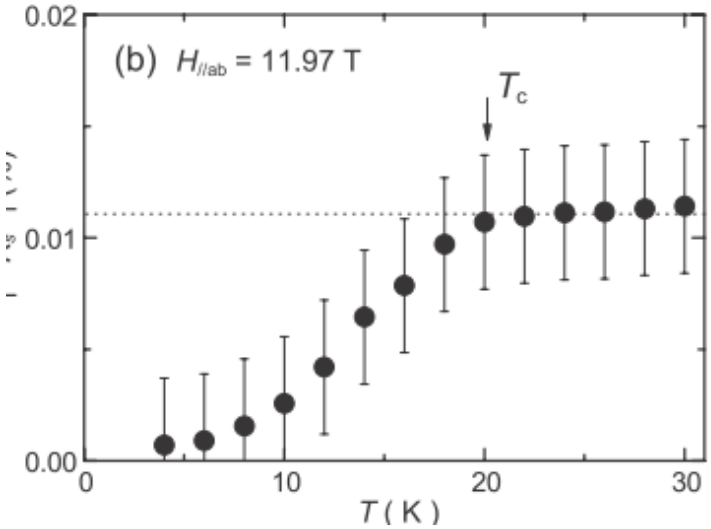
First principle calculations and superconductivity.

- Who are we and why have we had such a success in last decades?
- How do we deal with the *conventional* (electron-phonon) superconductivity?
- How do we predict anything (if at all)?
- How do we deal with an *unconventional* (spin-fluctuation) superconductivity?
- What do we know so far about the new Fe-based superconductors (review of the experiment)?

EXPERIMENTAL EVIDENCE: Singlet or triplet?



McMaster+Oakridge



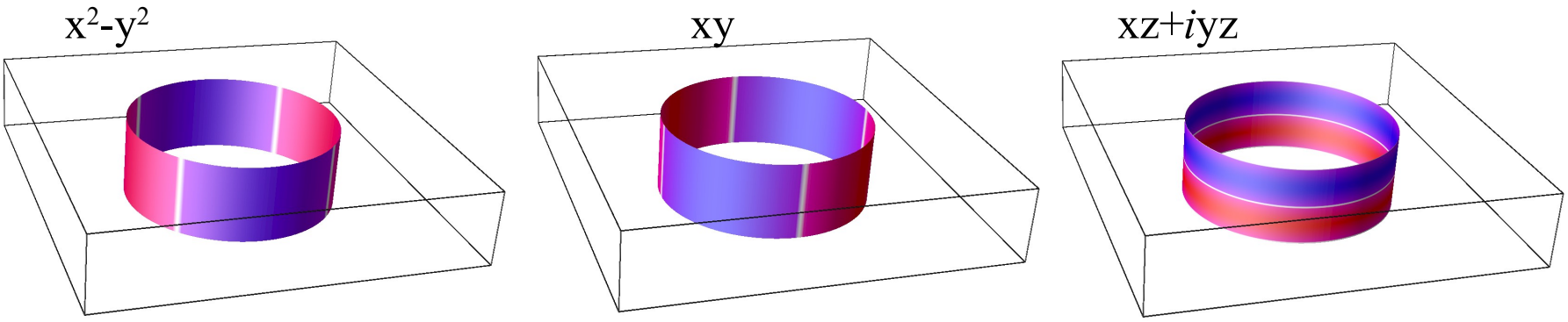
Osaka

It is singlet.

Remaining options for a tetragonal symmetry:

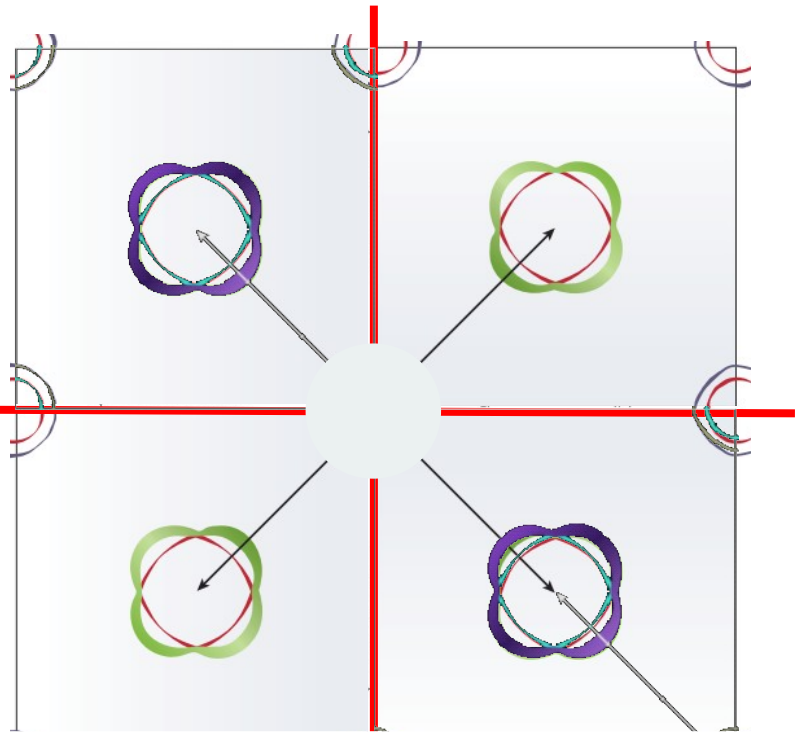
1. *L=0, s-wave*
2. *L=2, d-wave (*x -y , xy, *or* xz±*i*yz)

EXPERIMENTAL EVIDENCE: s-wave or d-wave?



1. d-wave ALWAYS has nodes (vertical or horizontal)

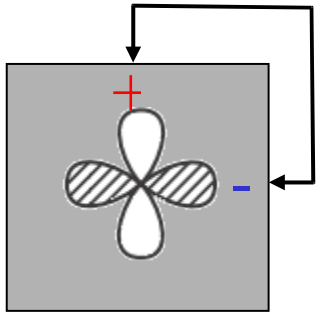
2. experimentally, at least *some* materials do NOT have any nodes, especially near the surface

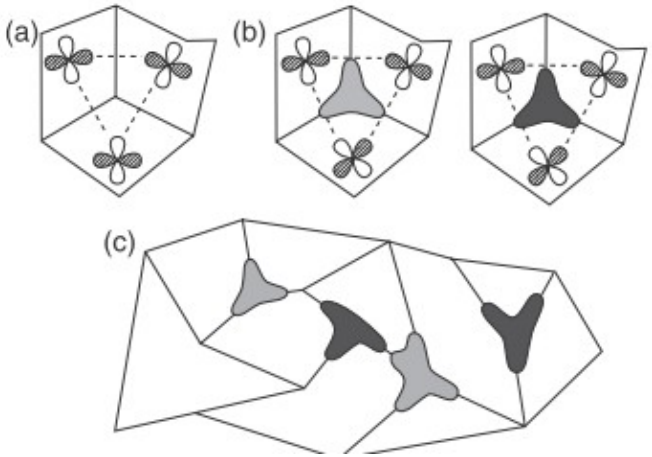


It is very unlikely to be d-wave.

Additional evidence against d-wave

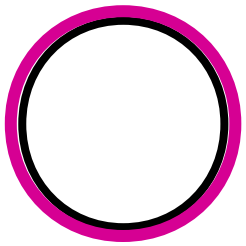
- **c-axis Josephson**: ***formally zero for all L≠0 symmetries observed (UMD group)***
- **Paramagnetic Meissner (Wohlleben) effect*; not observed (K.A. Moler et al, JPSJ)***
- **90-junctions**: ***unconfirmed reports (to-do list!)***

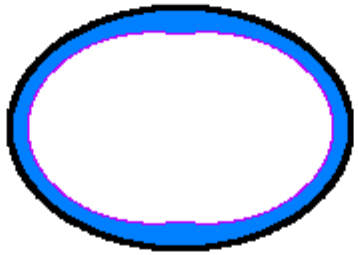




Experimental evidence: s_{++} or $s_{\pm}$?

