

Emergence of quantum phases in novel materials

SUPERCONDUCTIVITY II

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BIBLIOGRAPHY (BOOKS)

Collection of reviews

- Conventional SPC “Superconductivity” Edited by Parks. 1968.
- Conventional and unconventional SPC “Superconductivity” 2008 (Fe SPC not included)

“Many-body physics” Piers Coleman

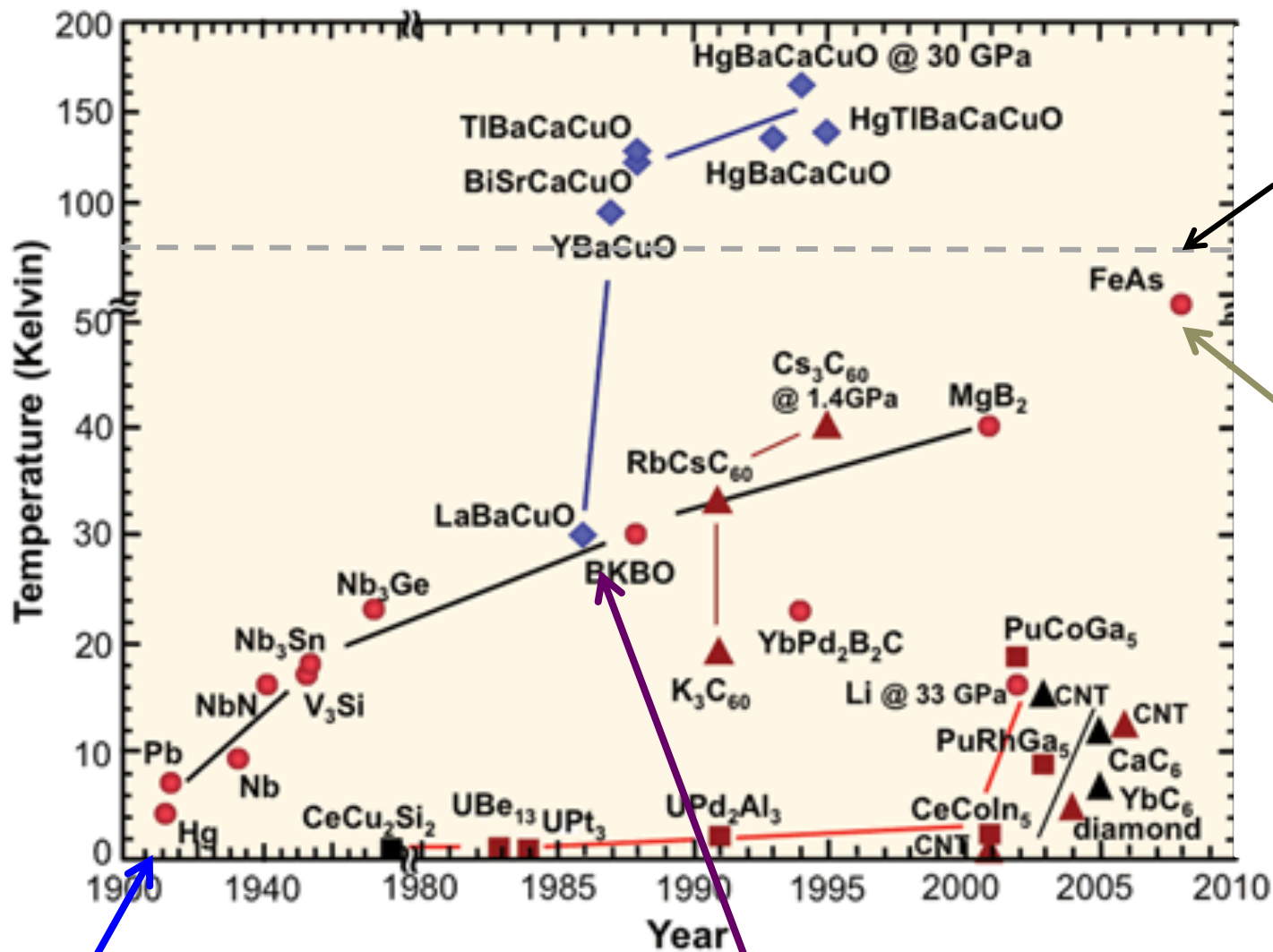
“Introduction to superconductivity” Tinkham

SPC history:

“Superconductivity: a very short introduction” S. Blundell

OUTLINE

- Superconductivity
 - Properties (zero resistivity, Meissner effect)
 - Understanding (pairing, BCS, Ginzburg-Landau)
 - Electron-phonon interaction (conventional superconductivity)
- **Unconventional superconductivity (unsolved)**
 - What are the new issues.
 - What are the proposals.



MATTHIAS'S RULES ?

Theory predicted superconductivity in hydrogen compounds (Ashcroft) and semiconductors (Cohen).

SrTiO_3 ($T_c=0.3\text{K}$); H_2S ($T_c=200\text{K}$)

High T_c

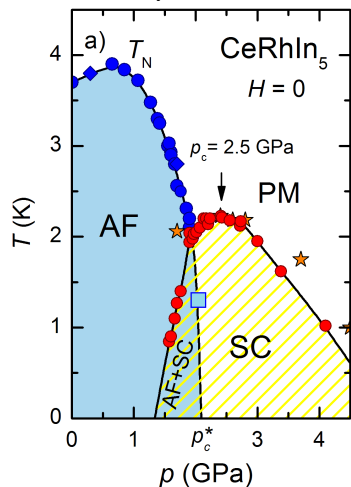
Cuprates

Fe-superconductors

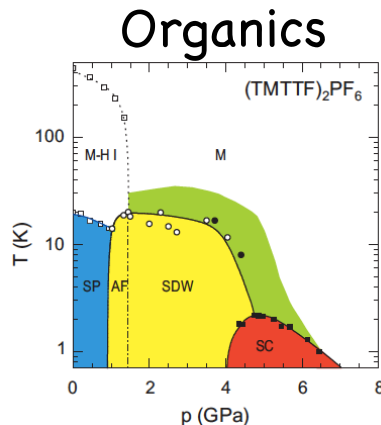
AF supercond.

Heavy fermions

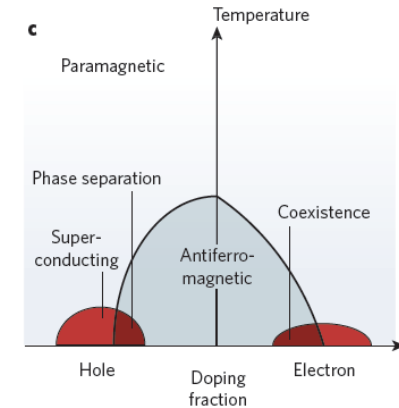
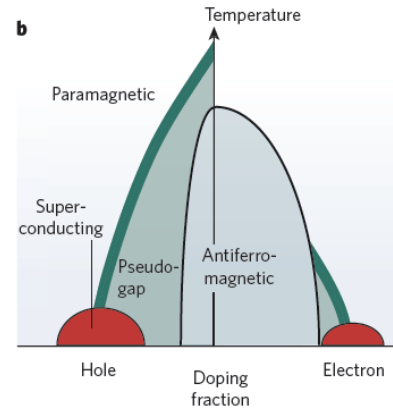
Oxides
Insulators
Magnetism



AF+SFC
Coexistence

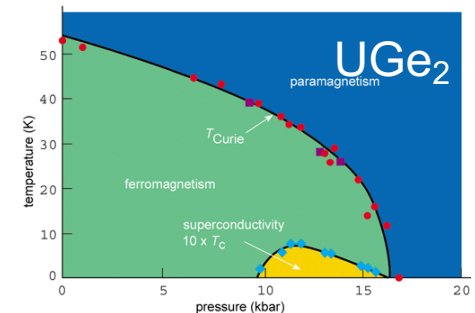
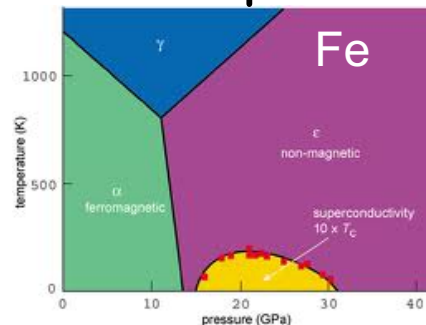


Eur. Phys. JB 21, 175



Nature 464, 183 (2010)

FM superconductors



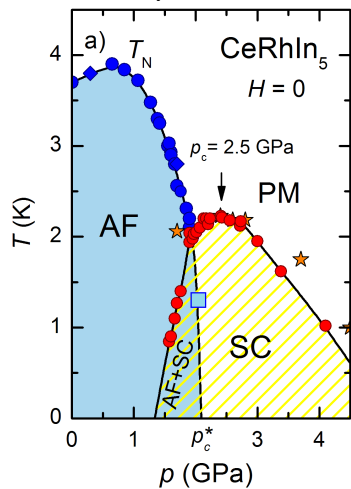
Physics World, Jan 2002

UNCONVENTIONAL SUPERCONDUCTORS

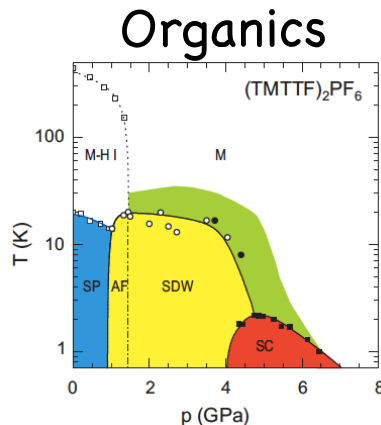
Not driven by conventional phonons.

AF supercond.
Heavy fermions

Oxides
Insulators
Magnetism



AF+SPC
Coexistence

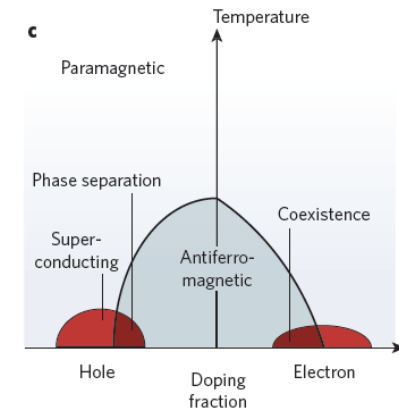
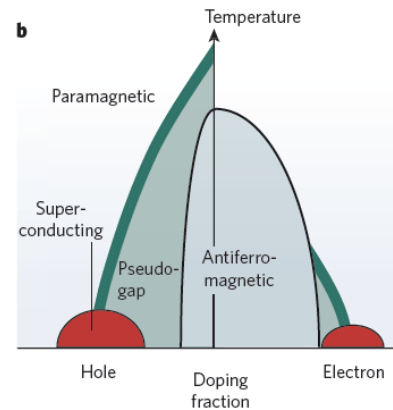


Eur. Phys. JB 21, 175

High T_c

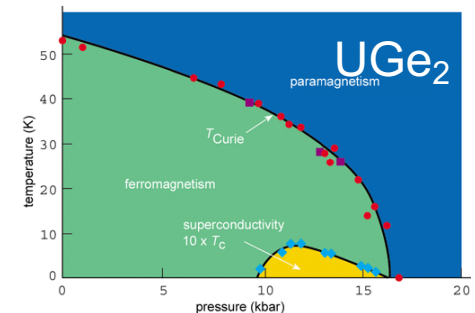
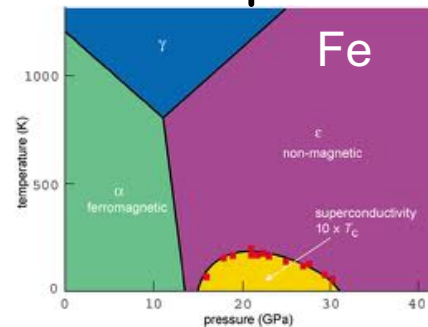
Cuprates

Fe-superconductors



Nature 464, 183 (2010)

FM superconductors

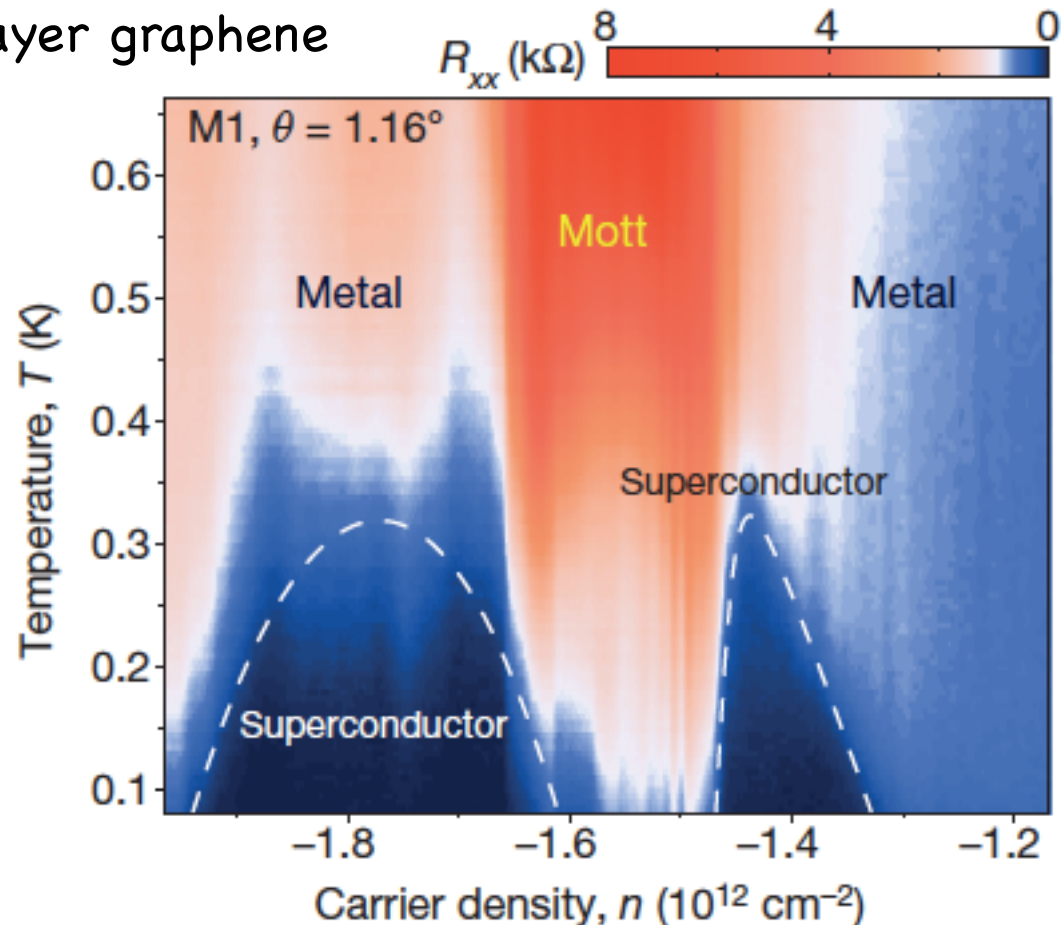


Physics World, Jan 2002

UNCONVENTIONAL SUPERCONDUCTORS

Not driven by conventional phonons?

