Lecture 7. Cuprates II: S-State Properties

(somewhat doping-dependent : will quote results at optimal doping unless otherwise stated)
Will compare with BCS predictions where possible. ("$\surd$" ="agrees with BCS")

1. Structural and elastic properties and electron density distribution :

essentially no change at T_c or below $\surd$

2.Macroscopic EM properties:

i) strongly type-II ii) strongly anisotropic ($\lambda_c \gg \lambda_{ab}$, $\xi_c \ll \xi_{ab}$)
extrapolated $H_{c2}(0) \sim 50$ T for $\boldsymbol{H}||\boldsymbol{c}$, 400 T for $\boldsymbol{H} \perp \boldsymbol{c}$
if interpreted by BCS, corresponds to $\xi_{ab}(0) \sim 15-30$Å, $\xi_c(0) \sim 2-3$Å.
(BCS : $\xi_{ab}(0) = 0.18\hbar v_F/k_B T_c \sim 30$Å for $m^*/m = 4$)

3. Specific heat + condensation energy :

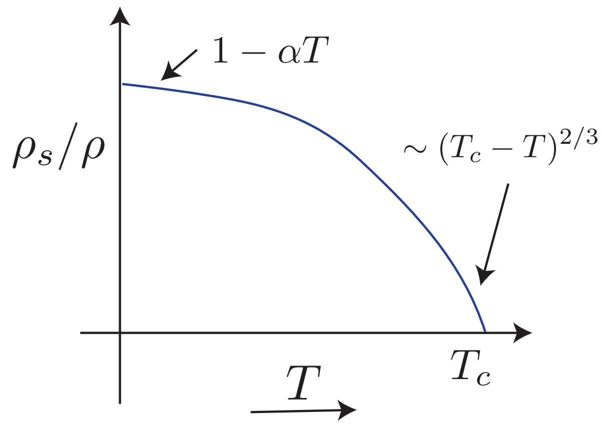
jump at T_c, $\Delta C_{n-s}/C_n \cong 1.6 - 2$ (BCS : 1.4)
for UD and OD, peak is considerably more rounded
for $T < T_c$ falls off sharply ($\surd$) but for $T \rightarrow 0$ power law T^n , probably consistent with $n = 1$.
Condensation energy : peaks sharply at $p = 0.19$ ($\Uparrow$ not "optimal" value 0.16), at a value $\sim$ 33J/mol, corresponding to $\Delta U_{ns}(0) \cong 2K/$ CuO_2 unit.

4. NMR :

T_1^{-1} drops precipitately below T_c, $\propto T^3$ for $T \rightarrow 0$
χ mostly BCS-like for $T \gtrsim 0.5T_c$.

5. Penetration depth :

methods : magnetization-related (unreliable for strong anisotropy)
Fraunhofer diffraction in Josephson junction (not widely used)
μSR (muon spin resonance)
*microwave surface impedance
i) ab-plane : behavior of ρ_s/ρ ($\propto \lambda^{-2}$)
near T_c probably $\propto (T_c - T)^{2/3}$ (3D XY model)
$T \to 0$, (pure) $(1 - \alpha T)$
(dirty) $(1 - \alpha' T^2)$
value of $\lambda(0)$:$\sim$ 1000Å (YBCO, optimal, b-axis)-4000Å (LSCO)
How well do data on $\lambda_{ab}(0)$ fit "naive" (quasi-London) prediction



$$\lambda^{-2}(0) = n_{3D} e^2 \mu_0 / m^* \quad ?$$

Can fit with $m^* = 4m$, $n_{3D} = 10^{22}\text{cm}^{-3} \times p_{\text{eff}}$ ← effective number of carriers per CuO_2 unit
provided that not $p_{\text{eff}} = p$ but

$$p_{\text{eff}} = 1 + p$$

i.e. all holes in Cu $3d^9$ band, not just the excess ones over parent compound.
One puzzle : in YBCO, $\lambda_a(0) \cong 1600$Å, $\lambda_b(0) \cong 1000$Å
$\Rightarrow$ chains appear to contribute (to ρ_s) 3/2 as much as both planes !!

ii) <u>c-axis</u>

$\lambda_c(0) \sim 11,000$Å (YBCO) - 100 μ (=0.1 mm !) (BSCCO 2212)

increases very rapidly with UD. Temperature-dependent at low T much weaker than *ab*-plane, may be fit by $\rho_{sc}/\rho \sim 1 - \alpha T^5$.

