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)?
<table>
<thead>
<tr>
<th>Post-cuprate Materials</th>
<th>Key concept</th>
<th>Band theorists</th>
<th>Many-body theorists</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{60}$</td>
<td>High-energy intramolecular modes</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>ZrZn$_2$</td>
<td>Sample inhomogeneity</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>MgCNi$_3$</td>
<td>Anharm. phonons suppressed by spin fluctuations</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>MgB$_2$</td>
<td>Two gaps</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Sr$_2$RuO$_4$</td>
<td>p-wave</td>
<td></td>
<td>+?</td>
</tr>
<tr>
<td>Hcp Fe under pressure</td>
<td>Unconventional, magnetism-driven</td>
<td>+?</td>
<td></td>
</tr>
<tr>
<td>CaC$_6$</td>
<td>C and intercalant phonons</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Fe-based</td>
<td>$S_{+/-}$</td>
<td>+?</td>
<td>-</td>
</tr>
</tbody>
</table>
• 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.

• 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)?
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 $\omega_\nu$, belonging to a phonon branch $\nu$.

$$g_{k,k+q,\nu} = q, \nu \gamma_{kk+q}^j \quad \text{and} \quad g_{k,k+q,\nu} = \langle k | dV / dQ_{q,\nu} | q \rangle$$

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:

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

Electron self energy is defined by the following diagram:
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, \( \alpha^2 F_{kk'}(\omega) \), and is, explicitly
This basic quantity is called the Eliashberg function, $\alpha^2 F_{kk'}(\omega)$, and is, explicitly

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

while its isotropic average is

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

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 $\lambda$ independent of complexity of crystal structure or even periodicity.
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

\[ \hat{H} = - \sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_{i,I} \frac{Z_I e^2}{|r_i - R_I|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} \]

\[ - \sum_I \frac{\hbar^2}{2M_I} \nabla_I^2 + \frac{1}{2} \sum_{I \neq J} \frac{Z_I Z_J e^2}{|R_I - R_J|} \]

- 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

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

- 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 $n = n_0$
- From Kohn-Sham

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

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

Equations for independent particles - soluble

Exchange-Correlation Functional – Exact theory but unknown functional!

- The new paradigm – find useful, approximate functionals
The Kohn-Sham Equations

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

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

Constraint – required
Exclusion principle for independent particles

\[ \frac{\delta E_{KS}}{\delta \psi_i^{\sigma\ast}(r)} = 0, \quad (1) \]

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

\[ (-\frac{1}{2} \nabla^2 + V_{KS}^\sigma(r), -\varepsilon_i^\sigma) \psi_i^\sigma(r) = 0 \quad (3) \]

\[ V_{KS}^\sigma(r) = V_{ext}(r) + \frac{\delta E_{Hartree}}{\delta n(r,\sigma)} + \frac{\delta E_{xc}}{\delta n(r,\sigma)} \]

\[ = V_{ext}(r) + V_{Hartree}(r) + V_{xc}^{\sigma}(r) \quad (4) \]

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

Self-Consistent Kohn-Sham Equations

1. Initial Guess
   - \( n^\uparrow(r), n^\downarrow(r) \)
2. Calculate Effective Potential
   - \( V_{eff}(r) = V_{ext}(r) + V_{Hart}[n] + V_{xc}[n^\uparrow, n^\downarrow] \)
3. Solve KS Equation
   - \( \left( -\frac{1}{2} \nabla^2 + V_{eff}(r) \right) \psi_\sigma^i(r) = \epsilon_\sigma^i \psi_\sigma^i(r) \)
4. Calculate Electron Density
   - \( n_\sigma(r) = \sum_i f^{\sigma}_i |\psi_\sigma^i(r)|^2 \)
5. Self-consistent?
6. Output Quantities
   - Energy, Forces, Stresses, 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:

\[ \psi_v = \sum_i A_v \phi_i; \quad \delta \psi_v = \sum_i \delta A_v \phi_i; \quad \text{or} \quad \delta \psi_v = \sum_i A_v \delta \phi_i \]

When ions shifts, atomic orbitals also shift and deform.
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)?
Recent applications: superconductivity in doped graphenes