Are we *closer* to the s_{++} limit (with possible nodes and patches of the "wrong" sign), or to $s_{\pm}$ limit (with possible nodes and patches of the "wrong" sign)?





And the correct question is…

No symmetry distinction – look f…s

Inversed coherence factors for c…

confirmed, but there are many other reasons

confirmed, but there may be another reason (claimed by Onari et al, PRB 60504)

…tructive coh…

…e for $\Delta_k\Delta_{k'}>0$, c…

$E_kE_{k'}$, …re as so… *…uctive for $\Delta_k\Delta_{k'}>0$, peaks as DOS*

This is reversed if $\Delta_k\Delta_{k'}<0$ (as known in cuprates)

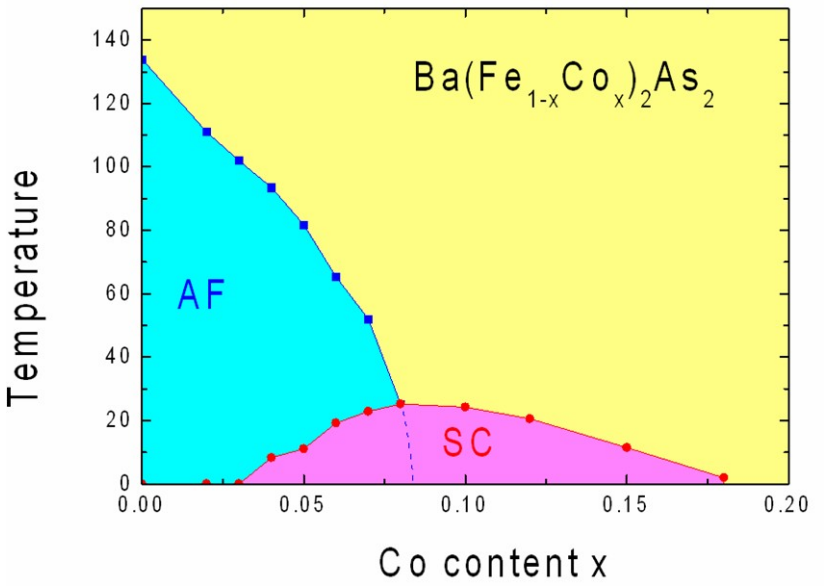
Expect no coherence peak in $1/TT_1$ (assuming main fluctuations at $Q=\{\pi,\pi\}$)

Expect a coherence peak in Imχ at $Q=(\pi,\pi)$

…more subtle (but maybe detectable) effects in phonon renormalization, quasiparticle scattering etc.

not yet

Coexistence of SDW and superconductivity



Unique opportunity: microscopic coexistence of SDW and SC at $0.04<x<0.08$

Thermal conductivity shows NO NODES there!

±

One can show that it is *only possible* in an s case (this is a <u>qualitative</u> result, D. Parker et al, PRB 80, 100508**).**

One can also argue that the very fact of coexistence is not

++

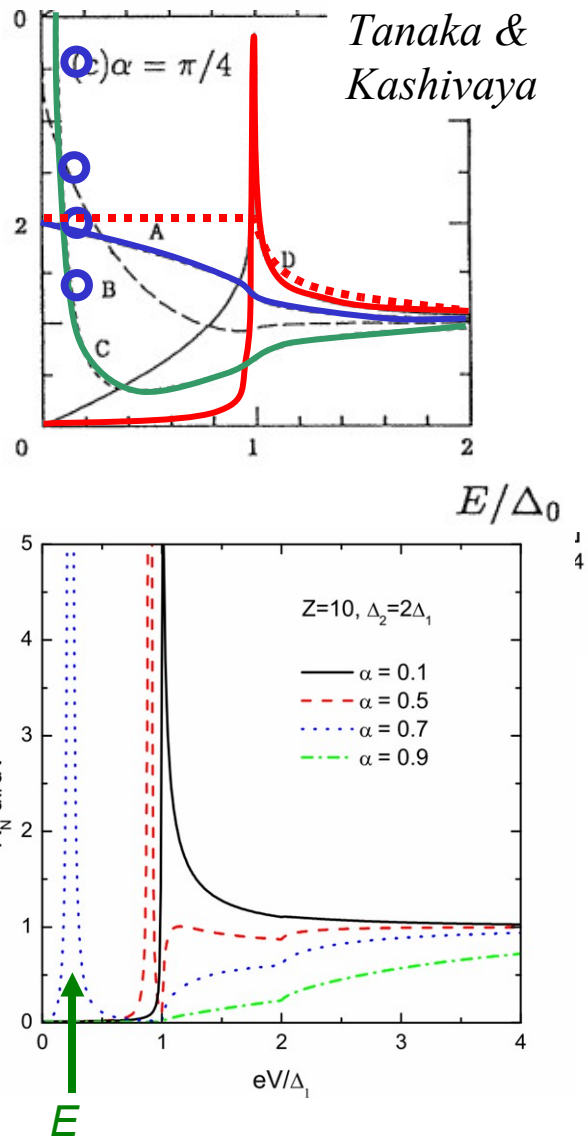
compatible with s (R.M. Fernandes et al, arXiv:0911.5183; M. Vavilov

Phase-sensitive tunneling effects: Andreev bound states

1. Recall s-wave: in the high-transparency limit $\sigma(0)=2$, in the low-transparency limit $\sigma(0)=0$

2. Recall d-wave: in the high-transparency limit $\sigma(0)=2$, in the low-transparency limit $\sigma(0)\rightarrow\infty$ (ZB bound state), and the result depends on angle.

3. In $s_{\pm}$ in the high-transparency limit $\sigma(0)<2$, in the low-transparency limit $\sigma(E)\rightarrow\infty$ (finite-bias bound state), and

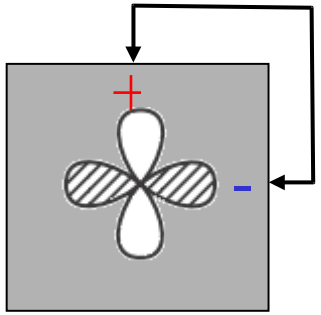


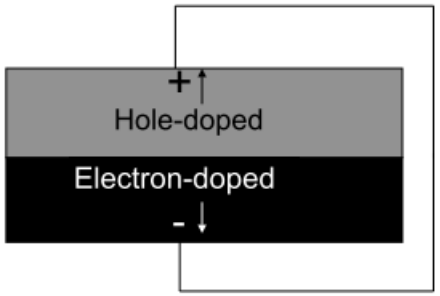
A. A. Golubov et al PRL **103**, 077003 (2009), and several other authors

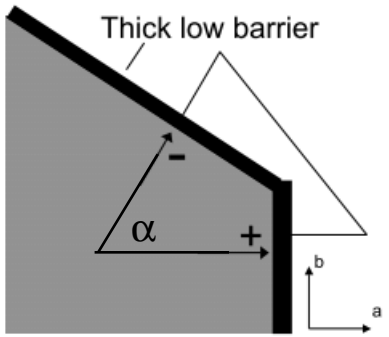
There are new effects, but they are very difficult to single out experimentally

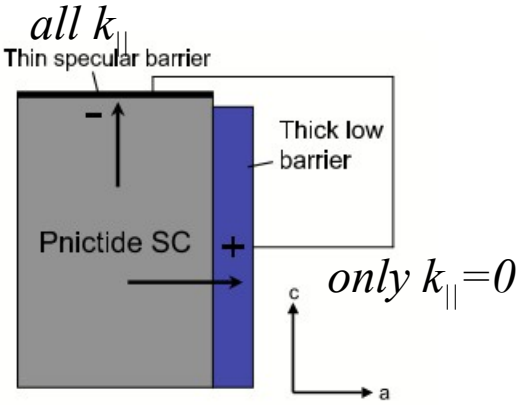
Phase-sensitive tunneling effects: corner junctions