If we model interlayer contact as Josephson junction and apply standard Ambegaokar-Baratoff formula $I_c(0)R_N = \pi\Delta(0)/2e$, we expect

$$\lambda_c^{-2}(0)\rho_c d_{\text{int}}/\Delta(0) = \text{const.} \quad (d_{\text{int}} \equiv \text{mean spacing between multilayers})$$

agrees reasonably well with experiment.

6. ac conductivity $(\sigma_1(\omega))$

complicated both in BCS superconductors and in cuprates, but 2 qualitative differences :

i) in cuprates, $\sigma_1(\omega)$ appreciable for $\omega < 2\Delta(0)$ (BCS : $\sigma_1(\omega) = 0$)

ii) for finite ω, $\sigma_1(\omega)$ rises immediately below T_c thereafter drops

$\Rightarrow$ suggests σ_1 limited by e-e scattering, and latter drops below T_c

7. Thermal conductivity

Kinetic-theory formula :

$$\kappa = \frac{1}{3} c_V \overline{v} \ell$$

$$\Rightarrow \quad \kappa_{\text{ph}}/\kappa_{\text{el}} \sim (T/\theta_D)^2 (\ell_{\text{ph}}/\ell_{\text{el}}) \quad (\text{for } \; p \sim 1, \text{since } \; c_s/v_F \sim \omega_D/\varepsilon_F)$$

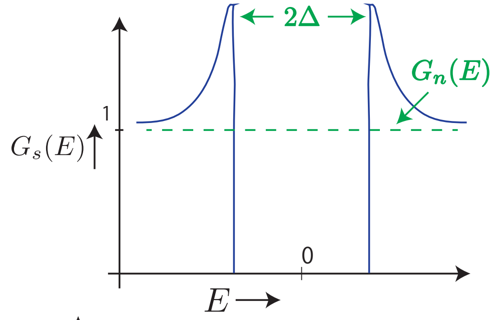
For BCS superconductors, $\kappa_{\text{ph}}/\kappa_{\text{el}} \ll 1$ at T_c, so $\kappa \sim \kappa_{\text{el}} \sim \rho_n \Rightarrow \kappa$ falls rapidly below T_c.

For cuprates $\kappa_{\text{ph}}/\kappa_{\text{el}} \gtrsim 1$, κ rises below $T_c \Rightarrow$ phonons dominant, limited by scattering by electrons which drops below T_c.

S-State Properties (cont.)
8. Tunneling

BCS: $G \equiv \partial I/\partial V$ flat in N state. In S state,

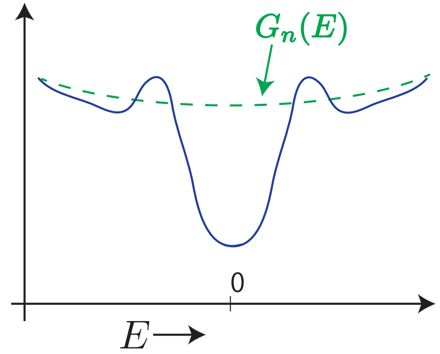
$$G_s(E)/G_n = \frac{\varepsilon}{\sqrt{\varepsilon^2 - \Delta^2}}\theta(\varepsilon - \Delta)$$



In cuprates:

(a) in N state, $G_n(E) \sim a + b(E)$

(b) in S state: $\Rightarrow$



note

i) "dip" beyond peak

ii) $G_s(0) \neq 0$

iii) peak-to-peak distance ("2Δ") typically $\sim 7 - 8 k_B T_c$ for ab-plane tunneling (BCS : 3.5 $k_B T_c$) but closer to BCS for c-axis tunneling (and overdoping).