Magic angle twisted bilayer graphene



Cao et al, Nature 556, 43 (2018); 556, 80 (2018)

UNCONVENTIONAL SUPERCONDUCTORS

The “normal” state is more complicated

- Proximity or coexistence with magnetism
- Strong correlations.
 - Competing orders (stripes).
 - Is there a Fermi surface? Doped Mott insulator. Non-Fermi liquid behaviour. Pseudogap phase in cuprates.
- Low dimensionality, anisotropies.

UNCONVENTIONAL SUPERCONDUCTORS

The superconducting state is different

The pairing function Δ_k may

- Be non-isotropic (including nodes, sign changes)
- Have a finite orbital momentum (p, d)
- Be spin-triplet
- High superconducting T_c
- $\lambda \gg \xi$ (type II)
- Anisotropies

$$\frac{2\Delta}{k_B T_c} \gg 3.53$$

Many theories.

2 distinct approaches to the problem:

- Stay within BCS but a new pairing (glue) mechanism is needed (maybe spin fluctuations, some kind of electron-phonon interaction).
- Start from the Mott state (no boson exchange required) and see how to gain energy from pairing
 - Resonating valence bonds
 - Kinetic energy driven
 - Quantum criticality...

Many theories.

2 distinct approaches to the problem:

- Stay within BCS but a new pairing (glue) mechanism is needed (maybe spin fluctuations, some kind of electron-phonon interaction).

A: We know how to deal with it.

D: Usually there is no Fermi surface. Note: Fe superconductors are not Mott insulators; their AF state is a metal.

Many theories.

2 distinct approaches to the problem:

- Start from the Mott state
 - Resonating valence bonds
 - Kinetic energy driven
 - Quantum criticality...

A: It seems, in principle, more self-consistent.

D: We need to properly treat the Mott state first!!

Is it possible to have a universal
theory of superconductivity?

Assume BCS is valid for non-conventional superconductors. Then we need some attractive interaction but we don't have the help of phonons anymore! Moreover, we have a very strong electron-electron repulsive interaction.
Is there a way around it??

PAIRING SYMMETRY

$$\psi(\vec{r}_1 s_1, \vec{r}_2 s_2) = \varphi(\vec{r}_1, \vec{r}_2) \chi(s_1, s_2)$$

Spatial

Spin

Pair wavefunction must be antisymmetric

Spin singlet $\rightarrow$ even parity orbital wave function s, d
Spin triplet $\rightarrow$ odd parity orbital wave-function p, f

s-wave: conventional spc

d-wave: cuprates

p-wave Superfluidity in ^3He

UPt₃

Sr₂RuO₄

p-wave
currently under
revision!

0.51K

0.93K

SUPERFLUIDITY IN ^3He (1972) $T_c=2.7$ mK

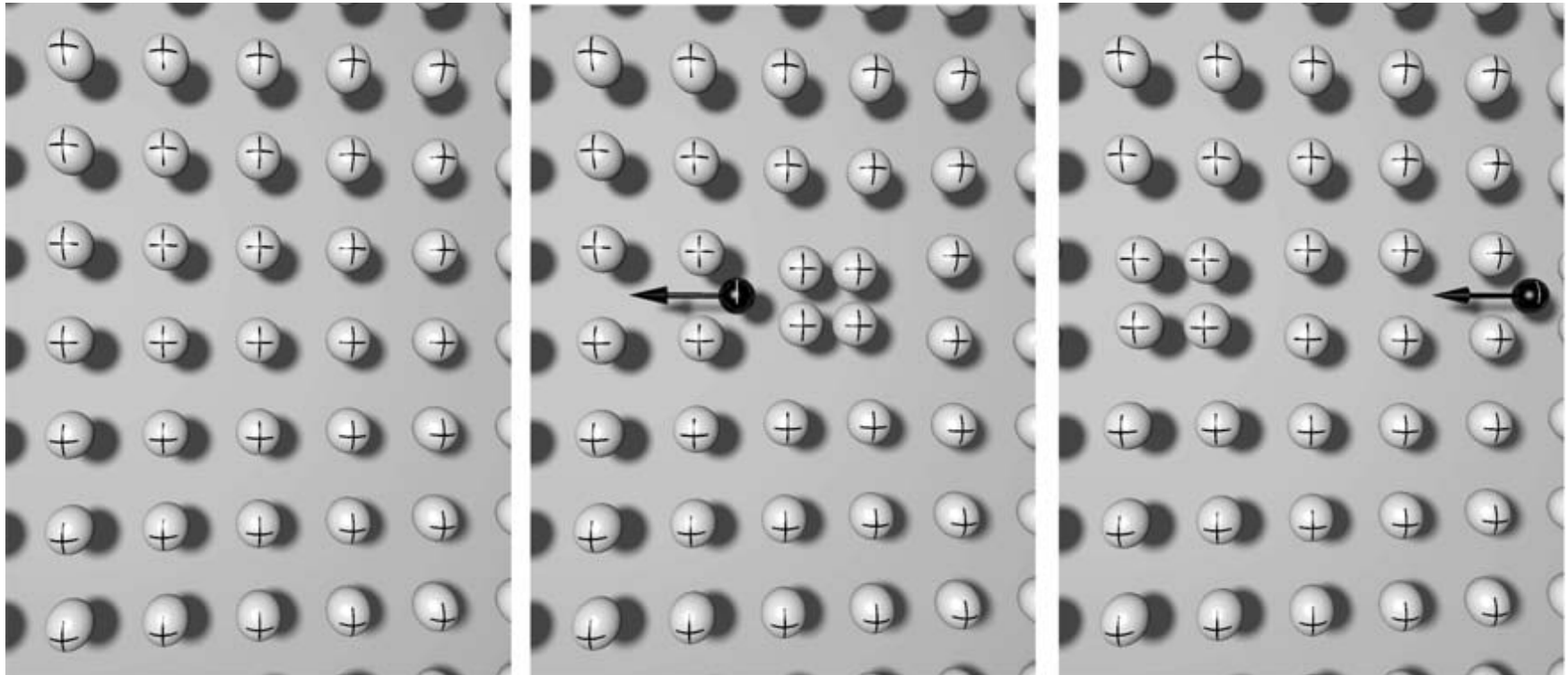
Pairing cannot be mediated by the lattice.
Nuclear forces are strongly repulsive in the core
→ no s-wave possible. Need of wavefunctions that vanish at $r \rightarrow 0$.

One possibility is mediation by ferromagnetic spin fluctuations: FM paramagnons (FM fluctuations suppress s-wave and enhance p-wave pairing).

SUPERFLUIDITY IN ^3He

Attractive interactions by ferromagnetic fluctuations:

FM clouds are formed which attract the ^3He quasiparticles (something like magnetic polarons instead of lattice polarons)



Blundell's book

High angular momentum pairing (p-wave) was proposed for ^3He as a way to overcome the short range repulsion (Pitaevskii 1959)

What about
non-conventional superconductors?

Mostly singlet pairs with mainly d-wave symmetry.

In iron superconductors both s and d are postulated.

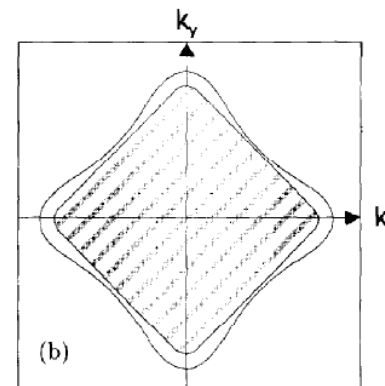
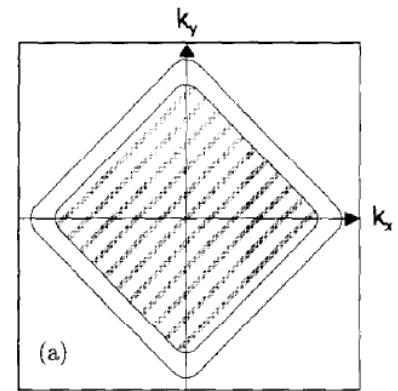
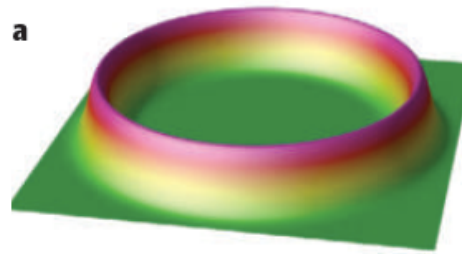
S-WAVE

Gap equation from BCS
(T=0)

$$\Delta_k = -\frac{1}{\Omega} \sum_{kk'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}}$$

For $V_{kk'}$ constant and attractive: isotropic gap $\Delta_k = \Delta$

s wave gap
(spherical symmetry)



More generally, s-wave gap
may be anisotropic with no
sign changes.

D-WAVE

Gap equation from BCS
($T=0$)

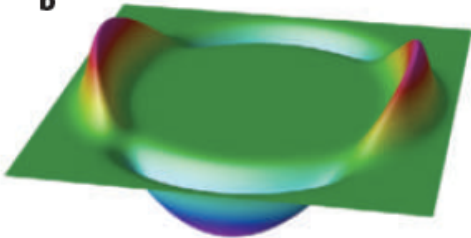
$$\Delta_k = -\frac{1}{\Omega} \sum_{kk'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}}$$

Repulsive $V_{kk'}$ $\longleftrightarrow$ Anisotropic Δ_k with sign change!

$$\text{sign}(\Delta_k) = -\text{sign}(V_{k,k'})\text{sign}(\Delta_{k'}).$$

For instance, d-wave

$$\Delta_k = \Delta_0 \cos(2\phi)$$



The gap has nodes
and sign changes

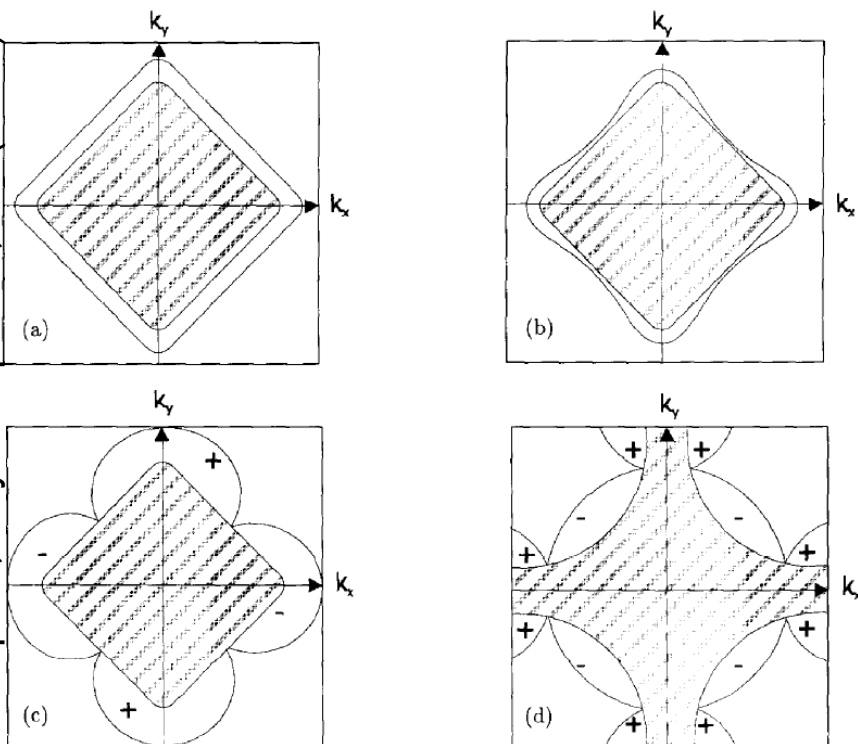
An anisotropic pair potential
leads to an anisotropic gap

$$V_{kk'} = -V_0 \gamma_k \gamma_{k'}$$

$$\Delta_k = \gamma_k \Delta_0$$

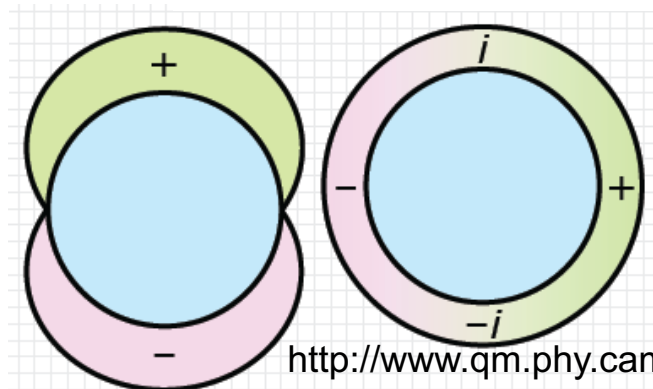
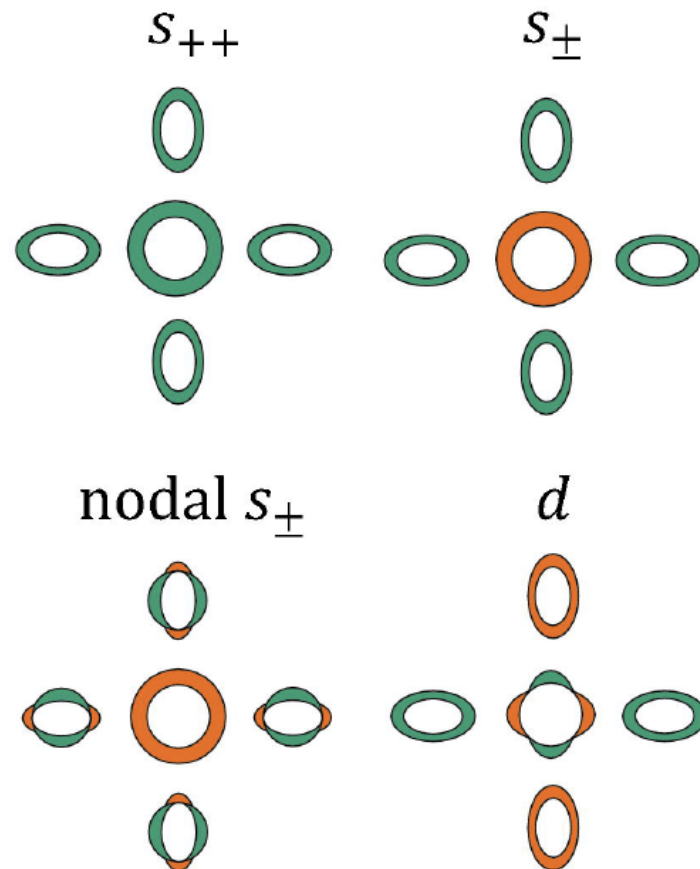
GAP SYMMETRIES...