- d-wave required by symmetry⇒NO means NO, YES means YES.
  s : only quantitative effect possible ⇒ YES



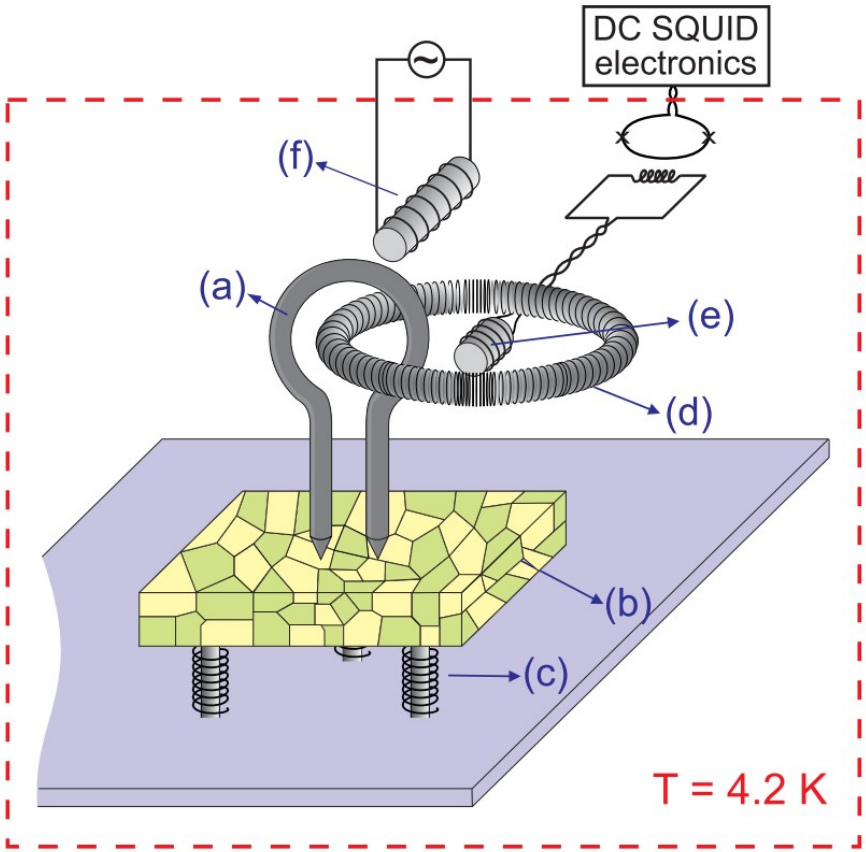






A “statistical alternative”

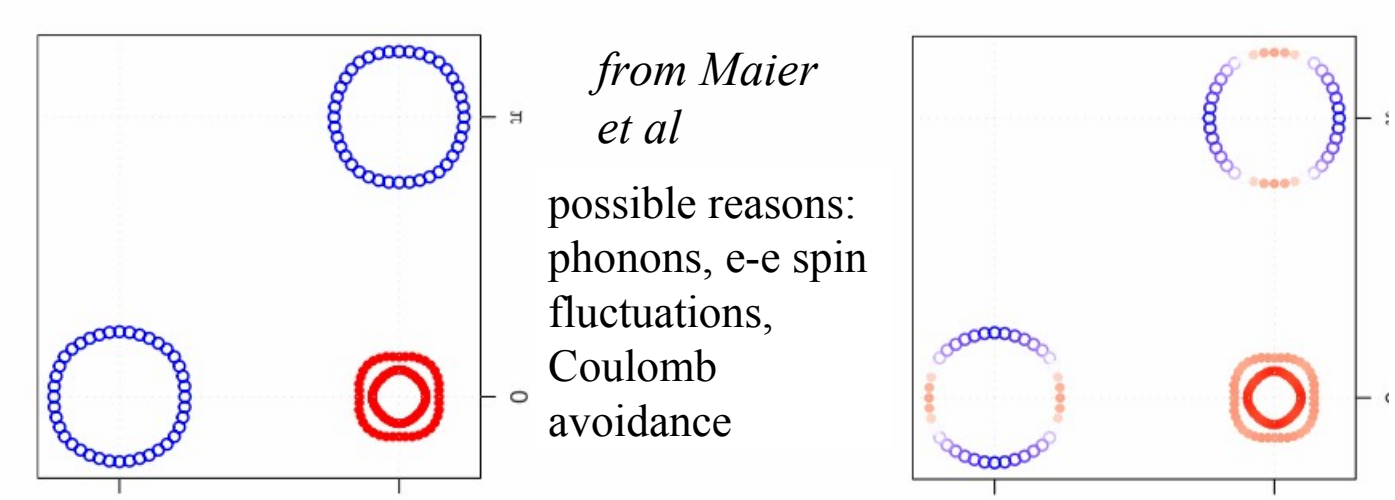
IBM group, cond-mat arXiv:0905.3571



Half-integer fluxes detected (in a small fraction of loops).

Various interpretations possible, but all of them require sign change of the order parameter

Nodes or no nodes?



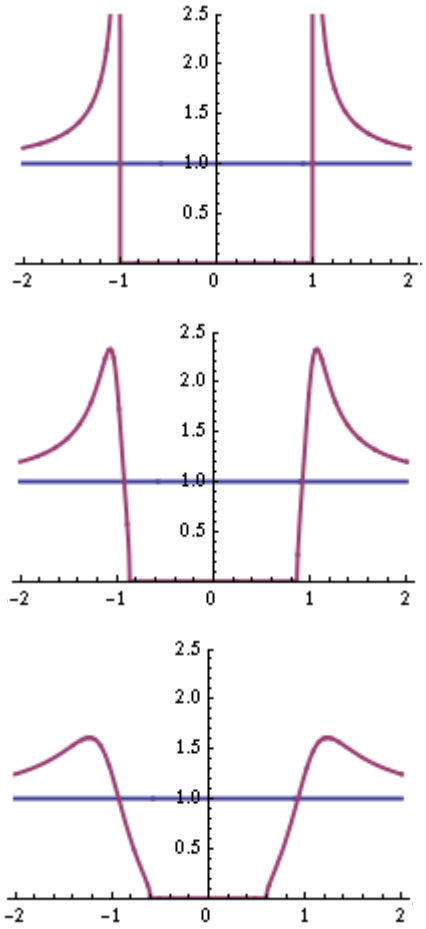
from Maier et al

possible reasons: phonons, e-e spin fluctuations, Coulomb avoidance

1. DOS probes (C/T, tunneling, penetration depth) – cannot distinguish between nodes and pair-breaking effects (which we do not entirely understand, still!)
2. ARPES (and tunneling) only probe the surface
3. Thermal conductivity – similar to DOS but more accurate and less sensitive to impurities

Thermal conductivity

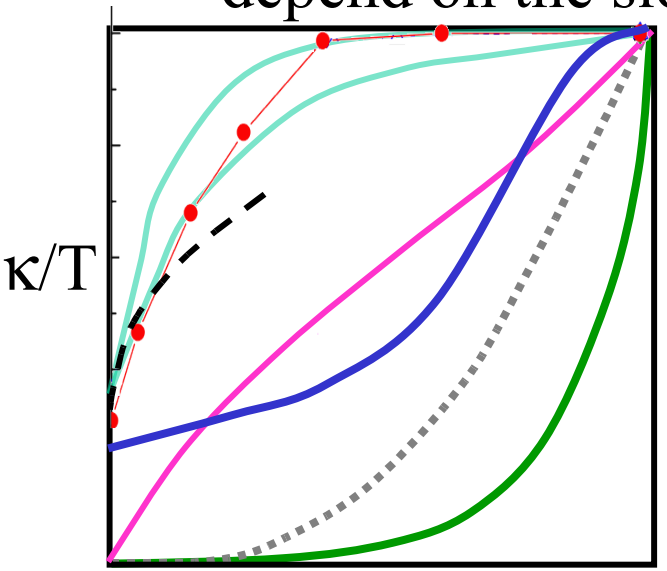
κ/T at T→0 probes DOS at E=0. How does it differ from non-transport probes?



$$\kappa / T \propto N(0)\sigma_{norm} \propto N(0)/\gamma$$

Near nodes, DOS increases linearly with impurity concentration.