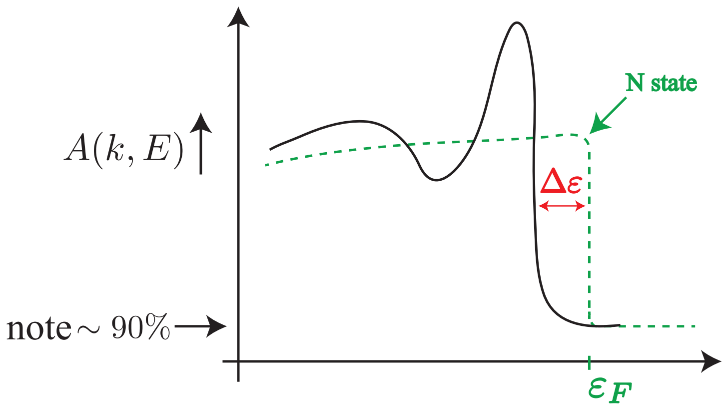
9. ARPES

Note

(a) drop at ε_F only $\sim 10\%$ in both N and S states

(b) dip beyond peak (c.f. tunneling)

(c) $\Delta\varepsilon(\pi, 0)$ ("pullback") $\sim 4 - 5k_BT_c$.

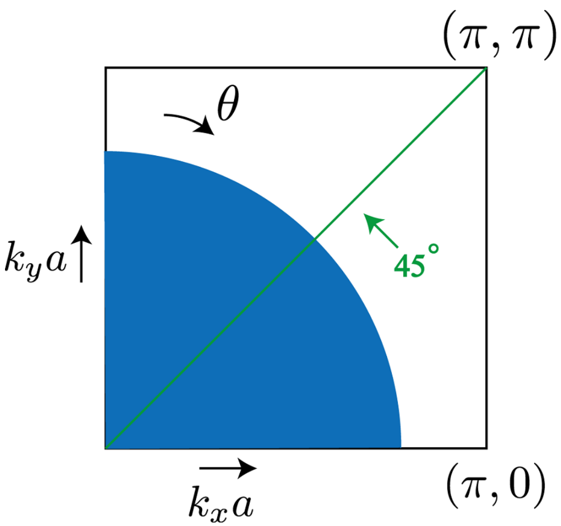


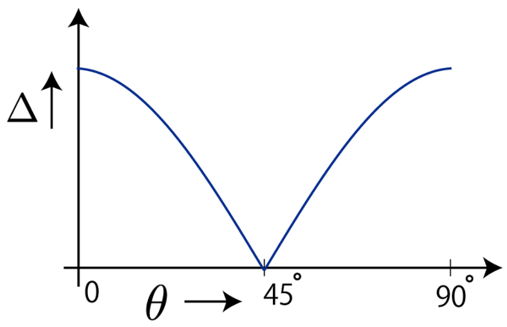
Most interesting feature ; dependence of $\Delta\varepsilon(\boldsymbol{n})$ and peak height on angle on Fermi surface.

Both height and pullback on maximum at $(\pi, 0)$ and almost certainly $\Rightarrow 0$ at (π, π)

i.e. at 45 to crystal axes

$\Rightarrow$ "gap " as seen in ARPES has nodes at (π, π).





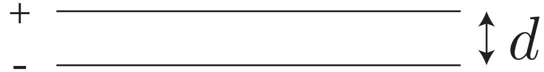
10. Neutron scattering (YBCO LSCO, Bi- 2212)

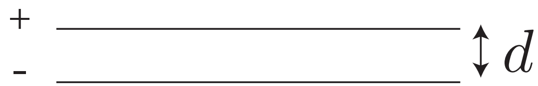
Recall : in N state, $\sigma(q, \omega)$ fairly strongly peaked as $f(q)$ at $(0.5, 0.5)$ (magnetic superlattice values) but featureless as $f(\omega)$.