Scalapino, Phys. Rep. 250,329 (1995)



Non-isotropic gaps lead to sensitivity of unconventional SPC to non-magnetic impurities

Hirshfield et al. 1106.3712



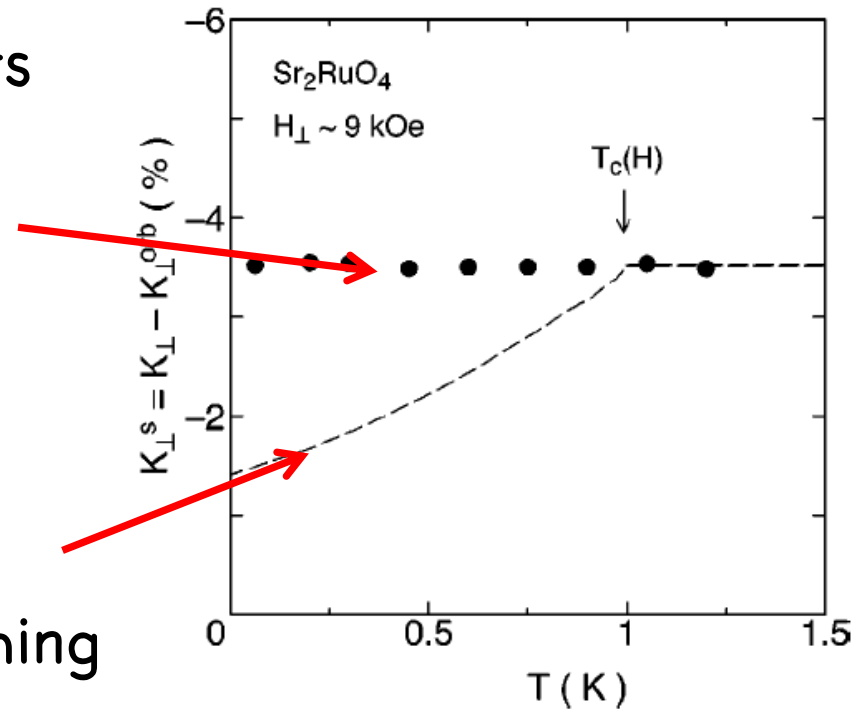
<http://www.qm.phy.cam.ac.uk/teaching/>

SINGLET-TRIPLET

From Knight shift experiments

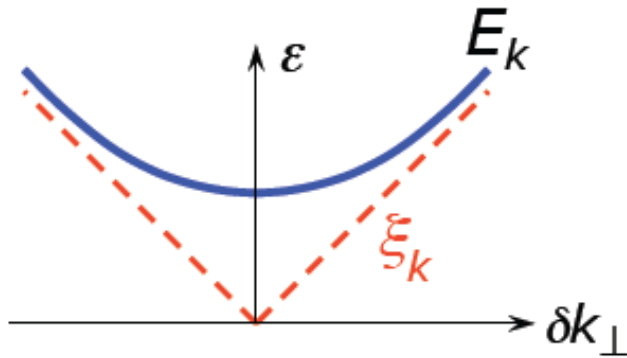
triplet

Singlet
(spin quenching
at low T)

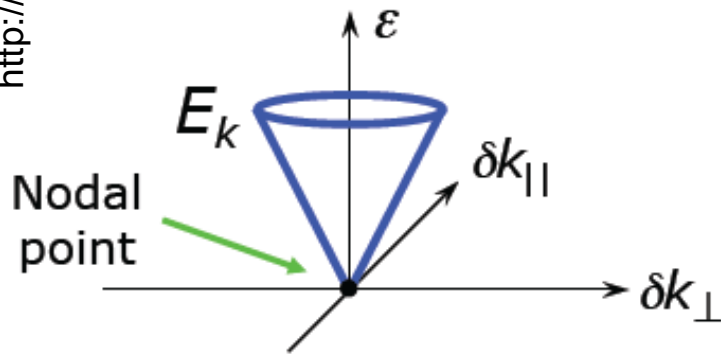
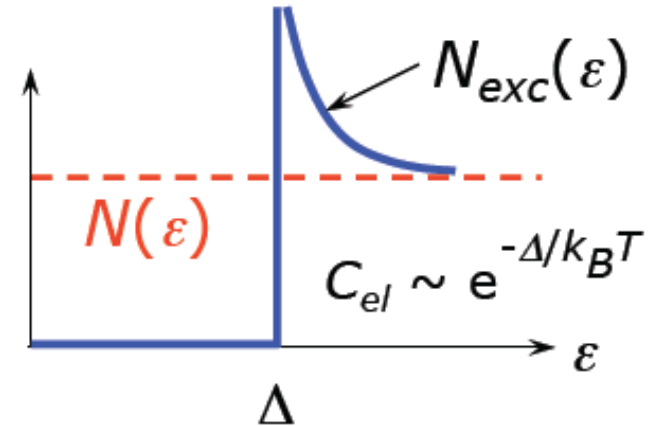


PRB 63, 060507 (2001)

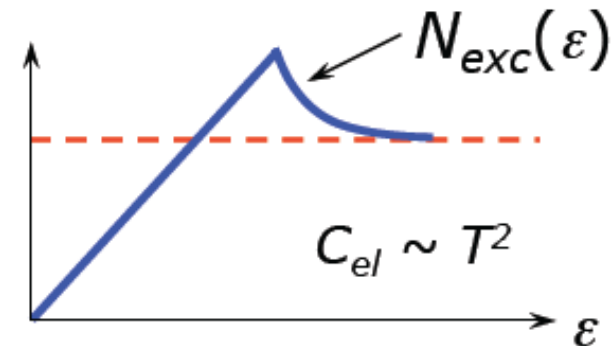
NODES VERSUS NODELESS



s-wave
pairing



d-wave
pairing

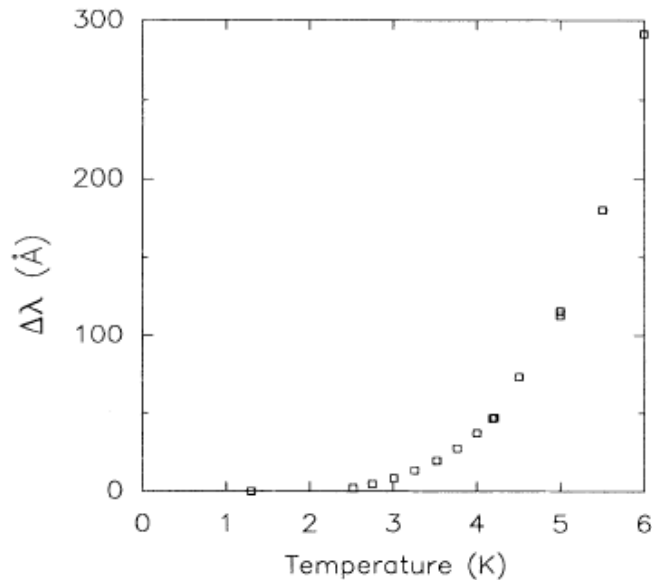


Without nodes: activated behavior (λ , specific heat...) With nodes: power law behaviors

Gap without nodes

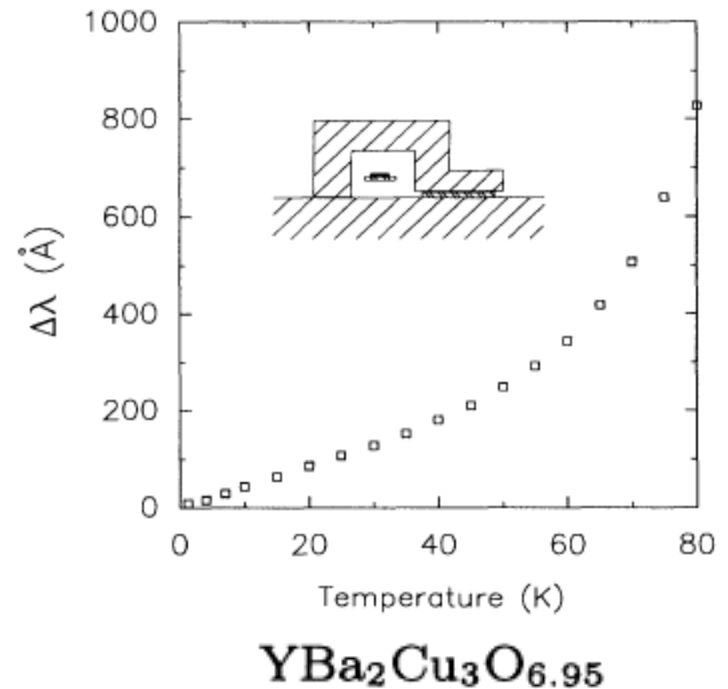
London penetration length within BCS

$$\frac{\Delta\lambda(T)}{\lambda(0)} \sim 3.33 \left(\frac{T_c}{T} \right)^{1/2} \exp(-1.76T_c/T)$$



Gap with nodes

Power law dependencies



Pb_{0.95}Sn_{0.05}

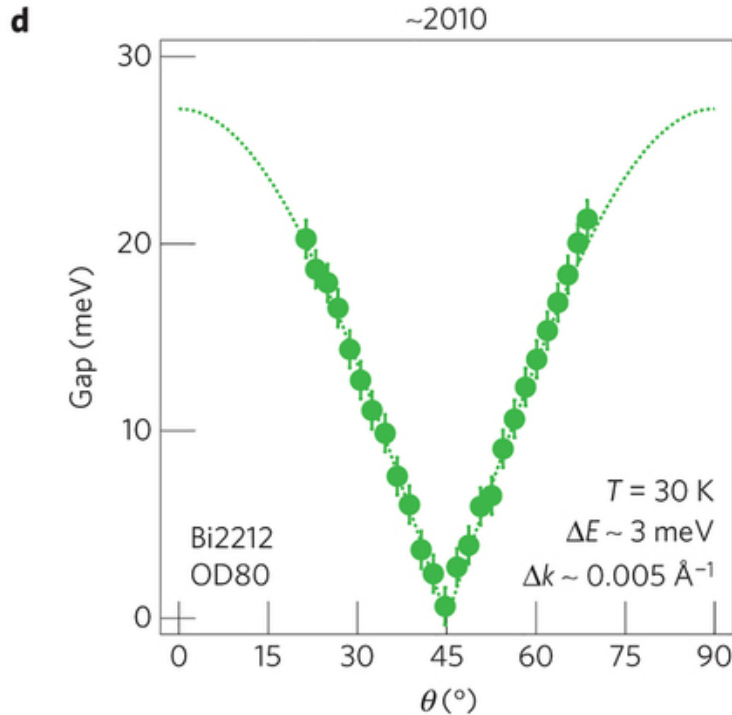
PRL 70, 3999 (1993)

(no phase information)

ARPES

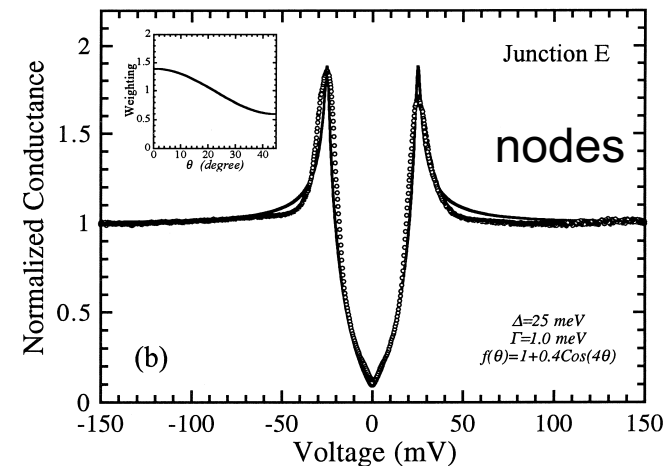
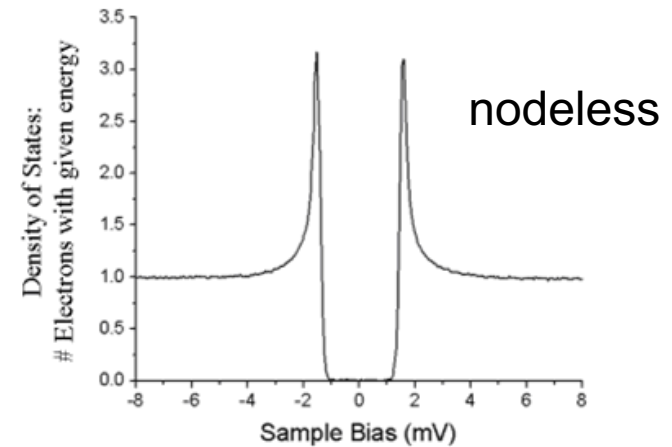
TUNNELING SPECTROSCOPY

www.personal.psu.edu/ewh10 Physica C 320, 9



Nature Physics 10, 483–495 (2014)