κ/T does not depend on γ, but does depend on the slope of Δ



Nb

InBi

Tl2201

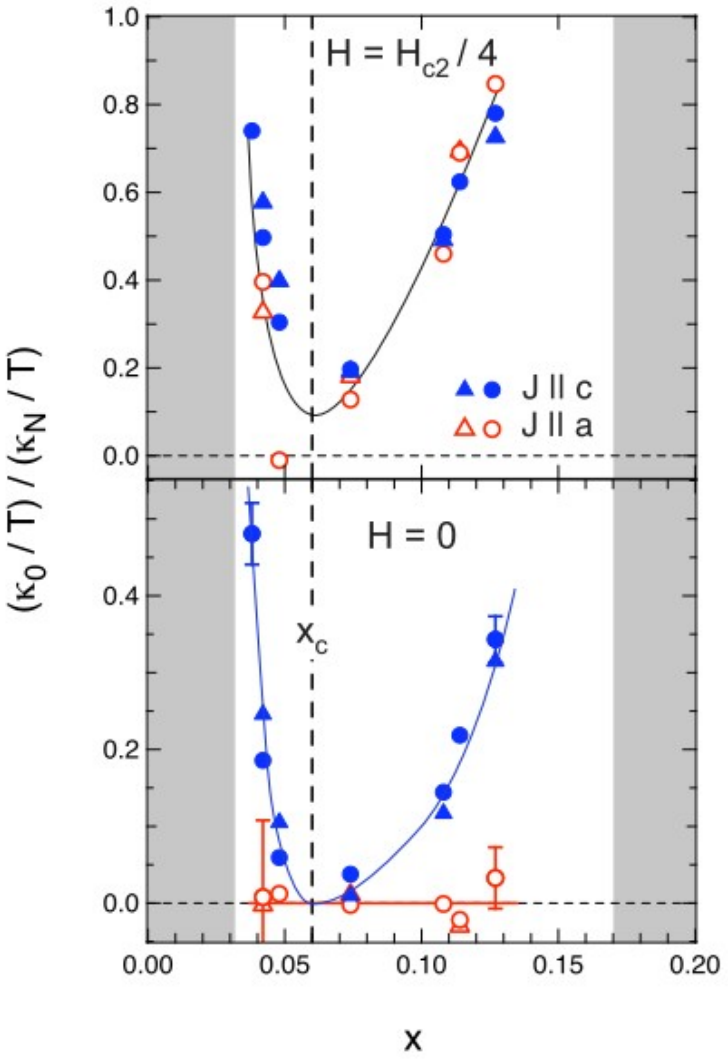
NbSe$_2$

BaFe$_2$(As,P)$_2$

LaFePO

Thermal conductivity

- In optimally doped $Ba(Fe,Co)_2As_2$ (also in $Ba_{0.5}K_{0.5}Fe_2As_2$, and in FeSe) thermal conductivity is inconsistent with nodes
- Thermal conductivity slope in $Ba(Fe,Co)_2As_2$ monotonically grows away from optimal doping
- The κ_c behavior is totally inconsistent with κ_{ab} behavior
- 5% of Ni (optimally doped) has the same effect as 4.8% Co (underdoped)
- Role of impurity states?

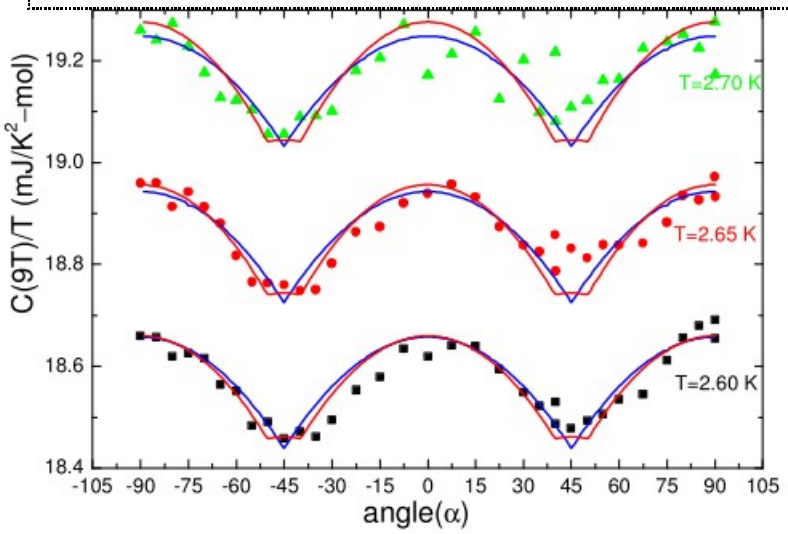


J.-P. Reid, M. Tanatar, …, L. Taillafer, unpublished

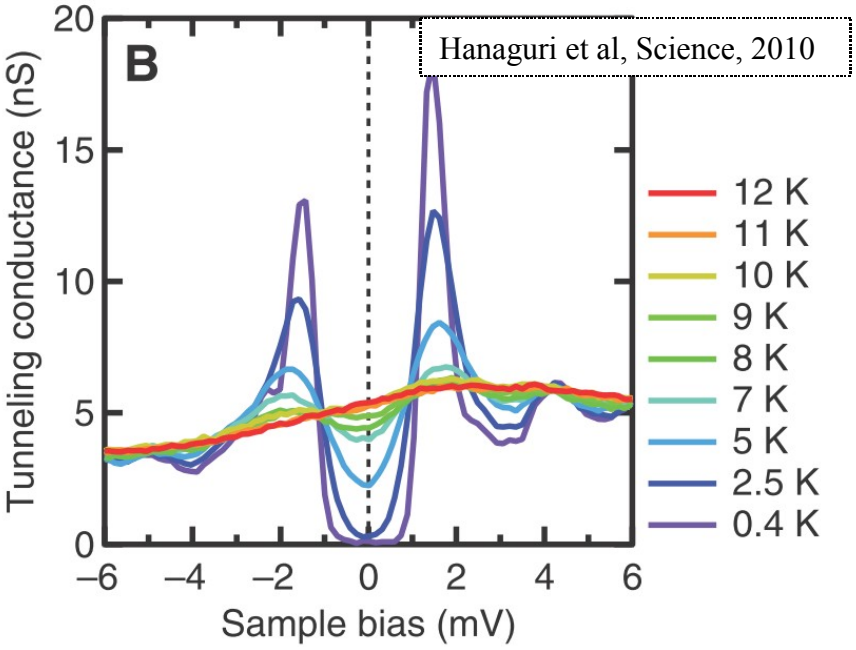
Angle-resolved probes

- Specific heat of Fe(Se,Te) in rotating magnetic field indicated nodes or deep minima along the (1,1) directions. Thermal conductivity and C(T) show no nodes. Tunneling shows a full gap.