In the S state in YBCO and Bi-2212, nothing changes in "even" channel, but in "odd" channel ($q_z = \pi/d$ $\leftarrow$ interlayer spacing) a striking peak is seen around $\boldsymbol{q} = (0.5, 0.5)$ with $\omega \cong 41$ meV. Not seen in (single) channel of LSCO.

In this peak peculiar to bilayer cuprates?

In any case, what is its significance?

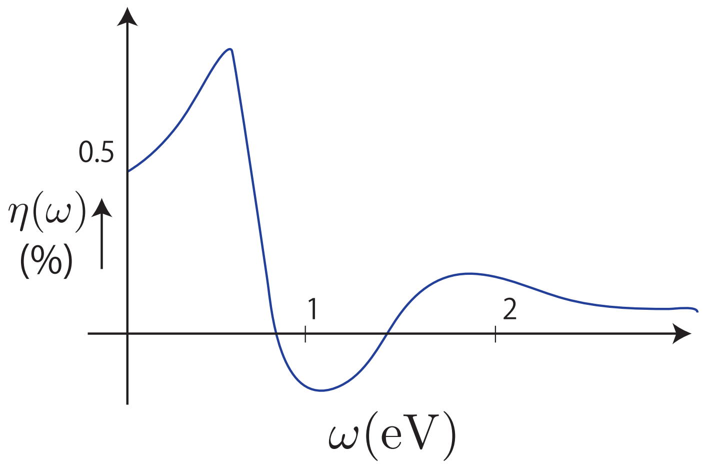




11. Optics

BCS-based prejudice : effect of superconductivity on optical behavior at frequency $\omega \gg \Delta$ should be $\lesssim (k_B T_c/\hbar\omega)^2$ ($\sim 10^{-4}$ for $\hbar\omega \sim 1$ eV) $\Rightarrow$ probably too small to see.
Fact : at $\hbar\omega \sim 1$ eV, changes in S state $\sim 1\%$!

Define ($R(\omega) \equiv$ reflectivity)
$\eta(\omega) \equiv \frac{R_S(\omega)}{R_N(\omega)} - 1$ then :
Note : zero crossing of $\eta(\omega)$ almost exactly where $R_N(\omega)$ has minimum. Suggests
$\eta(\omega) = -\delta(\partial R_N/\partial\omega)$ (∗)
where δ is average downward shift of "initial" state (no change in final state). But



(a) would require $\delta \sim \Delta$, .i.e. initial states strongly concentrated over energy range $\sim \Delta$ near ε_F (no obvious reason for this)
(b) while (∗) qualitatively fits data on reflectivity, does not seem to fit $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ (measured independently in ellipsometric experiment)

12. EELS

Published data for S states only for $\omega \lesssim 100$ meV : no particularly interesting feature seen (probably not surprising)

No date yet on MIR (mid-infrared) region ($\omega \sim 0.5 - 1$ eV)

WHAT DO WE KNOW FOR SURE ABOUT SUPERCONDUCTIVITY IN THE CUPRATES?

1. Flux quantization and Josephson experiments

   $\Rightarrow$ ODLRO in 2-particle correlation function, i.e., superconductivity due to formation of Cooper pairs, i.e., basic "topology" of many-body wave function is

$$\Psi_N \sim \mathcal{A}[\phi(\boldsymbol{r}_1\sigma_1;\boldsymbol{r}_2\sigma_2)\phi(\boldsymbol{r}_3\sigma_3;\boldsymbol{r}_4\sigma_4)\cdots\phi(\boldsymbol{r}_{N-1}\sigma_{N-1};\boldsymbol{r}_N\sigma_N)],$$

   where ϕ is the same "molecular" wave function for all pairs (quasi-BEC!)