(no phase information)

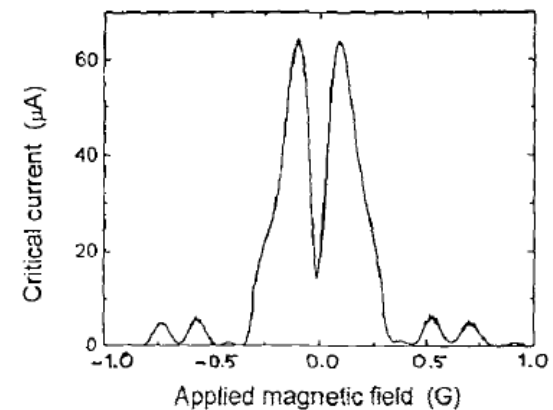
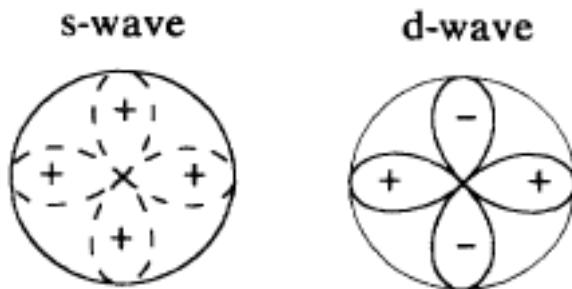
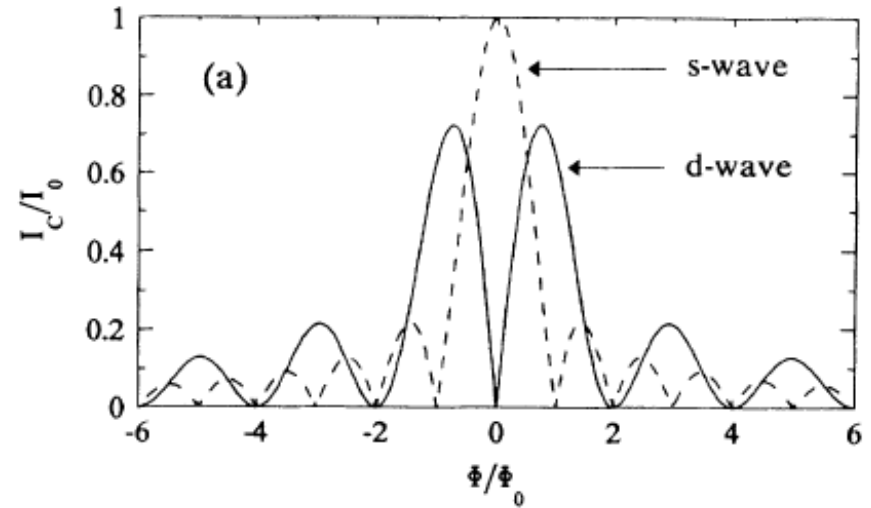
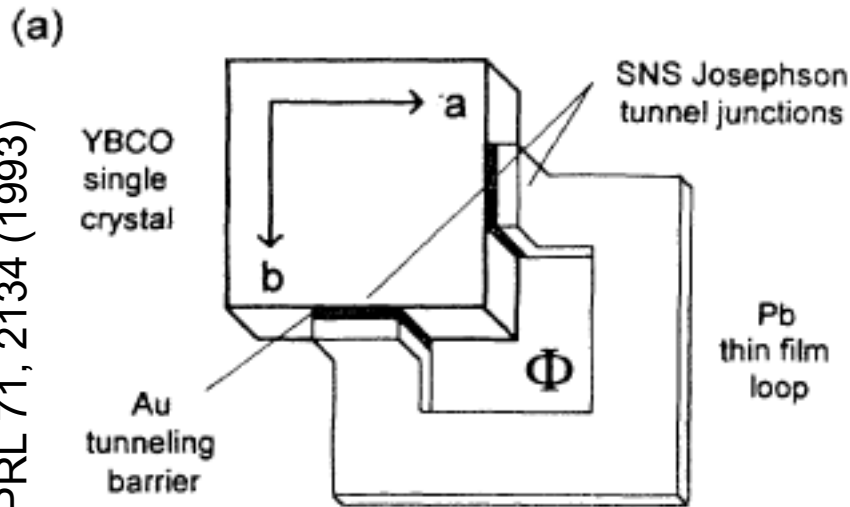


SENSITIVITY TO THE PHASE: JOSEPHSON EFFECT

$$I_s = I_c \sin \Delta\varphi$$

Calculated critical current

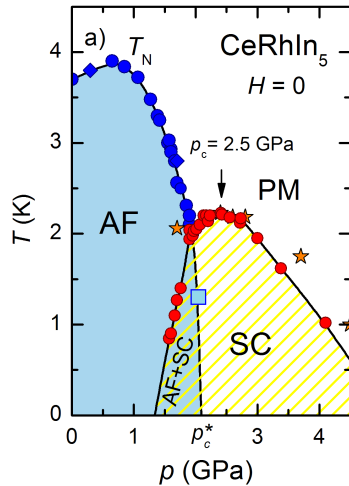
PRL 71, 2134 (1993)



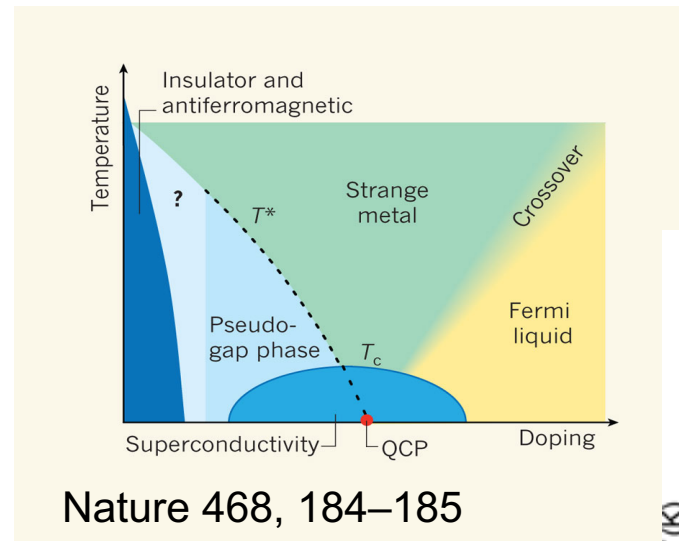
A FEW WORDS ABOUT THE MATERIALS

SOME TYPICAL PHASE DIAGRAMS

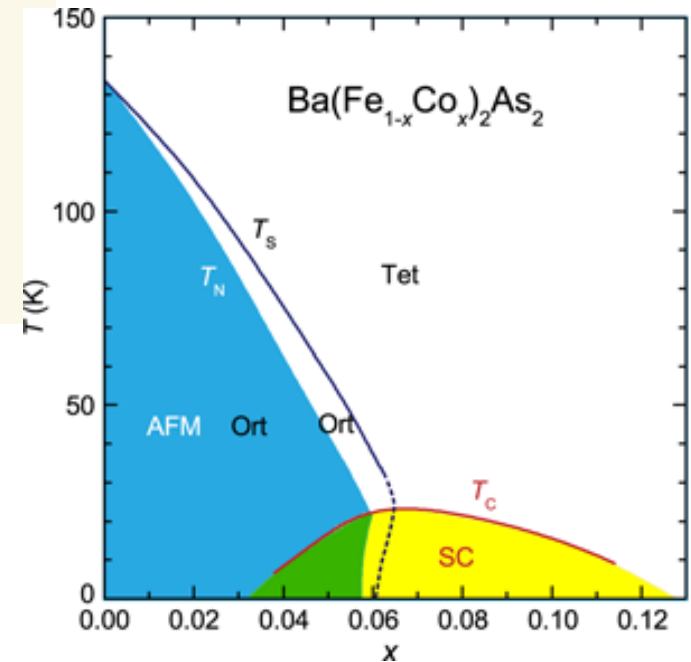
Heavy fermions



Cuprates

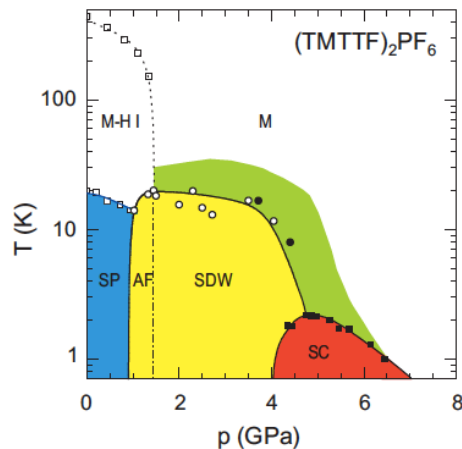


Fe-superconductors



Nandi et al, PRL 104, 057006 (2010)

Organics



In common:
(AF)magnetic
phases

HEAVY FERMIONS (1979)

“Our experiments demonstrate for the first time that superconductivity can exist in a metal in which many-body interactions, probably magnetic in origin, have strongly renormalized the properties of the conduction-electron gas.”

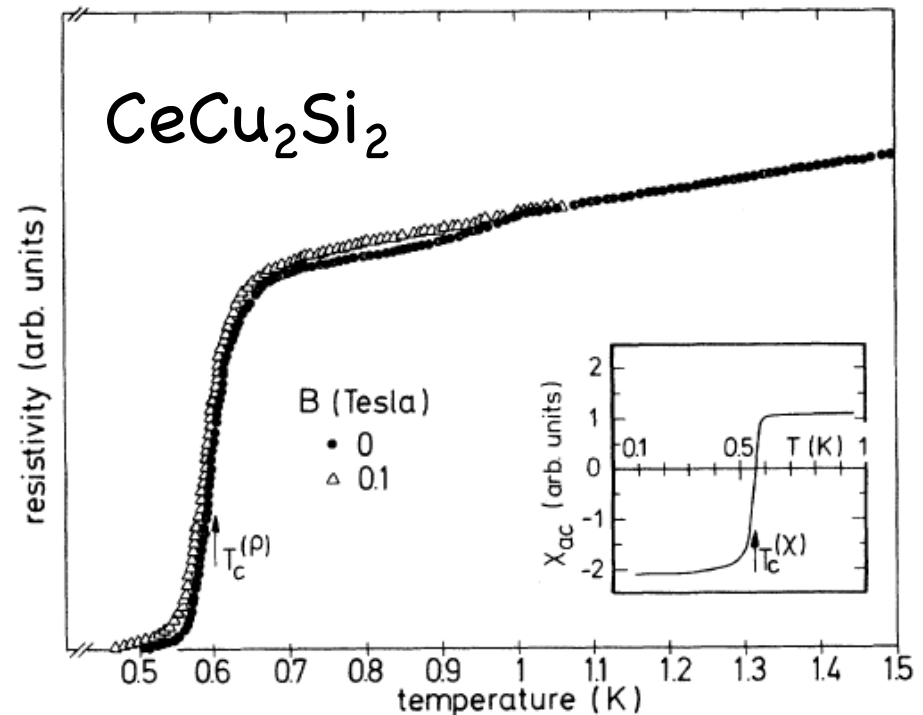
PRL 43, 1892 (1979)

Coexisting AF + SPC

Reentrant SPC due to competition with Kondo

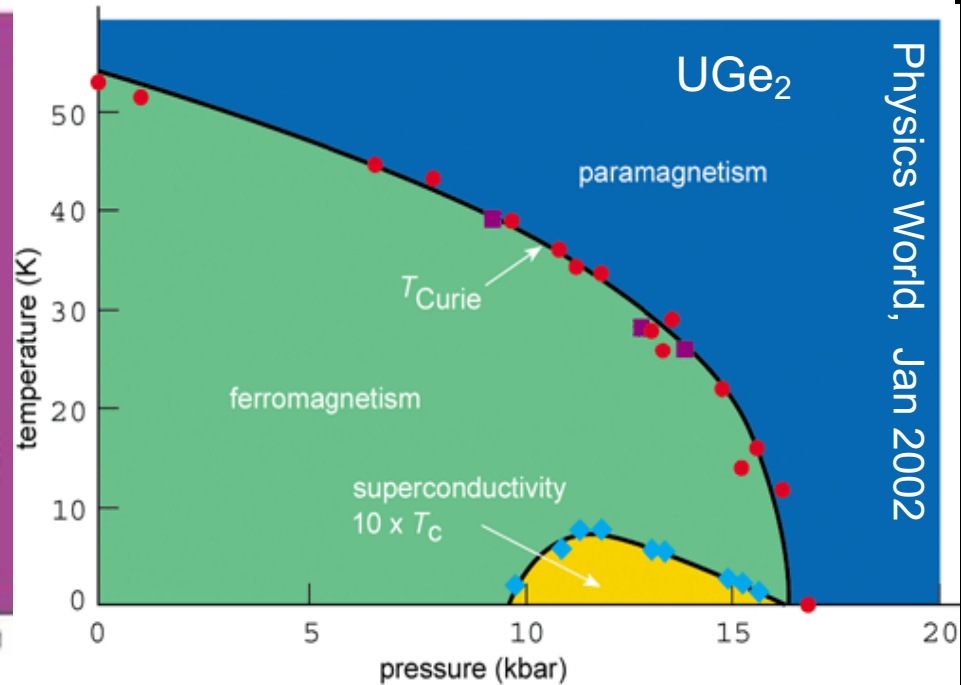
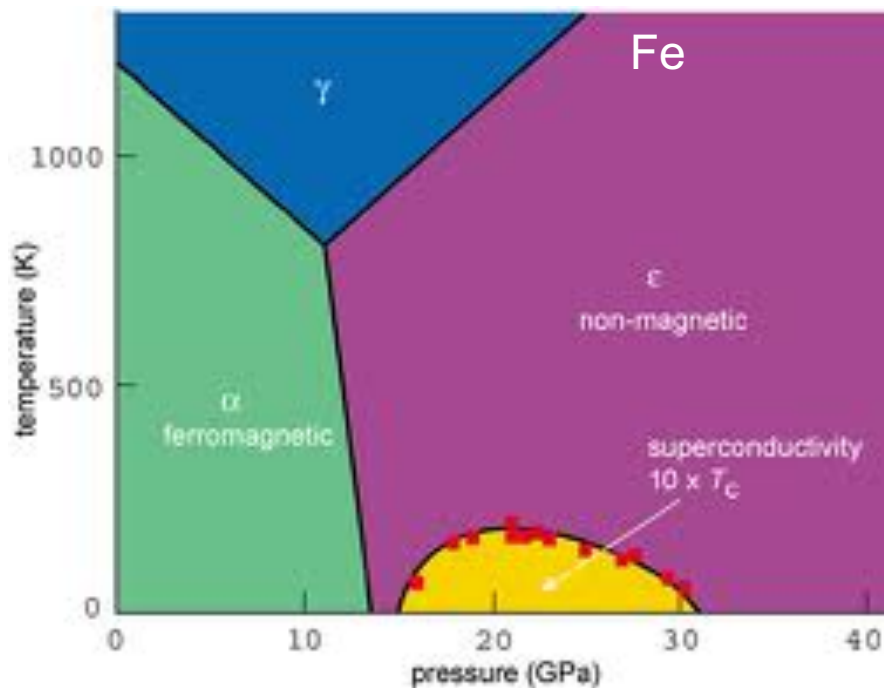
Quantum criticality

Nat. Phys. 4, 186



PRL 43, 1892 (1979)

FERROMAGNETIC SUPERCONDUCTORS



Physics World, Jan 2002

Proximity of quantum critical point can lead to coexistence
Triplet pairing?