B. Zheng, … IIM, … H-H Wen, arXiv:1004.2236

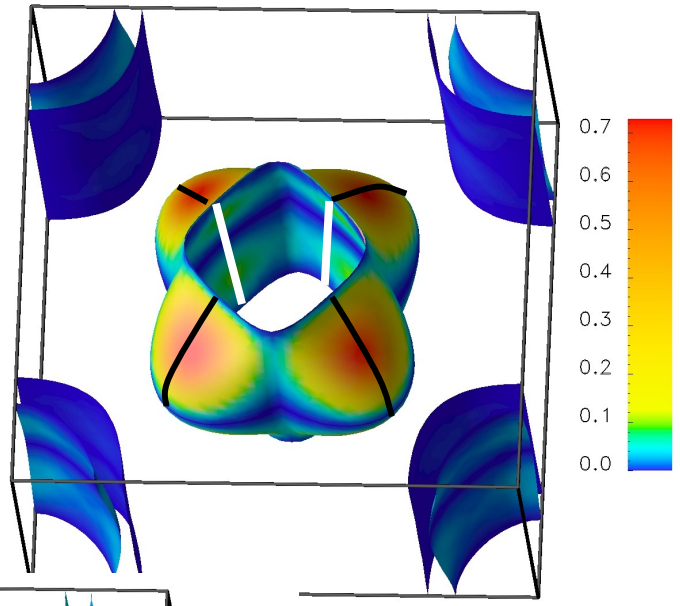


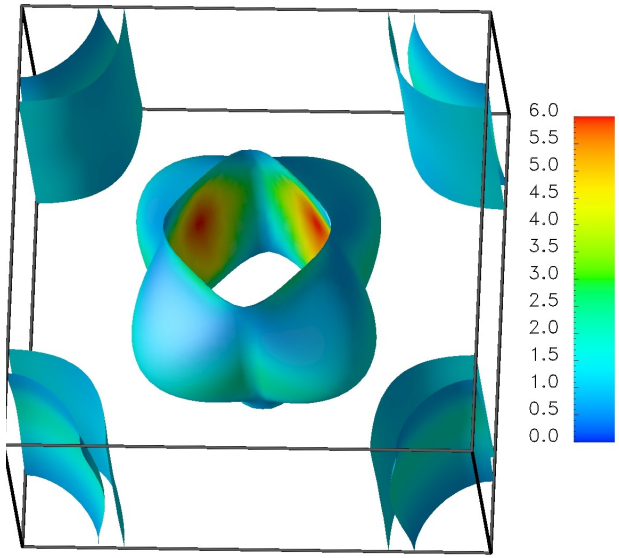
Hanaguri et al, Science, 2010



Angle-resolved probes

- Where are nodes?
- Hole surface: unlikely (no model provides those)
- Electron outer: contardicts STM
- Electron inner: consistent with both STM and thermal conductivity.





Angle-resolved probes

- Thermal conductivity of $BaFe_2(As,P)_2$ in rotating magnetic field indicated nodes or deep minima along the (1,1) directions. Thermal conductivity and C(T) show no nodes.

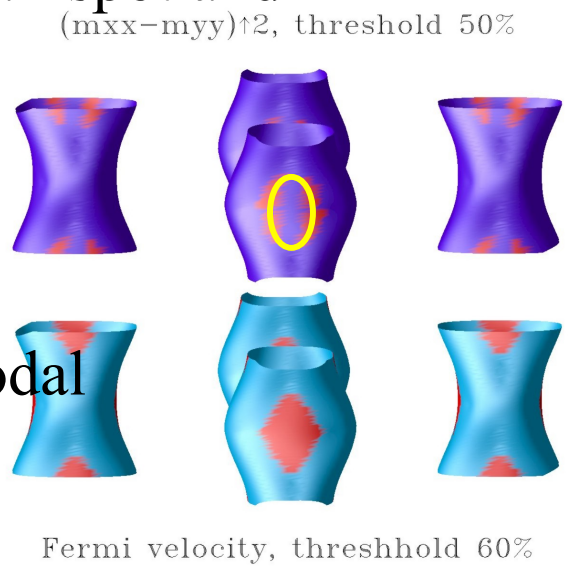
Matsuda et al, unpublished

- Their interpretation: Thermal conductivity is controlled by light electrons (corroborated by other experiments), specific heat controlled by heavy holes (>80%; not corroborated). Nodes live on the e-surface.
- *cf.* Sherbrook data: κ_c is controlled by a small spot and accidentally nodes live exactly there.
  Too many accidents?

- Electronic Raman scattering does not see any gap for the B_{1g} polarization – nodal ellipses.

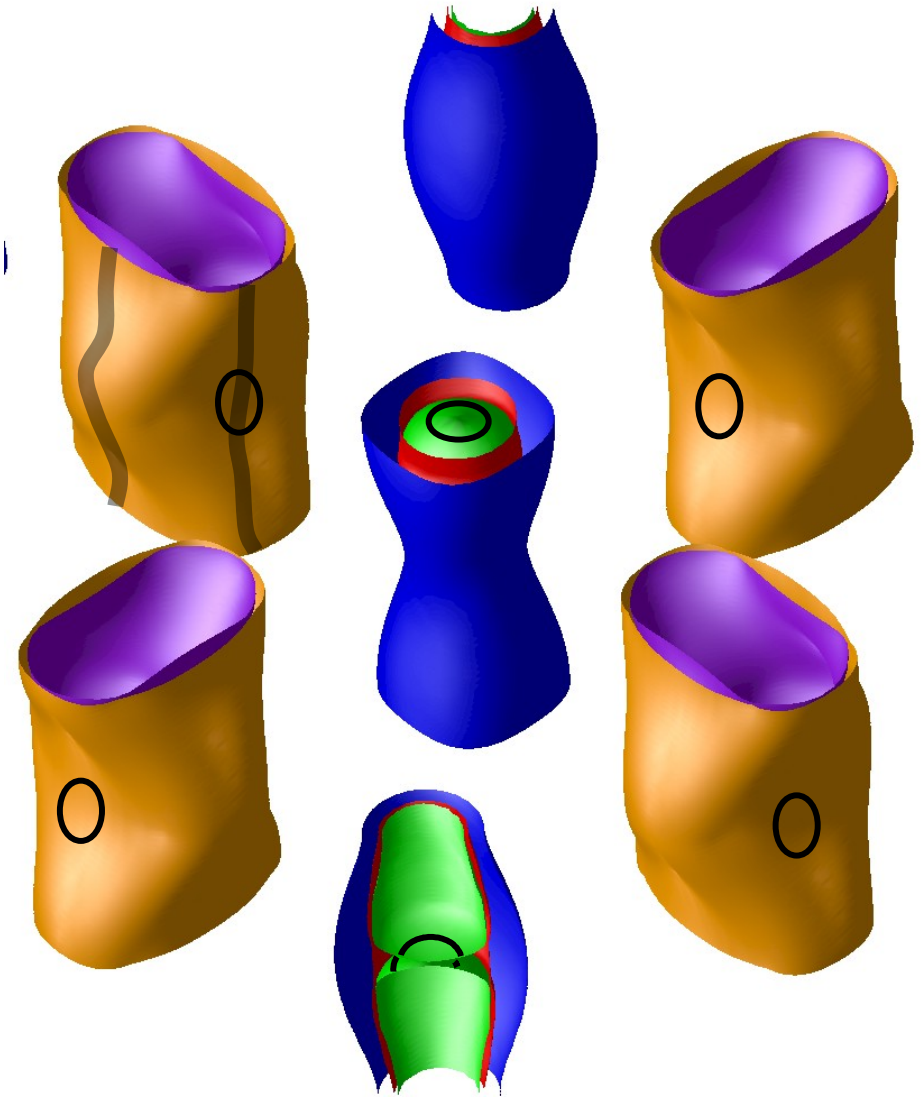
Muschler, Hackl, Devereaux et al, PRB 80, 180510 (2009)

IIM, Hackl, Devereaux et al, unpublished



Summary of all four experiments:

1. $BaFe_2(As,P)_2$, thermal conductivity in rotating magnetic field – (1,1) directions, *and maximal Fermi velocity in the same direction*
2. $Ba(Fe,Co)_2As_2$, thermal conductivity along c – nodal circles on the FS caps
3. $Ba(Fe,Co)_2As_2$, electronic Raman scattering – nodal ellipses around (1,1,0), *where the Fermi velocity is maximal.*



CONCLUSIONS (Current status)

Pairing symmetry:

- definitely singlet

- nearly definitely not *d*

- most likely sign-changing

$\pm$

-

- strong evidence for $s^{\pm}$ (but only **indirect** so far)

Presence (in most cases) of subgap quasiparticles, with a complicated DOS – more work needed.

