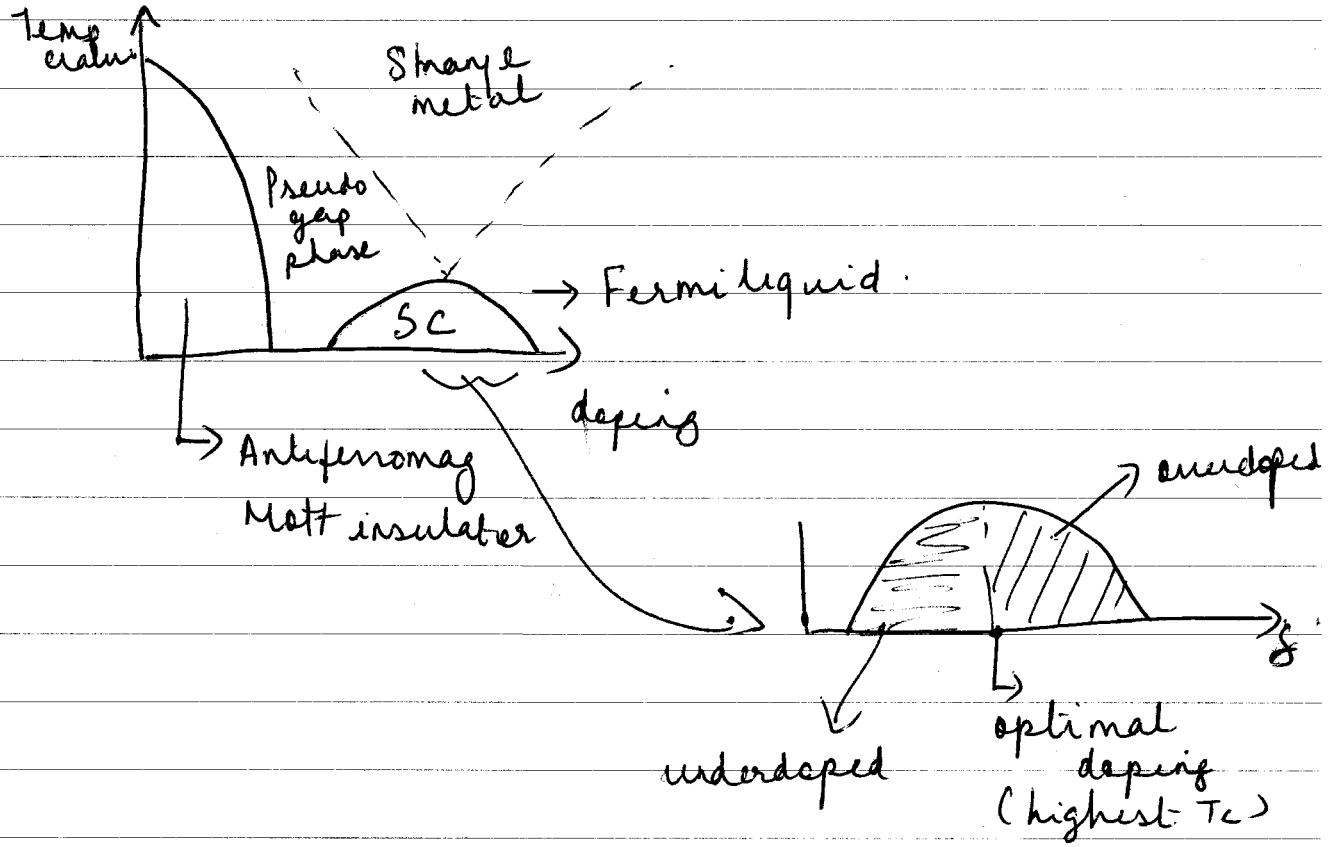
Unconventional SC → high T_c cuprates, MgB_2, C_{60}) organics ruthenates, pnictides ... heavy fermions ...