PRL 94, 097003 (2005)

CUPRATES

Layers of CuO_2 . Different related structures. But note!: SPC requires coherence in 3dim.

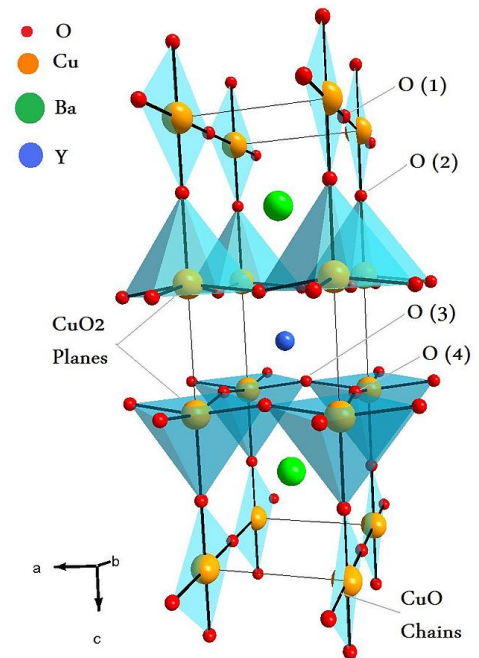
Highest T_c 134K (at ambient pressure).
 T_c increases with number of CuO_2 planes in the unit cell (up to $n=3$).

Pairs were found to be singlets.

d-wave pairing was proposed in the cuprates early on.

Scalapino, Phys. Rep. 250, 329 (1995)

Undoped cuprates are correlated insulators and AF (π, π).

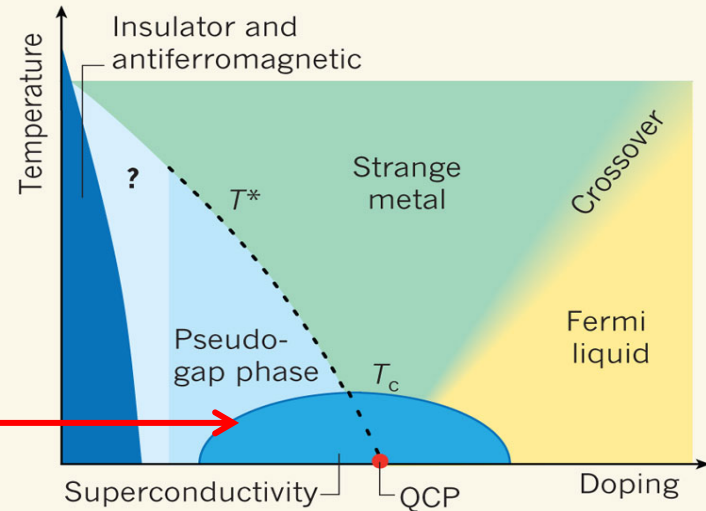


wikipedia

PSEUDOGAP

Spin quenching sets up at T^* .

underdoped



Nature 468, 184–185

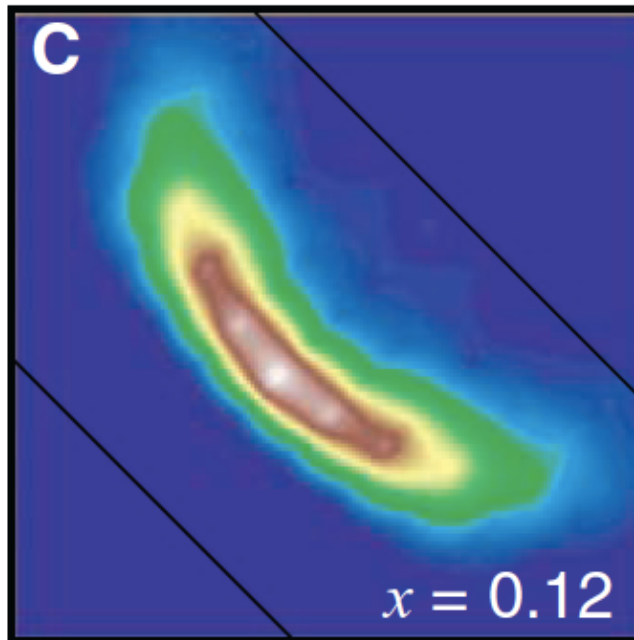
Origin?: spin-singlet formation (Anderson), pairing with short range order (preformed pairs), antiferromagnetic fluctuations, charge density wave

Is it due to fluctuations or is it a new phase (with a related broken symmetry)? Transition or crossover?

PSEUDOGAP

In other words:

Is it a precursor or a competing phase?



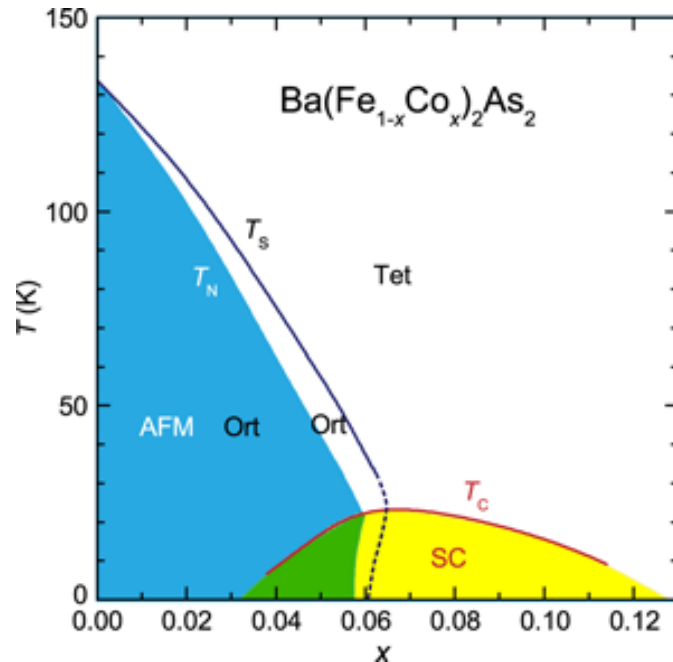
Science 307, 901

Norman, cond-mat:0507031

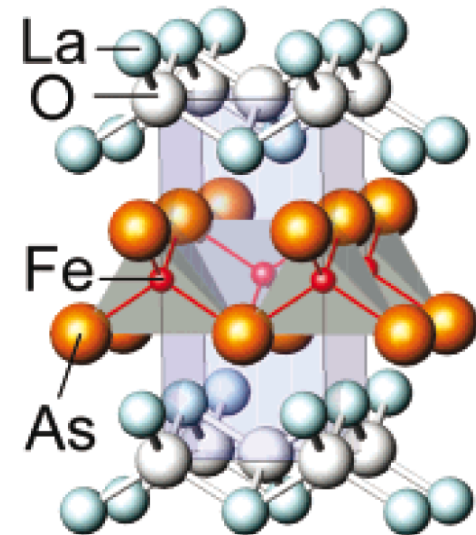
<http://www.msd.anl.gov/files/msd/cuprates-columbia.pdf>

FE BASED SUPERCONDUCTORS

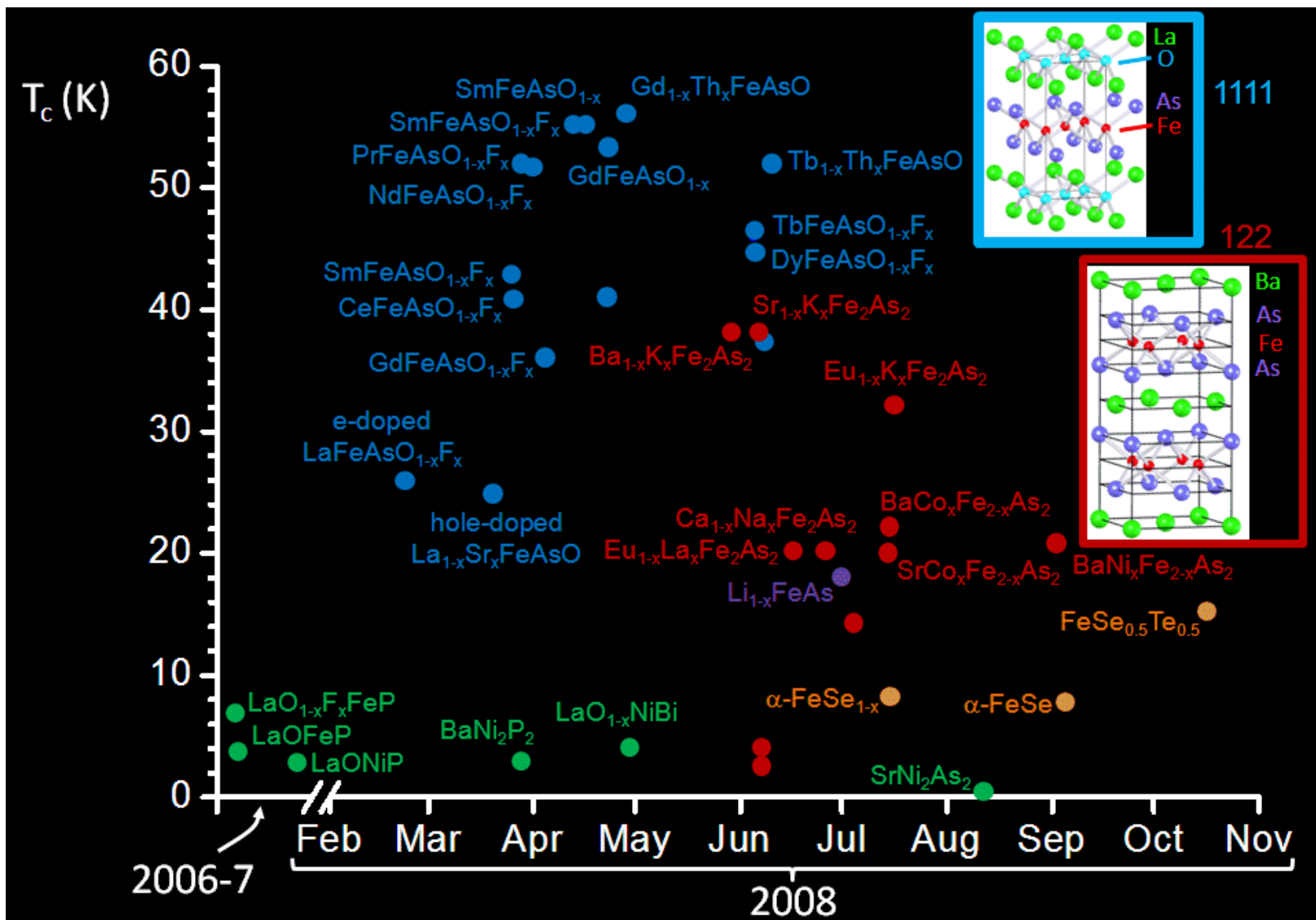
Many different families discovered, all sharing a Fe plane



Nandi et al, PRL 104, 057006 (2010)