What is the nature of structure of these quasiparticles? Are they nodal? Are they impurity driven? – intuition and knowledge derived from the old good one-band d-wave in cuprates looks like hopelessly out of place…

To be strict is better than to be lax... though this pairing sounds natural enough in some localities.

Rhymes and Meters, A Practical Manual for Versifiers, by Horatio Winslow, 1909

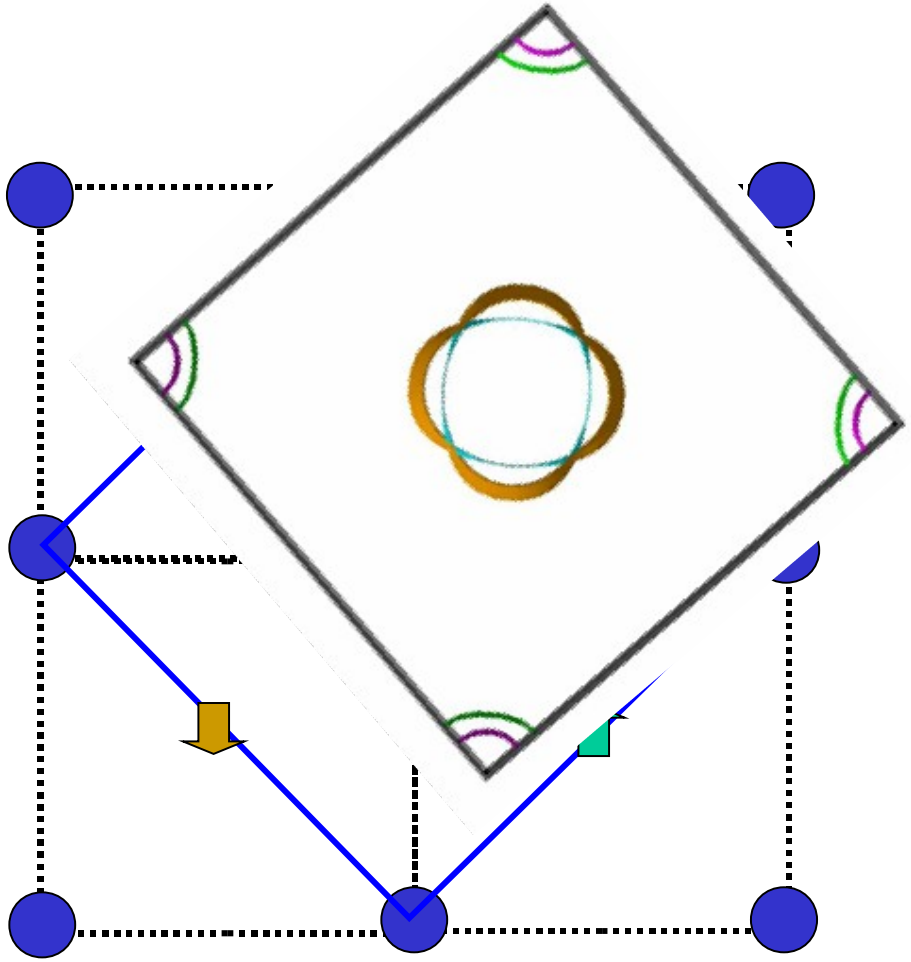
POST-CONCLUSIONS (Future experiments)

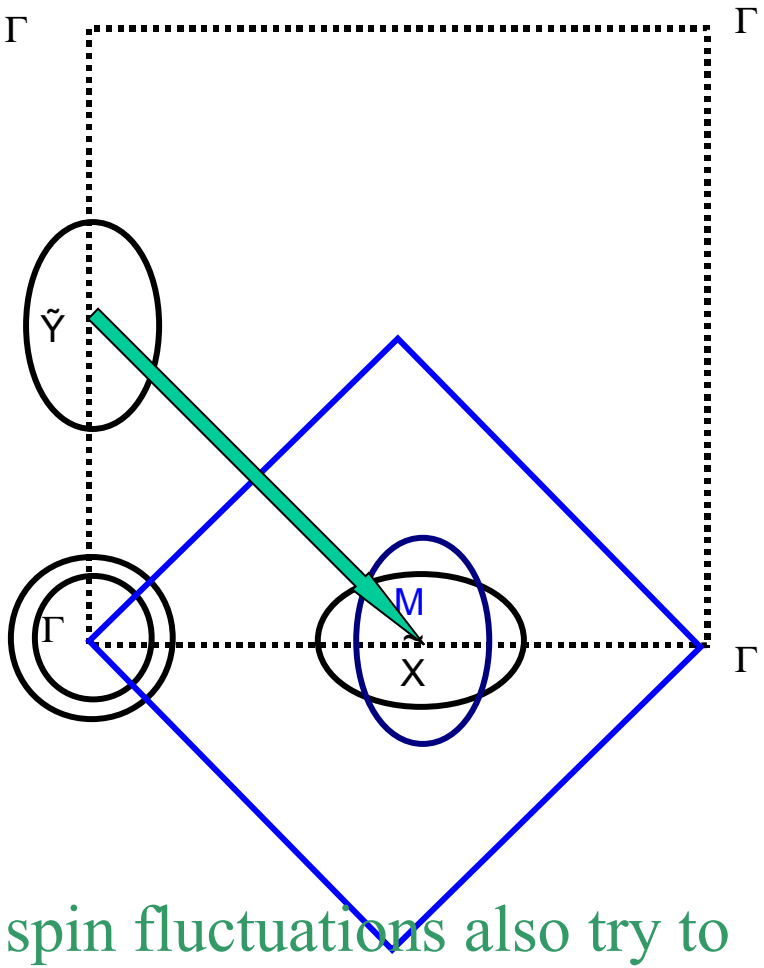
1. **Phase-sensitive experiments.**
   - Any indication of π-shift is a strong argument; absence thereof isn't.
   - "Standard" 90 corner junctions still unverified!
   - The only *qualitative* test: epitaxial sandwich.