Cuprate superconductivity: ('87, Bednorz + Müller)

- ceramics with Cu–O planes playing primary role in SC.
- highly anisotropic materials.
- parent compound → antiferromagnetic and insulating

General phase diagram for hole doping



Consider La_2CuO_4 (insulating parent compound)

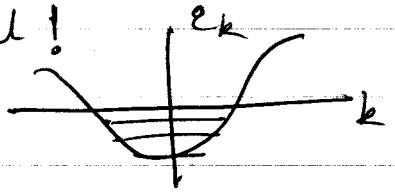
valences are La^{3+} O^{2-} $Cu^{2+} \longrightarrow 3d^9$

$O^{2-} \rightarrow 2p^6$ complete

$Cu \rightarrow 3d^9$ state $\Rightarrow$ single hole (10 electrons in a d shell)

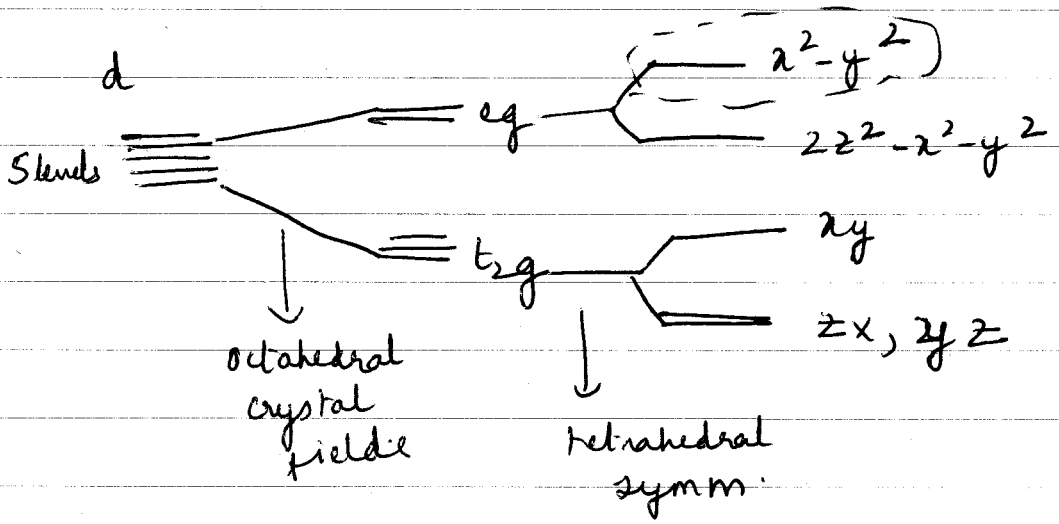
La_2CuO_4 expected to have one hole/unit cell $\rightarrow$ half-filled band

predicted to be a paramagnetic metal!



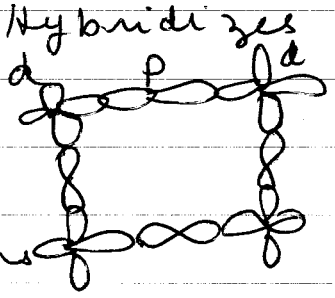
But it is an insulator $\longrightarrow$ failure of Band theory.

Crystal field splittings:



[xy, zx .... denote nature of orbitals]

$d_{x^2-y^2}$ state plays fundamental role! with O p level to generate hopping



⁂ Interactions matter!!

Consider Coulomb interactions between electrons

E = kinetic energy + potential energy.

For strong interactions energy is minimized by localizing the electrons. This is essentially a Mott insulator.

~~Minimal~~ Model to describe high T_c:

3-band model of p (O) + d (Cu) levels.

$$H = -t_{pd} \sum_{\langle ij \rangle} \left(p^{\dagger}_{j\sigma} d_{i\sigma} + h.c \right) - t_{pp} \sum_{\langle ij \rangle} \left(p^{\dagger}_{j\sigma} p_{i\sigma} + h.c \right)$$

$$+ \varepsilon_d \sum_i n_i^d + \varepsilon_p \sum_i n_i^p + U_{dd} \sum_i n^d_{i\uparrow} n^d_{i\downarrow}$$

$$+ U_{pp} \sum_i n^p_{i\uparrow} n^p_{i\downarrow} + U_{pd} \sum_i n_i^d n_i^p$$

$$n_i^{\alpha} = n^{\alpha}_{i\uparrow} + n^{\alpha}_{i\downarrow} \qquad n_p^i = \sum_{\sigma} p^{\dagger}_{i\sigma} p_{i\sigma} \qquad n^d_i = \sum_{\sigma} d^{\dagger}_{i\sigma} d^{\infty}_{i\sigma}$$

t_{pd}, t_{pp} → hopping matrix elements from hybridization of orbitals

ε_d, ε_p → fermi levels of p & d levels

U_{dd}, U_{pp}, U_{dp} → Coulomb repulsion

Model is defined on a square lattice where each site has both p & d levels

If $\Delta \equiv \varepsilon_p - \varepsilon_d > 0$ then first hole doped into system will prefer a d level

↳ Complicated model to solve.