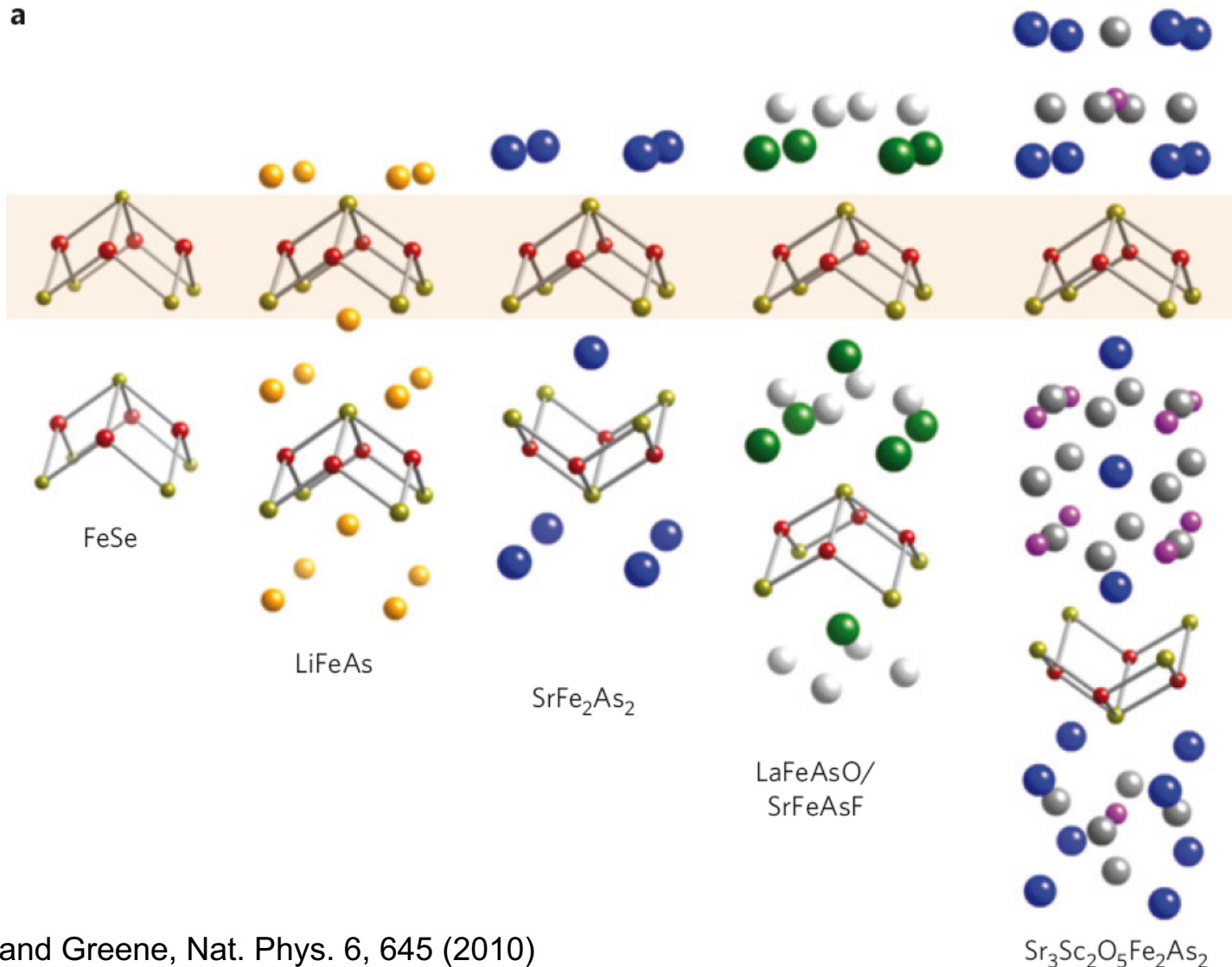


An important breakthrough because it could help understand cuprates



Fe-As or Fe-Se planes

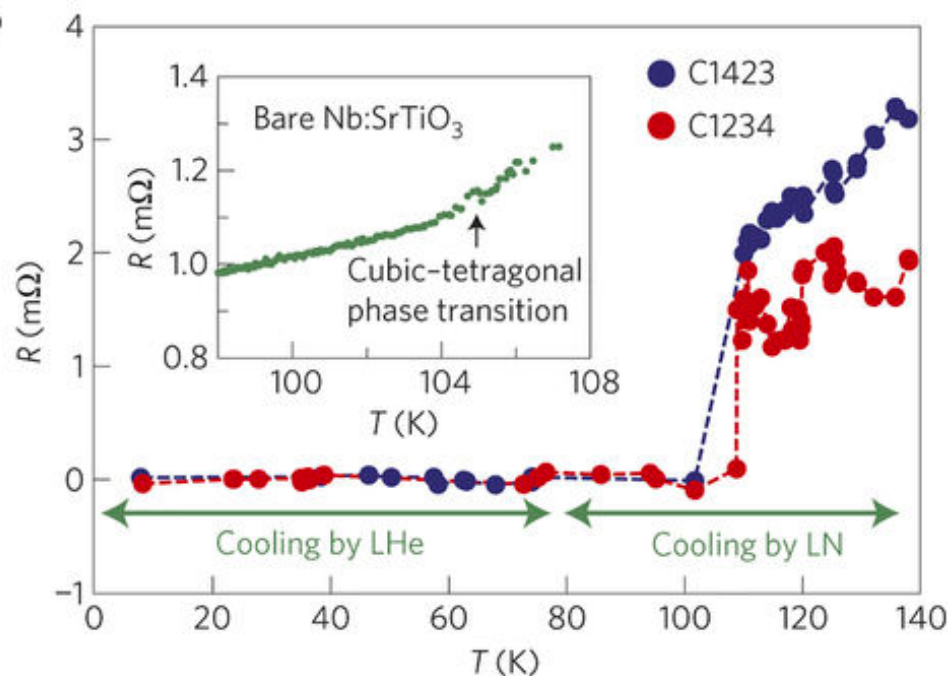
a



Paglione and Greene, Nat. Phys. 6, 645 (2010)

HIGHEST TC IN FE SUPERCONDUCTORS

Single layer FeSe on SrTiO₃
(interface superconductivity)



Nature Materials 14, 285–289 (2015)

FE BASED SUPERCONDUCTORS

Differences with cuprates:

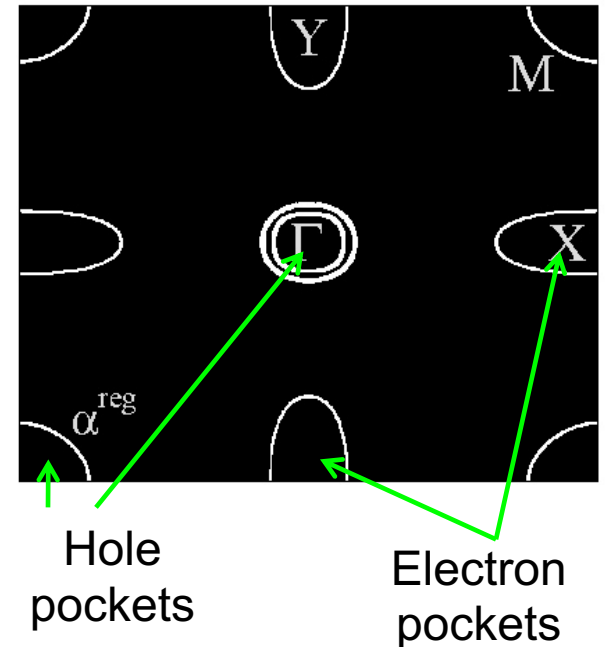
- The AF state is metallic (not Mott insulator): Hund metal (correlations).
- Multiorbital system (more than 1 gap possible)
- SPC can be achieved without chemical doping.
- More 3dim-like (less anisotropy in c-direction)

Proposed mechanisms for superconductivity

- Spin fluctuations ($\pi, 0$)
- Orbital fluctuations

Gap symmetry

Extended BZ (1 Fe unit cell)



Family	Full gap	Highly anisotropic	Strong nodal
1111	PrFeAsO _{1-y} [52K] [293] SmFeAs(O,F) [55K] [295]	LaFeAs(O,F) [26K] [214] NdFeAs(O,F) [214]	LaFePO [6K] [203, 204, 294]
122	(Ba,K)Fe ₂ As ₂ [40K] [146, 236, 296, 242] Ba(Fe,Co) ₂ As ₂ [OP,23K] [238, 208]	Ba(Fe,Co) ₂ As ₂ [OD] [238, 241]* Ba(Fe,Ni) ₂ As ₂ [297]* Ba(Fe,Co) ₂ As ₂ [UD] [241]*	KFe ₂ As ₂ [4K] [211, 309] BaFe ₂ (As,P) ₂ [OP,31K] [205, 149] (Ba,K)Fe ₂ As ₂ [UD] [242]
111	LiFeAs [18K] [298, 258]		LiFeP [6K] [299]
11		Fe(Se,Te) [27K] [231, 246]	

arXiv:1106.3712

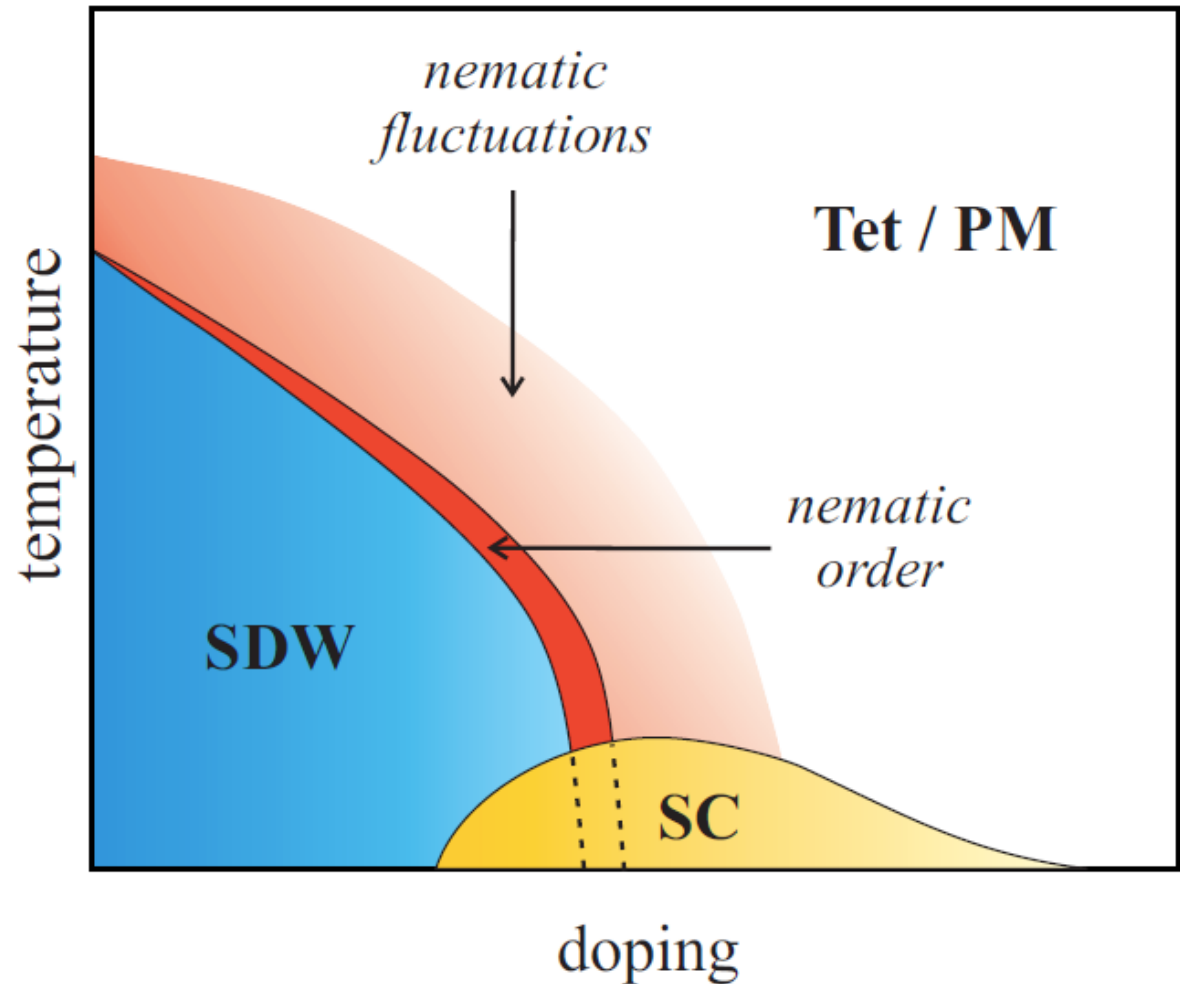
FE BASED SUPERCONDUCTORS

Role of nematicity?

Breaks the tetragonal symmetry.

Related to
magnetic
fluctuations.

Nematic order
postulated for
the pseudogap
in cuprates.

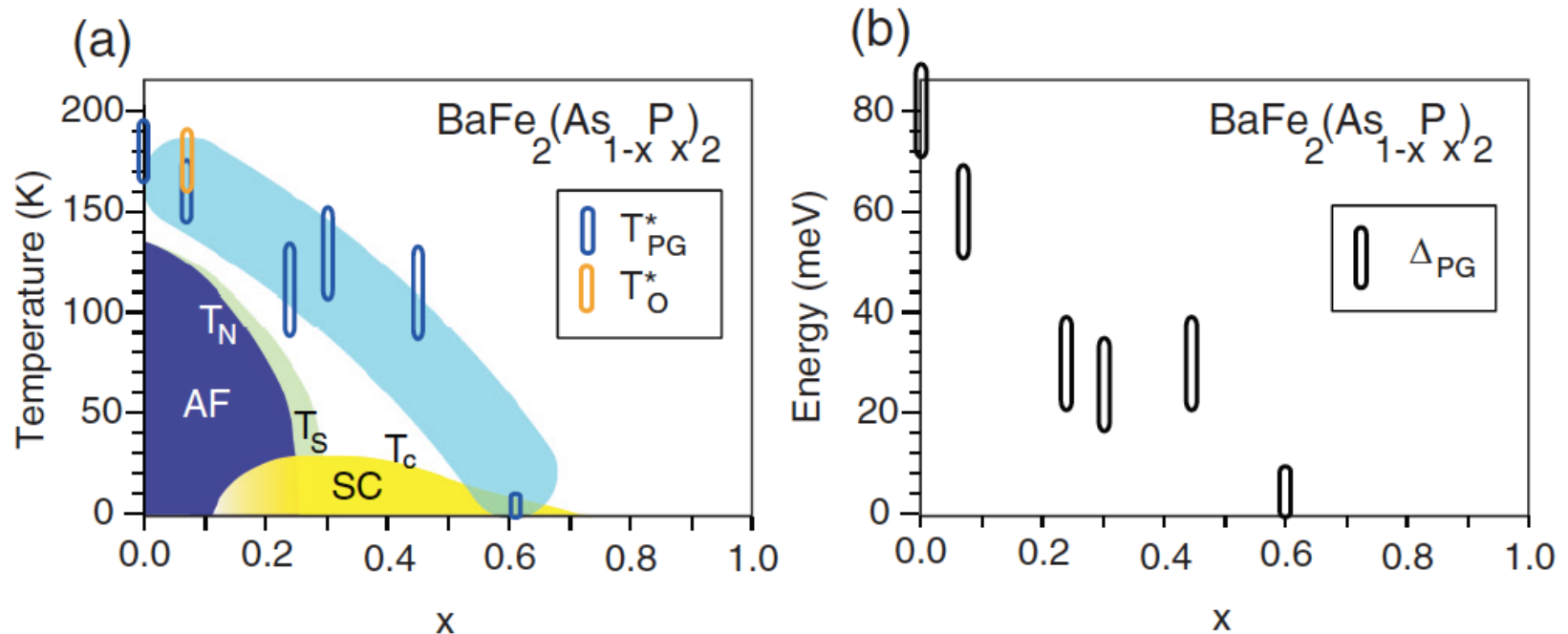


<http://www.ifsc.usp.br/coloquio/2013/Fernandes.pdf>

FE BASED SUPERCONDUCTORS

Pseudogap

Gap opening due to spin fluctuations:
Nat. Comm. **2**, 392 (2011)



Accompanied by orbital ordering. PRB **89**, 045101 (2014)

MECHANISMS

SPIN-FLUCTUATION MECHANISM

Spin fluctuations play the role of phonons (à la BCS).