**MgB$_2$**

**Graphite:**
- ABABAB

**LiC$_6$:**
- A$\alpha$A$\alpha$A$\alpha$A

**YbC$_6$:**
- A$\alpha$A$\beta$A$\alpha$A

**CaC$_6$:**
- A$\alpha$A$\beta$A$\gamma$A

**MgB$_2$:**
- A($\alpha$+$\beta$+$\gamma$)A

LiC$_6$
Intercalated graphene: electronic structure

Formation of the electronic structure

- $C_{px,y}$
- $C_{pz}$
- intercalant orbitals (s, d, f… )
- “nearly-free-electron” states
MgB$_2$: $\sigma$-band + $\pi$-band

MgB$_2$ differs from graphite only the Fermi level position (and by the “unimportant” $\zeta$-band)

No Mg states at $E_F$
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 $q < q_{\text{max}}$. 

Bond-stretching $E_{2g}$ mode: main player
It seems like the $\pi$ 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.

\[
\begin{bmatrix}
0.95-1.0 & 0.16-0.17 \\
0.21-0.23 & 0.3-0.45
\end{bmatrix}
\]

$\lambda_{ij} \approx 1-1.05; \lambda_{av} = 0.87-0.9$
3D band: free electrons or intercalant states?

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

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

CaC₆

carbon $p(z)$

C₆

Ca/empty $s$
CaC$_6$: $\pi$-band + $\zeta$-band

CaC$_6$ : fcc Ca + C$_6$

- Ca states

Cf. MgB$_2$ -- $\sigma$-band + $\pi$-band.

Is it possible to create a material with all three types of carriers? XXX -- $\sigma$-band + $\pi$-band + $\zeta$-band?
Full DFT calculations

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

Note that most of the coupling comes from the free-electron-like spherical FS (the $\zeta$-band).
MgB$_2$ + CaC$_6$ = ?

CaC$_6$: $\pi$-band + $\zeta$-band
MgB$_2$: $\sigma$-band + $\pi$-band
Li$_2$B$_2$: $\sigma$-band + $\zeta$-band!

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

Where have all the $\pi$-electrons gone??

In terms of the $\pi$-band, Li$_2$B$_2$ is an exact analogue of the undoped graphite
Better to see once than to be told about thrice

(Russian proverb)

Fermi surfaces

MgB$_2$

CaC$_6$

Li$_2$B$_2$
Why do we need that π-band, after all???

Electron-phonon coupling with π-electrons softens the “working” phonon in MgB$_2$ from 81 meV to 67: a 50% enhancement of $\lambda$!

Calculated $T_C \sim$ 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 $\pi$-band can!

Doping of 0.15 electrons per formula (e.g., Li$_2$B$_{1.85}$C$_{0.15}$) raises the Fermi level

...and raises the density of $\pi$-states up to a value comparable with that of MgB$_2$. 
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

Charge fluctuations (phonons) mediate attraction; spin fluctuations mediate repulsion.

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

Superexchange interaction is peaked at $Q=(\pi, \pi)$

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.

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

Fermi surface of BSCCO measured by ARPES (http://en.wikipedia.org/wiki/Fermi_surface)
Cooking an $s^{\pm}$ state: ingredient 1 - Fermiology

In all actual materials there is some “poor” nesting of the Fermi surfaces.
Cooking an $s_{\pm}$ state: ingredient 2 – spin fluctuation

$$\text{Re} \chi_0(q, \omega \to 0) = \sum_k \frac{f_{k+q} - f_k}{\varepsilon_{k+q} - \varepsilon_k} \quad \text{Im} \chi_0(q, \omega) \bigg|_{\omega \to 0} = \sum_k \delta (\varepsilon_{k+q} - E_F) \delta (\varepsilon_k - E_F)$$

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

FOUND EXPERIMENTALLY!
Origin of spin fluctuations: not important!

\[ \chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - J(q, \omega) \chi_0(q, \omega)} \]

For a Mott-Hubbard system, \( J(q, \omega) \) 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

\[ \chi_0(q, \omega) = \sum_k \frac{f(\epsilon_{k+q}) - f(\epsilon_k)}{\epsilon_{k+q} - \epsilon_k - \omega - i\delta} \]

**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

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


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
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 the $s^\pm$ 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)?
It is singlet.