→ for small values of doping physics of above model captured by t-J model.

Parent of t-J model is the Hubbard model

→ MINIMAL MODEL FOR Electrons/holes interacting on a lattice.

$$H^{Hub} = -\sum_{\langle ij \rangle} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \mu \sum_i c_{i\sigma}^{\dagger} c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}.$$

$\mu \rightarrow$ chemical potential — fixes filling.

Consider the half-filled case: $n = 1$ [one particle / site on average]

On bipartite, non frustrated lattices, do Hartree-Fock mean field theory.

$$U n_{i\uparrow} n_{i\downarrow} \Longrightarrow U \left[\langle n_{i\uparrow} \rangle n_{i\downarrow} + \langle n_{i\downarrow} \rangle n_{i\uparrow} \right] + \text{other terms}.$$

If we have an antiferromagnetic order in ground state

then, antiferro moment

$$m_i = \langle n_{i\uparrow} - n_{i\downarrow} \rangle = 2\delta (-1)^i$$
$$\equiv m_0 \cos(\vec{Q} \cdot \vec{R_i})$$

where $\vec{Q} = (\pi, \pi, \pi)$

i.e $\langle n_{i\sigma} \rangle = 1 + \sigma (-1)^i \delta$

↳ Neel ordering vector.

Just like BCS theory, we diagonalize the Hamiltonian and get a gap equation for the ground state

$$\delta = U\delta$$

$$\delta = \frac{\delta U}{(2\pi)^2} \int \frac{d^2k}{\left(\varepsilon_k^2 + \Delta^2\right)^{1/2}}$$

[Two dimensions]

Trivial soln $\delta = 0$, non-trivial soln $\delta \neq 0$.

Non-trivial soln exists

⇒ gap is opened in dispersion by the formation of antiferro ordering (insulator) $\Delta \sim a\sqrt{t/u}$.

$$E_k = \pm\sqrt{\varepsilon_k^2 + \Delta^2} \qquad \Delta \sim te$$

$t \rightarrow$ nearest neighbor hopping

$a \rightarrow$ coefficient.

System goes antiferromagnetic and insulating for arbitrary small repulsive interactions.

[Result is true beyond mean field].

Explains the parent compound.

→ Dope the parent compound!

Theoretical study of doped Hubbard model in $d=2$ is quite complex → numerical method. Dynamical Mean field theory . . .

In the limit of large U (where meanfield fails), the Hubbard models at half filling maps onto the Heisenberg model for spin-half

$$H^{Heis} = \sum_{\langle ij \rangle} J_{ij}\, \vec{S}_i \cdot \vec{S}_j \qquad J_{ij} = \frac{2|t_{ij}|^2}{U}.$$

where $\vec{S}_i = c^\dagger_{i\alpha} \left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta} c_{i\beta}$ where the electrons localize completely.

Mermin - Wagner theorem states no magnetic order at finite temperature for a $d=2$ system!

Finite temperature order is stabilized by other planes in the full 3-d system.

[No good explanation for pseudogap and strange metal phases]

Superconducting phase [cond-mat/0209476]

- $\frac{h}{2e}$ flux quantization observed (Josephson effect)
- $S=0$ singlet pairing (magnetic susceptibility $\chi(T) \to 0$ as $T \to 0$)
- "Gap" shows $\Delta(k) = \Delta_0 [\cos k_x - \cos k_y]/2$ d wave structure. changes sign!

Look at slides

- Sharp quasiparticles observed below $T \ll T_c$ → absent above T_c (pseudogap + strange metal)
- Transport and other properties show high anisotropy.
- Extreme-type II materials B_{c2} very high. coherence length $\xi \sim 3-10$ lattice spacings
- C-axis resistivity shows Cooper pairs in different layers effectively independent.
- absence of substantial isotope effect ⇒ non phononic pairing mechanism.

Possible attraction channels :

→ spin fluctuations
→ stripe ordering
→ excitons
→ and many others !!

Fundamental Egg or chicken question :

" Is superconductivity a consequence of anomalous high temperature normal phase or vice versa ? "

NO CLEAR ANSWER !.

Symmetry of order parameter.