The “normal” state can be described as a nearly AF Fermi liquid (unconventional Fermi liquid close to an AF instability).

Note: calculating the effective interaction is not trivial because vertex corrections can be important (Migdal's theorem doesn't apply)

SPIN-FLUCTUATION MECHANISM

If the magnetic susceptibility has a peak at q (remember nesting) the interaction is also peaked at q and positive.

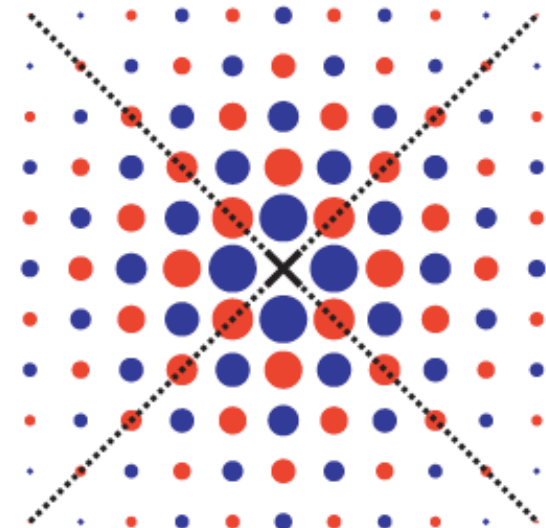
$$\Gamma_s(\mathbf{k}, \mathbf{k}') = \frac{3}{2}U^2 \frac{\chi_0(\mathbf{q})}{1 - U\chi_0(\mathbf{q})}$$

If you look at the interaction in real space

It changes sign with position!!

Attractive interaction by
space avoidance

$q=(\pi,\pi)$



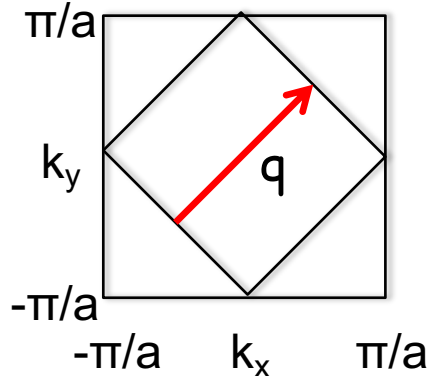
● Repulsion ● Attraction

Scalapino, Phys. Rep. 1995
Hirshfield et al. 1106.3712

Nature 450, 1177 (2007)

SPIN-FLUCTUATION MECHANISM

Square lattice at half-filling:



At $q=(\pi,\pi)$ the spin susceptibility is maximal (nesting)

$$V_{k,k'} = V_{k-k'} = V_q \propto \chi_q > 0 \quad q = (\pi, \pi)$$

To fulfil the gap equation, you need an anisotropic gap such that

$$\Delta_k = -\frac{1}{\Omega} \sum_{kk'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}}$$

$$\text{sign}(\Delta_k) = -\text{sign}(V_{k,k'}) \text{sign}(\Delta_{k'}).$$

d-wave

Scalapino, Phys. Rep. 1995
Hirshfield et al. 1106.3712

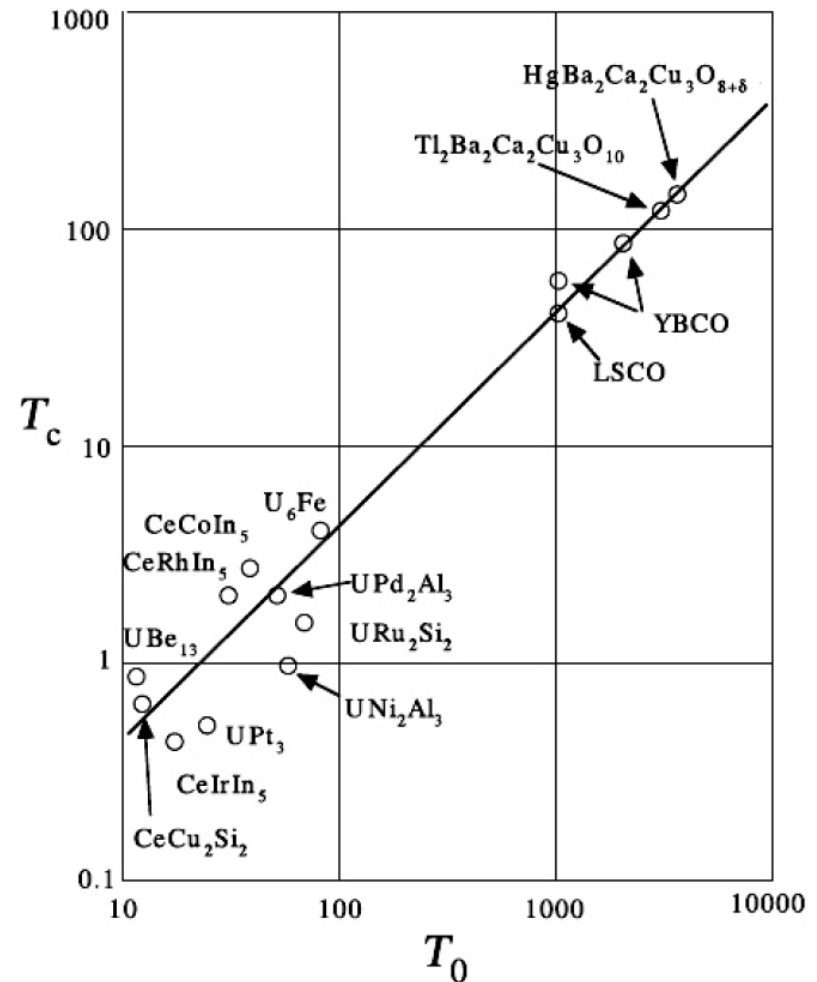
$$\Delta_k = \frac{\Delta_0}{2} (\cos k_x - \cos k_y)$$

$$\Delta_{k+(\pi,\pi)} = \frac{\Delta_0}{2} (-\cos k_x + \cos k_y) = -\Delta_k$$

SPIN-FLUCTUATION MECHANISM

Correlation between T_c and a typical energy scale of spin fluctuations.

In the Scalapino approach, the t-J model is the basis for understanding.



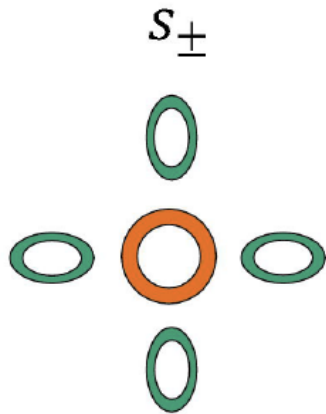
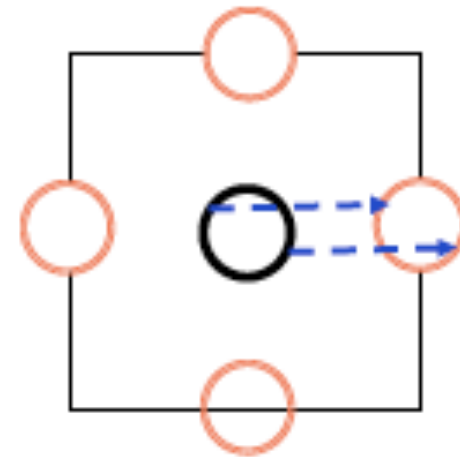
Moriya-Ueda, Rep. Prog. Phys. 66, 1299 (2003)

Scalapino, Rev. Mod. Phys. 84, 1383 (2012)

SPIN-FLUCTUATION MECHANISM

For a multiorbital system (as Fe-superconductors)

For instance, spin fluctuations related to nesting between electron and hole pockets: $q=(\pi,0)$



This would lead to an $s_{\pm}$
(as the order parameter averages to zero on the Fermi surface, you also get “Coulomb avoidance”)

ELECTRON-PHONON

Not discarded!

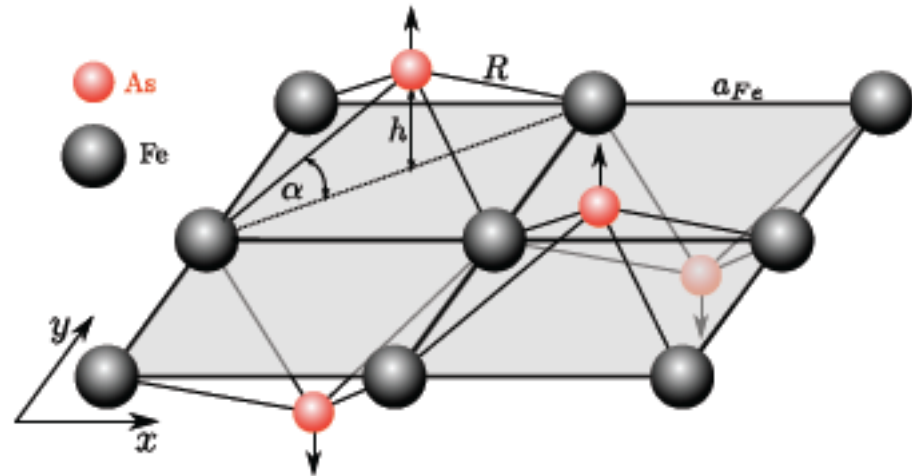
For cuprates: Phys. Rev. Lett. 105, 257001

Maybe coupled to other degrees of freedom?

For Fe-superconductors

Spin-phonon?

Adv. in Cond. Matt. Phys.
2010, 164916 (2010)



PRB 88, 165106 (2013)

Orbital fluctuations induced by electron-phonon.

PRL 104, 157001

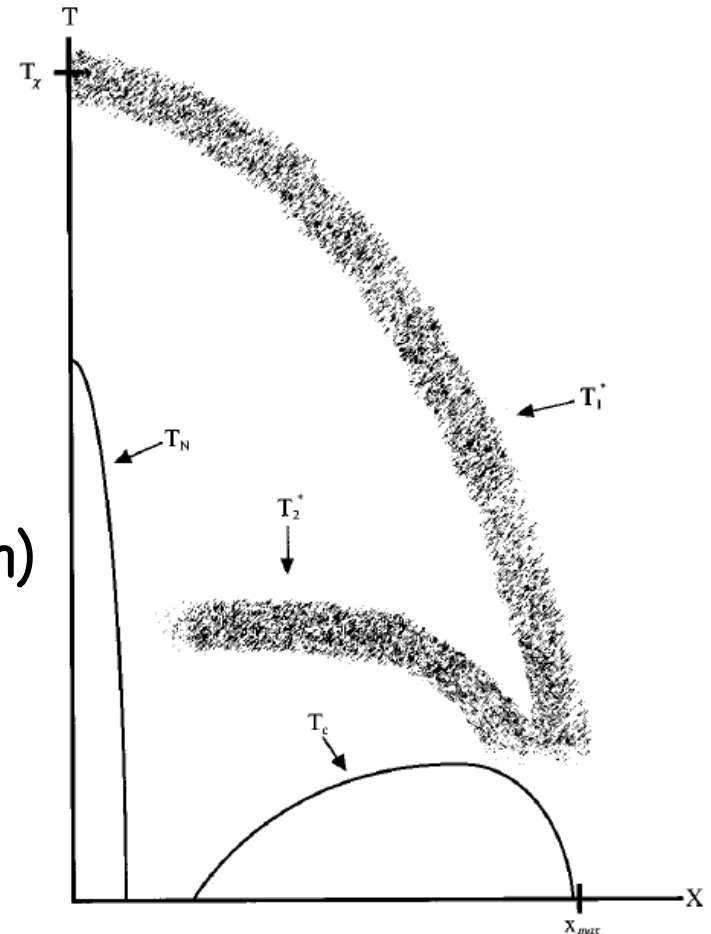
KINETIC ENERGY DRIVEN MECHANISM

Different energy scales involved for underdoped cuprates

T^* : Phase transition or crossover (no exp. evidence of phase transition)

$$T_c < T^*_{\text{pair}} < T^*_{\text{stripe}}$$

Carlson et al, Chapter 21



PRB 56, 6120

KINETIC ENERGY DRIVEN MECHANISM

Carlson et al, Chapter 21

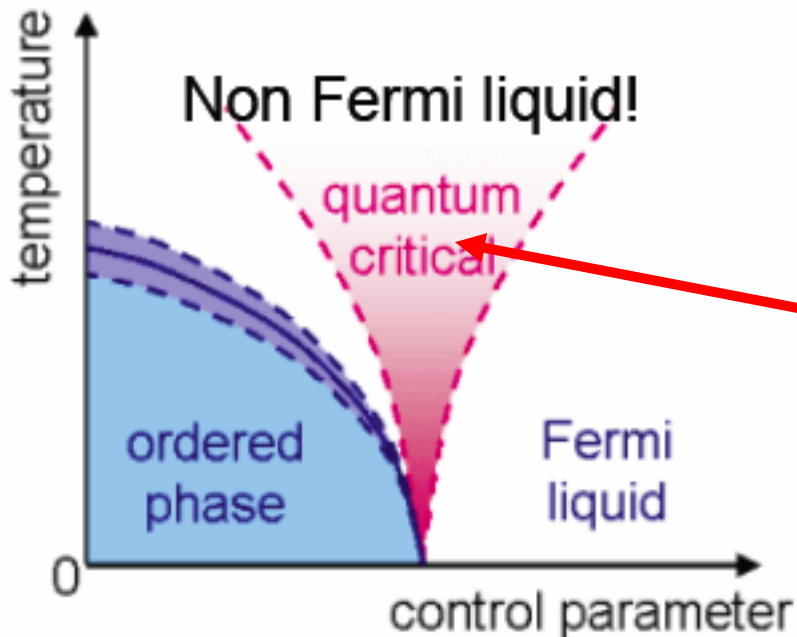
Different energy scales involved for underdoped cuprates
At T^*_{stripe} : stripe formation. Stripes are rivers of charge where holes can move (gain kinetic energy in 1dim). In between, AF regions where the carriers are localized.