1. **More angular dependent experiments**

1. **STM quasiparticle scattering?** – Not Bragg peaks, but real quasiparticles! (no data yet, AFAIK)

Unfolding the Brillouin zone





Zone-center [$\equiv J$ superexchange] spin fluctuations also try to

Coulomb avoidance

d-wave:

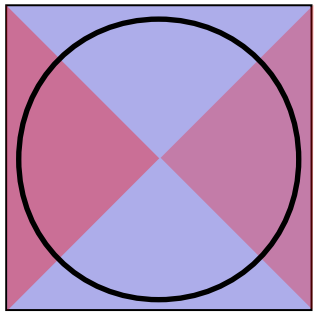
$$\Delta_k = \Delta_0[\cos(k_x a) - \cos(k_y a)]$$

$$\Delta(\mathbf{r}) = \Delta_0[\delta(x \pm a) - \delta(y \pm a)]$$

$s_{\pm}$-wave

$$\Delta_k = \Delta_0[\cos(k_x a)\cos(k_y a)]$$

$$\Delta(\mathbf{r}) = \Delta_0\delta(x \pm a)\delta(y \pm a)$$

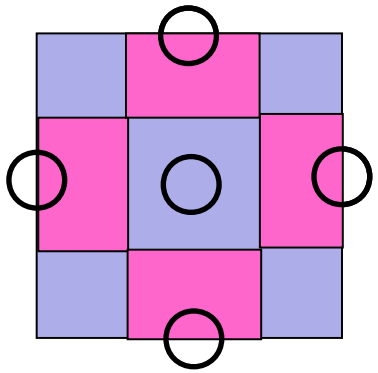


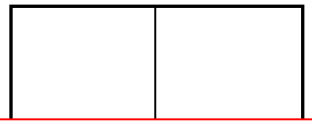
Condition for complete avoidance (Hubbard repulsion):

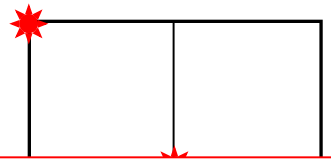
$<\Delta>=0$

If $\Delta_1/\Delta_2=\alpha$, $U\rightarrow\infty$

$\lambda/\lambda_0=2/(\alpha^{-1}+\alpha)\gtrsim 0.8$







Δ_1/Δ_2 is set by the DOSs.

Therefore Coulomb wants to create nodes on the FS with the larger gap

(Scalapino, Hirschfeld et al, Chubukov et al, Kuroki et al)