Consider 2 particle wave function like in Cooper pair problem.

$$\Psi(\vec{\rho}, \vec{R}) = \Phi(\vec{\rho})\, \chi_{\alpha\beta}\, \Psi(\vec{R})$$

$\Phi(\vec{\rho})$: relative coordinate
$\chi_{\alpha\beta}$: spin
$\Psi(\vec{R})$: centre of mass

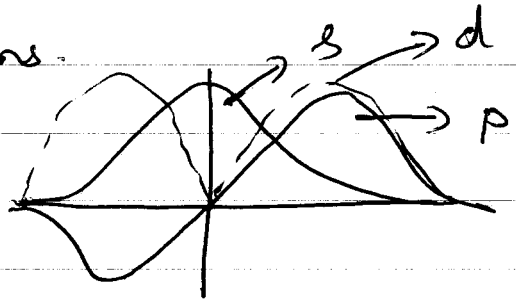
$$\Phi(\vec{\rho}) \equiv R(\rho)\, Y_{lm}(\theta, \phi)$$

In general Y_{lm} replaced by functions related to crystal symmetry

Antisymmetry implies :

$l = 0$, spin singlet → s wave SC.
$l = 1$, spin triplet → p wave SC.
$l = 2$, spin singlet → d wave SC.

from the point of view of wave fns.



d-wave fn has nodes !.

SC → order operator

$$\hat{\Delta}^{+}_{d_{x^2-y^2}} = \sum_{\vec{R}} \Delta_{d_{x^2-y^2}}(\vec{k})\, c^{\dagger}_{\vec{R}\uparrow}\, c^{\dagger}_{-\vec{R}\downarrow}$$

$$= \frac{\Delta_0}{2} \sum_{i} \Big[c^{\dagger}_{i+x\uparrow} c^{\dagger}_{i\downarrow} - c^{\dagger}_{i+x\downarrow} c^{\dagger}_{i\uparrow} - \left(c^{\dagger}_{i+y\uparrow} c^{\dagger}_{i\downarrow} - c^{\dagger}_{i+y\downarrow} c^{\dagger}_{i\uparrow}\right) + \left(c^{\dagger}_{i-x\uparrow} c^{\dagger}_{i\downarrow} - c^{\dagger}_{i-x\downarrow} c^{\dagger}_{i\uparrow}\right) - \left(c^{\dagger}_{i-y\uparrow} c^{\dagger}_{i\downarrow} \cdots\right) \Big]$$

$\vec{x}$ & $\vec{y}$ are unit vectors on square lattice.

$\hat{\Delta}$ is a linear combination of spin singlets between a site "i" and its nearest neighbors.

d-wave gap goes to zero at certain points on Fermi surface !.

what are the consequences ?.

Consider density of states $\rho(E) = \sum_k \delta(E - E_k)$.

$$\rho(E) \propto \int \frac{d\Omega_k}{4\pi} \frac{E}{\sqrt{E^2 - |\Delta_k|^2}}\, \theta(E - |\Delta_k|)$$

($d\Omega_k$ ⇒ angular integral)

for s-wave $\Delta_k = \Delta \quad \forall\, k$

and $\rho(E) \propto \dfrac{|E|}{\sqrt{|E|^2 - \Delta^2}}$ (gap in spectrum)

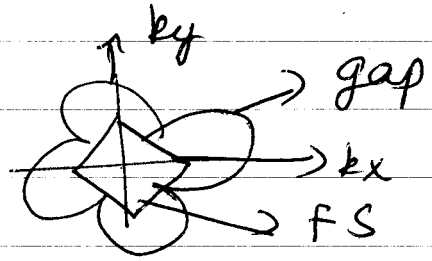
High - Tc : d wave. $\Delta(k) \sim \Delta_0 \cos 2\phi_k$.

$$P(E) \propto \int_0^{E/\Delta_0} d\phi \frac{E}{\sqrt{E^2 - \Delta_0^2 \phi^2}} \sim \frac{|E|}{\Delta_0}.$$

(no gap in density of states !)

→ Jump in specific heat at Tc is also much reduced in d-wave materials.

→ $\langle \Delta_{k_{x^2-y^2}}(\vec{k}) \rangle_{\text{Fermi surface}} = 0$



$\langle \Delta_{s\text{wave}}(\vec{k}) \rangle \neq 0$
Fermi surface.

This suggests that any disorder or impurities which scatter the e^-s or holes tend to isotropize the system and tends to suppress Tc !

[experimentally verified]