At T^*_{pair} : local pairing (spin-gap) within the 1DEGs (stripes). Pairs can tunnel to neighboring 1DEG (which in principle has another k_F). This way the system gains kinetic energy in a perpendicular direction as well. There is finite Δ but not fixed phase.

At T_c : phase coherence sets in (Josephson coupling between stripes) $\rightarrow$ superconductivity.

$$T_c < T^*_{\text{pair}} < T^*_{\text{stripe}}$$

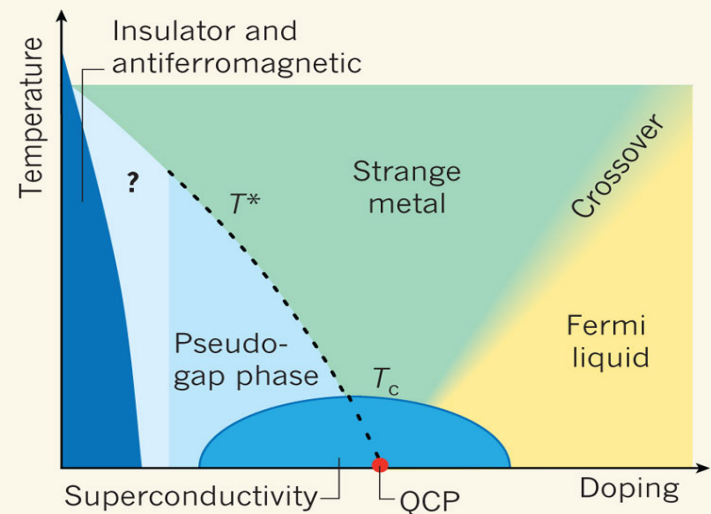
QUANTUM PHASE TRANSITIONS

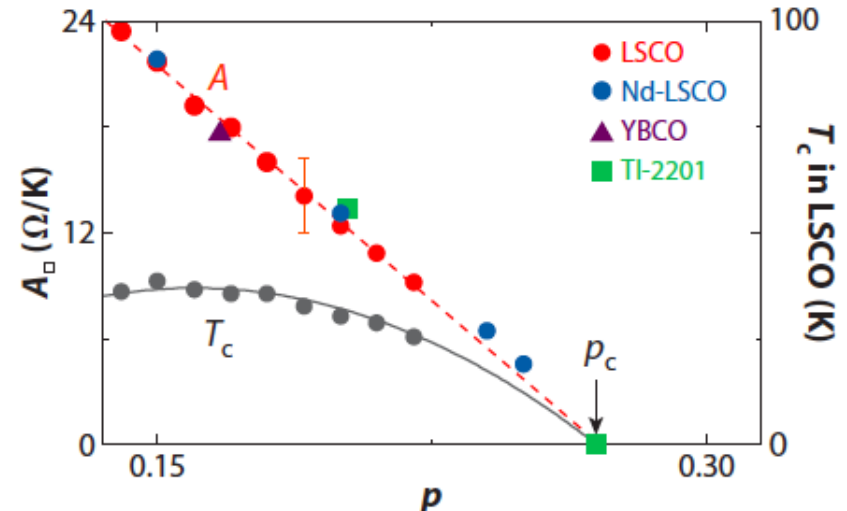
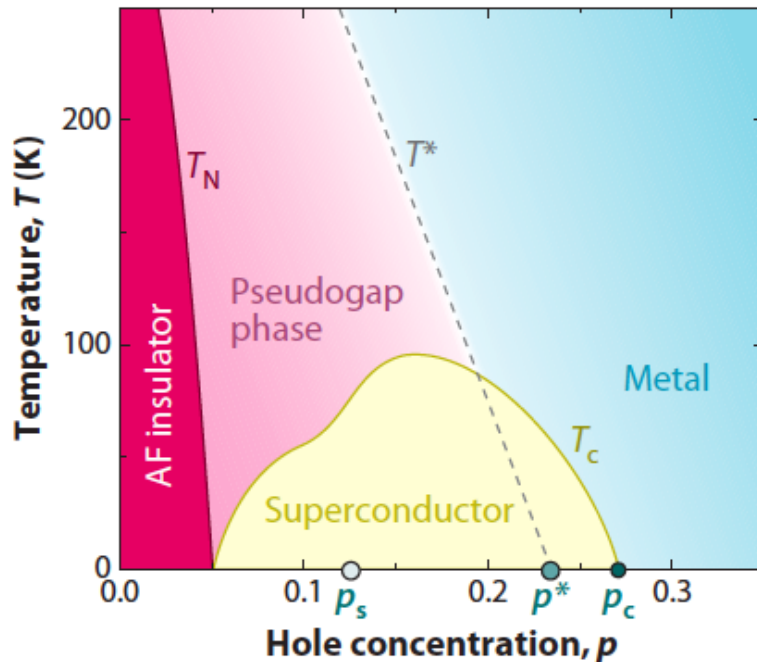


Region in which thermal and quantum fluctuations are equally important

Transition at $T=0$ with consequences for $T>0$.

Divergence of time coherence.





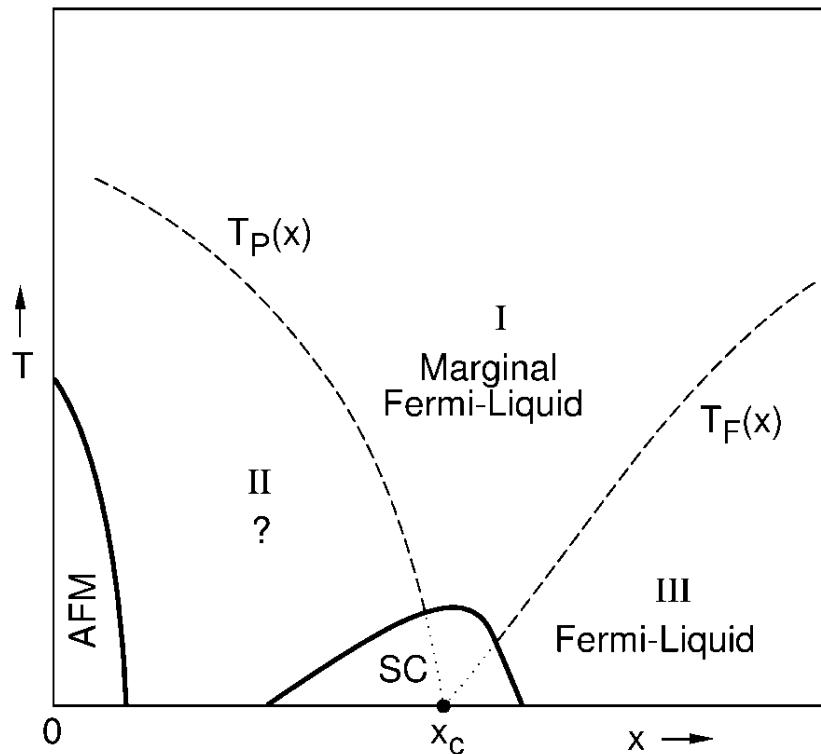
Resistivity linear with T above the spc phase appears at p_c (doping at the Quantum Critical Point).

Linear T resistivity coming from fluctuations in the pseudogap phase (spin density wave order).

In organic spc and Fe pnictides, similar phenomena coming from spin fluctuations.

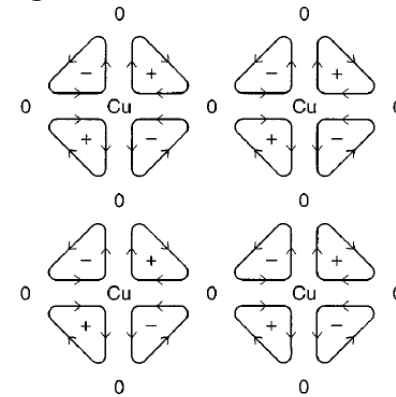
HIDDEN ORDER

Idea: the pseudogap phase is in fact a gapped phase (pseudo in experiment due to imperfections or dynamic effects)



PRL 83, 3538

Circulating currents, PRB 55, 14554



Charge order PRL 87, 056401

d-density wave PRB 63, 094503

Nematic phase arXiv:1404.0362

RESONATING VALENCE BONDS

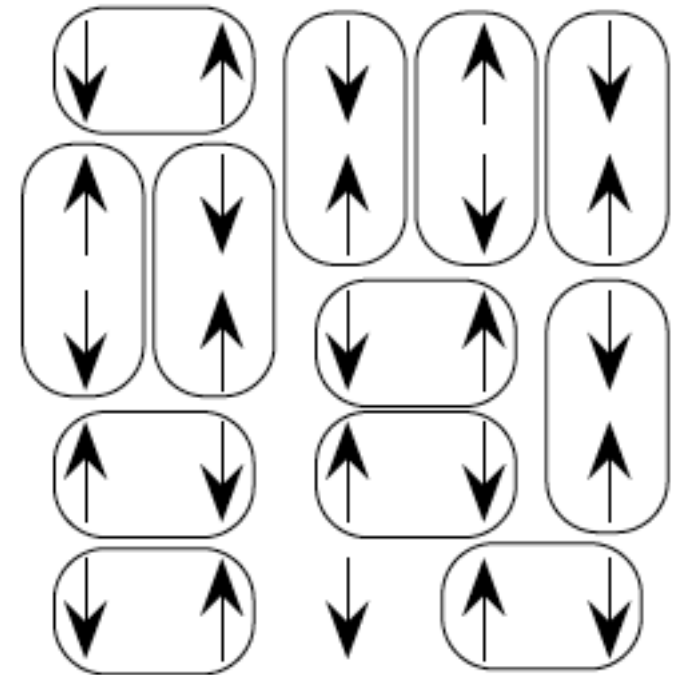
(Anderson)

Mottness from the start.

Pairing scale very large
(related to T^*)

Quantum fluctuations
destroy long range order
leading to a spin liquid of
singlets.

However, spin liquid not
found on cuprates.



<http://www.msd.anl.gov/files/msd/cuprates-columbia.pdf>

POST HIGH T_c PRINCIPLES TO FIND SPC

MAZIN, NATURE 464, 183 (2010)

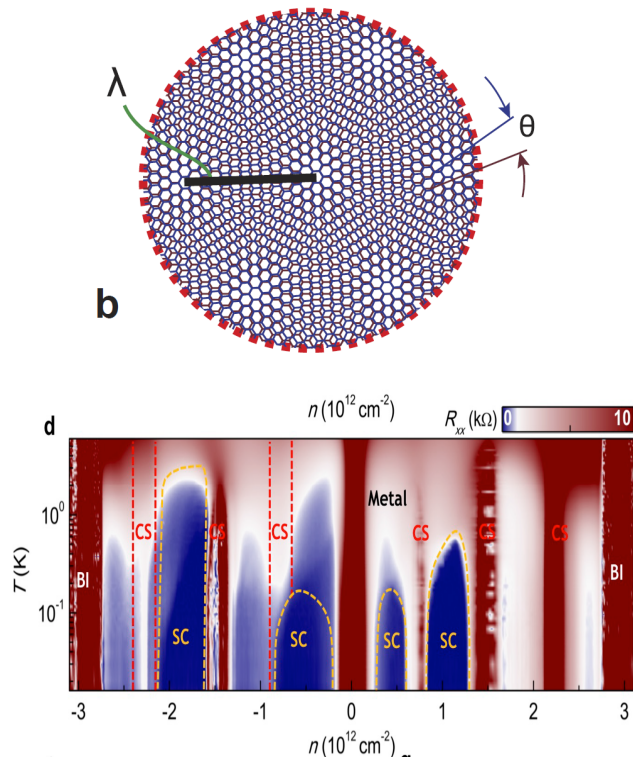
- Layered structures
- Carrier density should not be too high (compared to conventional metals)
- Transition metals of the fourth period (3d) are good
- Magnetism is essential
- Proper Fermi surface geometry is essential (in relation to spin excitations)

Corollary: work with solid state chemists (you need complex chemical compounds)

.... Really?

SUPERCONDUCTIVITY IN MULTILAYERED GRAPHENE (2018-)

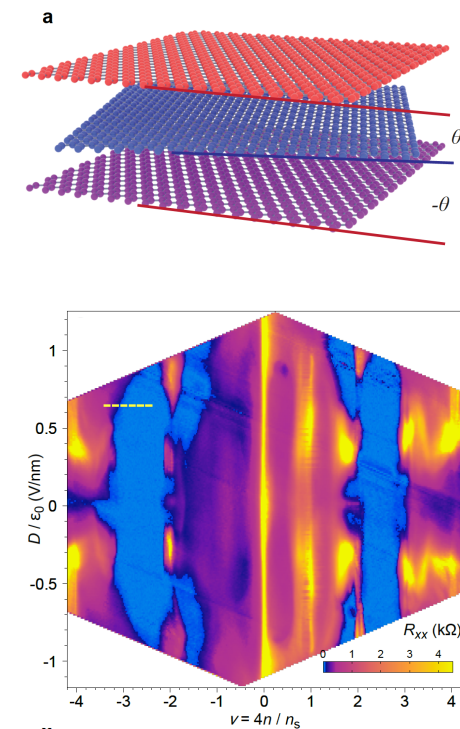
Twisted bilayer graphene



Cao et al, Nature 556, 80 (2018);
Nature 556, 43 (2018)
Lu, et al Nature 574, 653 (2019)

M.J. Calderón calderon@icmm.csic.es

Mirror-symmetric twisted trilayer graphene



Park et al, Nature 590, 249 (2021)

OUTLINE

- **Superconductivity**
 - Properties (zero resistivity, Meissner effect)
 - Understanding (pairing, BCS, Ginzburg-Landau)
 - Electron-phonon interaction (conventional superconductivity)
- **Unconventional superconductivity (unsolved)**
 - What are the new issues.
 - What are the proposals.