Remaining options for a tetragonal symmetry:
1. $L=0$, $s$-wave
2. $L=2$, $d$-wave ($x^2-y^2$, $xy$, or $xz\pm iyz$)
The text discusses experimental evidence to differentiate between s-wave and d-wave. It states:

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 $L \neq 0$
  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…
Inversed coherence factors for $q=(\pi, \pi)$ scattering

Constructive and destructive coherence factors:

$E_k E_{k'} - \Delta_k \Delta_{k'}$: destructive for $\Delta_k \Delta_{k'} > 0$, cancels DOS

$E_k E_{k'} + \Delta_k \Delta_{k'}$: constructive 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 $\text{Im}\chi$ at $Q=(\pi, \pi)$

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

Confirmed, but there may be another reason (claimed by Onari et al, PRB 60 504)

No symmetry distinction – look for $s^\pm$-specific properties

Confirmed, but there are many other reasons
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 $s\pm$ case (this is a qualitative result, D. Parker et al, PRB 80, 100508).

One can also argue that the very fact of coexistence is not compatible with $s\mp$ (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 $\sigma(0)\to\infty$ (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 $\sigma(E)\to\infty$ (finite-bias bound state), and

---

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

---

A. A. Golubov et al PRL 103, 077003 (2009), and several other authors
• d-wave required by symmetry $\Rightarrow$ NO means NO, YES means YES.

$s$ : only quantitative effect possible $\Rightarrow$ 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?

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

\( \kappa / T \) at \( T \to 0 \) probes DOS at \( E = 0 \). How does it differ from non-transport probes?

\[
\kappa / T \propto N(0) \sigma_{\text{norm}} \propto N(0) / \gamma
\]

Near nodes, DOS increases linearly with impurity concentration.

\( \kappa / T \) does not depend on \( \gamma \), but does depend on the slope of \( \Delta \)

\[
\kappa / T \propto H / H_{c2}
\]

- \( \text{Nb} \)
- \( \text{BaFe}_2(\text{As},\text{P})_2 \)
- \( \text{InBi} \)
- \( \text{LaFePO} \)
- \( \text{Tl}_2\text{2201} \)
- \( \text{NbSe}_2 \)
Thermal conductivity

- In optimally doped Ba(Fe,Co)$_2$As$_2$ (also in Ba$_{0.5}$K$_{0.5}$Fe$_2$As$_2$, and in FeSe) thermal conductivity is inconsistent with nodes
- Thermal conductivity slope in Ba(Fe,Co)$_2$As$_2$ monotonically grows away from optimal doping
- The $\kappa_c$ behavior is totally inconsistent with $\kappa_{ab}$ 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
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.

Hanaguri et al, Science, 2010
Angle-resolved probes

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

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: $\kappa_c$ 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.
Summary of all four experiments:

1. $\text{BaFe}_2(\text{As,P})_2$, thermal conductivity in rotating magnetic field – (1,1) directions, and maximal Fermi velocity in the same direction

2. $\text{Ba(Fe,Co)}_2\text{As}_2$, thermal conductivity along c – nodal circles on the FS caps

3. $\text{Ba(Fe,Co)}_2\text{As}_2$, 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
  
- **$\pm$**
  
- 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 $\pi$-shift is a strong argument; absence thereof isn’t.
   - “Standard” 90$^\circ$ 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)
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 $\Delta_1/\Delta_2 = \alpha$, $U \rightarrow \infty$

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

$\Delta_1/\Delta_2$ 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)
“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)

\[
\begin{align*}
\Delta_1(1 + \lambda_{12}) &= \lambda_{12}\Delta_2 \ln(1.13\omega_c / T_c) \\
\Delta_2(1 + \lambda_{21}) &= \lambda_{21}\Delta_1 \ln(1.13\omega_c / T_c)
\end{align*}
\]

\[
\frac{\Delta_1(T)}{\Delta_2(T)} = -\sqrt{N_2 / N_1} \left(1 + \frac{\sqrt{\lambda_{12}\lambda_{21}}}{4} \ln\left(\frac{N_2}{N_1}\right) + \frac{\lambda_{21} - \lambda_{12}}{2}\right)
\]
Detailed calculation of the doped compound are necessary to verify that it is indeed superior to MgB$_2$.

But one conclusion can be made: first principle calculations are mature enough (a XXI century thing!) to make quantitative predictions regarding conventional superconductors (not unconventional, alas!)

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