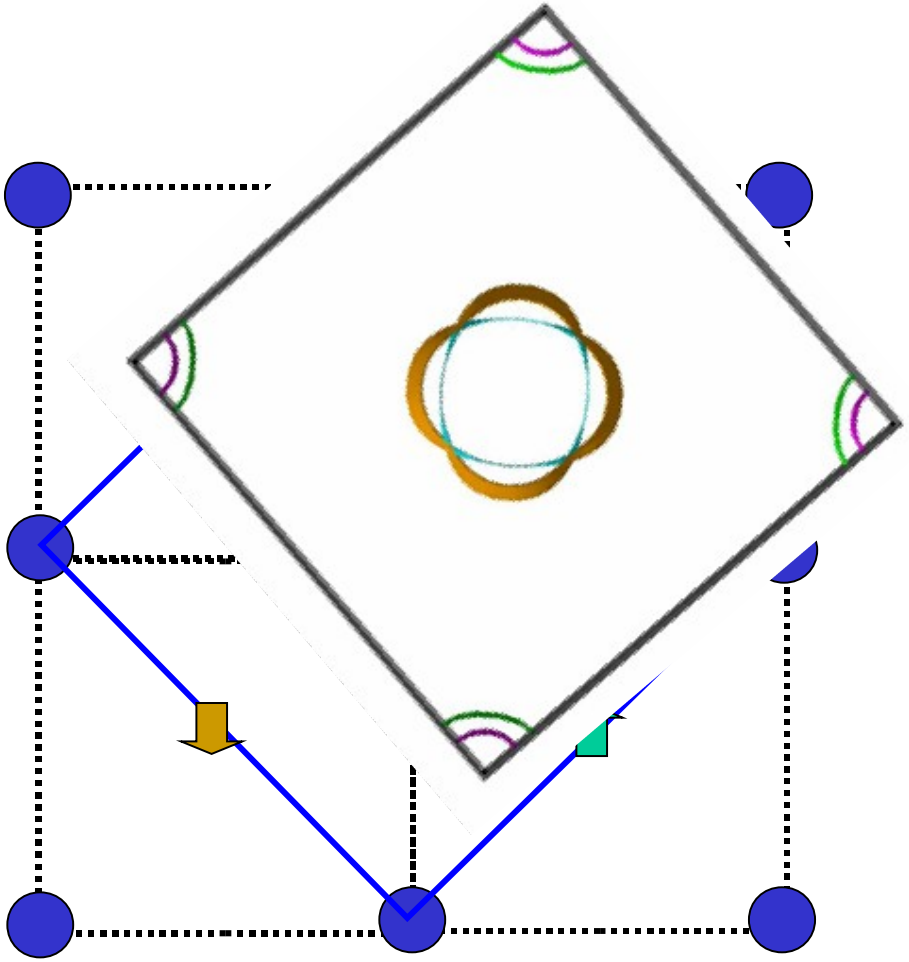
NA304012

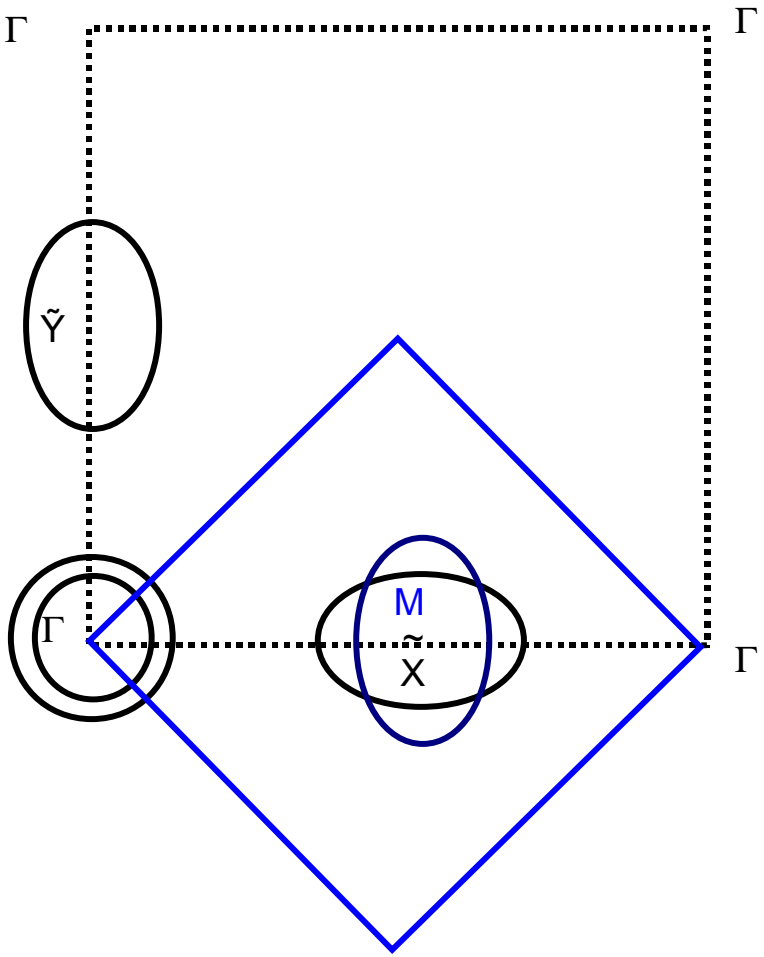
Lawrence Durrell

JUSTINE

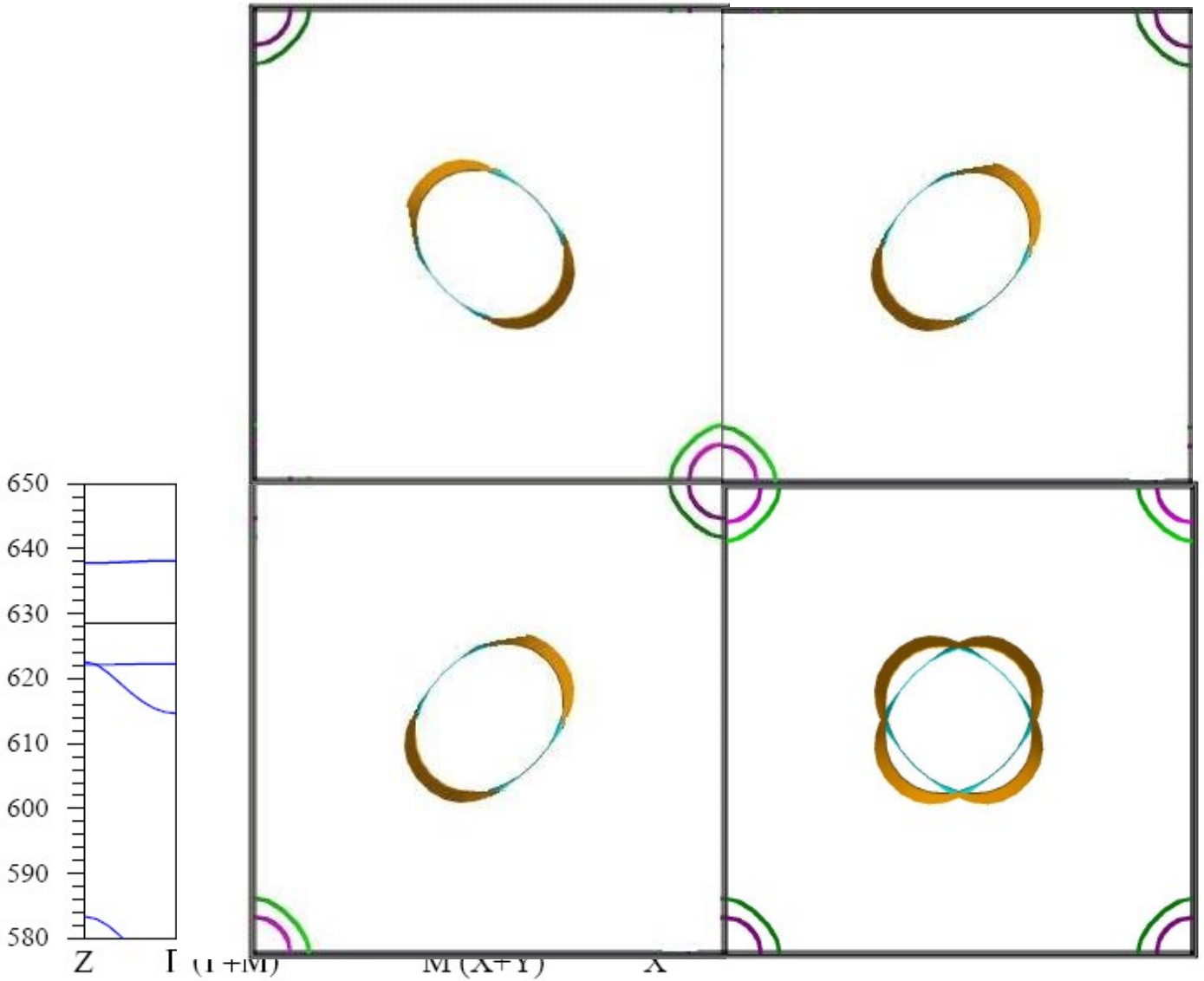
“It is mentally vulgar to spend one’s time being so certain of first principles…”

Unfolding the Brillouin zone

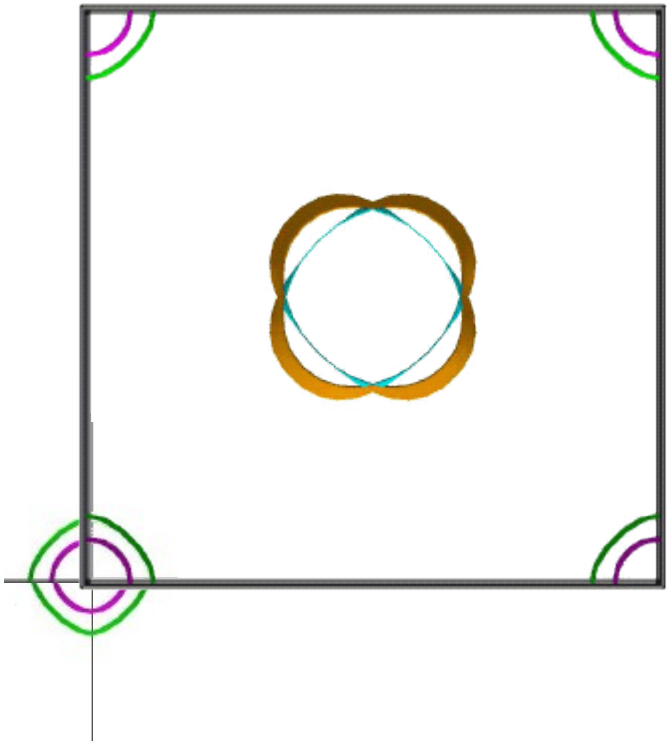


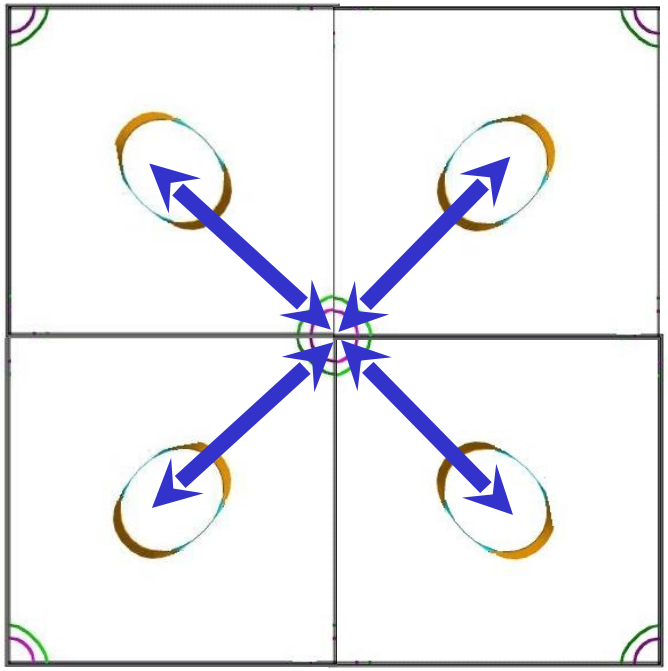


Crystal and electronic structure



Spin fluctuations





Gap ratio

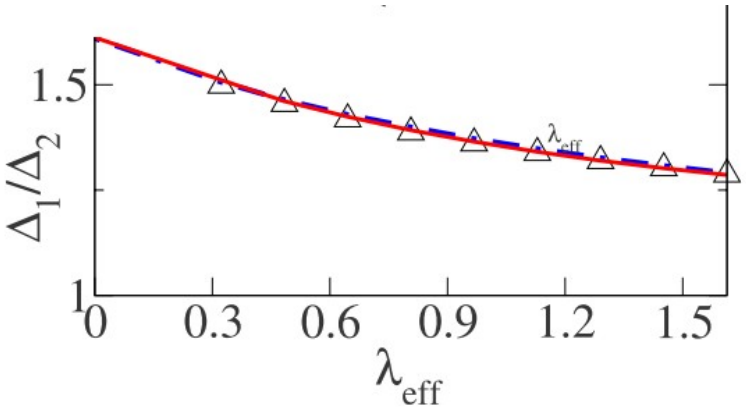
BCS (weak coupling)

It is not that easy to provide a gap ratio of 2!

- three (four) band effects are important
- other interactions (phonons, intraband spin fluctuations etc) are important

Eliashberg (strong coupling)

$$\begin{cases} \Delta_1(1+\lambda_{12} = \lambda_{12}\Delta_2 \ln(1.13\omega_c / T_c) \\ \Delta_2(1+\lambda_{21}) = \lambda_{21}\Delta_1 \ln(1.13\omega_c / T_c) \end{cases}$$



$$\frac{\Delta_1(T)}{\Delta_2(T)} = -\sqrt{N_2/N_1}\left(1+\frac{\sqrt{\lambda_{12}\lambda_{21}}\ln(N_2/N_1)}{4}+\frac{\lambda_{21}-\lambda_{12}}{2}\right)$$

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