   For most purposes, it is more convenient to work in terms of related quantity

$$F(\boldsymbol{r}_1,\boldsymbol{r}_2,\sigma_1,\sigma_2) = \langle\psi^\dagger_{\sigma_1}(\boldsymbol{r}_1)\psi^\dagger_{\sigma_2}(\boldsymbol{r}_2)\rangle \quad \text{("pair wave function" (anomalous average))}$$

   Note: "Macroscopic wave function" of Ginzburg and Landau, $\Psi(\boldsymbol{R})$, is just $F(\boldsymbol{r}_1,\boldsymbol{r}_2,\sigma_1,\sigma_2)$ for $\sigma_1=-\sigma_2=+1$, $\boldsymbol{r}_1=\boldsymbol{r}_2=\boldsymbol{R}$, i.e. wave function of COM of Cooper pairs.

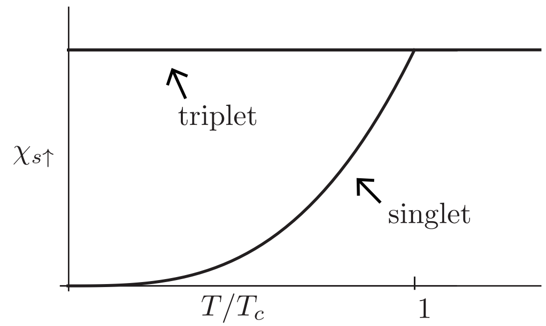
2. "Universality" of high-T_c superconductors in cuprates with very different chemical compositions, etc.

   $\Rightarrow$ Main actors in superconductivity are electrons in CuO_2 planes.

3. NMR ($\chi_s, T_1, ...$) (note: Spin Orbit interaction very small)

   $\Rightarrow$ spin wave function of Cooper pairs is singlet not triplet, i.e.

$$F(\boldsymbol{r}_1, \boldsymbol{r}_2, \sigma_1, \sigma_2) = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)F(\boldsymbol{r}_1, \boldsymbol{r}_2)$$



4. Absence of substantial FIR (far infra-red) absorption above gap edge

   $\Rightarrow$ pair from time-reversed states (but cf. J. Tahir-Kheli)

5. Order-of-magnitude estimates from (a) T_c and (b) H_c

   $\Rightarrow$ (in-plane) "radius" of Cooper pairs $\sim$ a few lattice spacings. (thus, $\xi_0/a \sim$ 3-10: contrast $\sim 10^4$ for Al.)

   ξ_0: pair radius; a: inter-cond. electron spacing

   $\Rightarrow$ fluctuations much more important than in e.g. Al.

6. c-axis resistivity

   $\Rightarrow$ hopping time between unit cells along c-axis $\gg \hbar/k_B T$

   $\Rightarrow$ pairs in different multilayers effectively independent.(but cf. Anderson Interlayer Tunneling theory).

7. Absence of substantial isotope effect (in higher-T_c cuprates) + "folk-theorems" on T_c

   $\Rightarrow$ phonons do not play major role in cuprate superconductivity (but cf. Newns and Tsuei).

WHAT DO WE KNOW FOR SURE... (cont.)

SYMMETRY OF THE ORDER PARAMETER (GAP)

In BCS theory, $\Delta(\boldsymbol{n})$ (fermionic gap) has (almost) same $\boldsymbol{n}$-dependence as $\Psi(\boldsymbol{n})$ (order parameter $\equiv$ pair wave function). In a more general theory this is not guaranteed (but seem unlikely to be qualitatively different) .

As we have seen, NMR experiments $\Rightarrow$ order parameter is spin singlet, i.e.

$$F(\boldsymbol{r}_1, \boldsymbol{r}_2, \sigma_1, \sigma_2) = \frac{1}{\sqrt{2}}(\uparrow_1\downarrow_2 - \downarrow_2\uparrow_1)F(\boldsymbol{r}_1, \boldsymbol{r}_2)$$

where $F(\boldsymbol{r}_1, \boldsymbol{r}_2)$ even-parity $\Rightarrow F_{\boldsymbol{k}}$ even-parity. Assume relevant symmetry is that of CuO_2 plains, i.e. (approximately) tetragonal. Then symmetry group is C_{4v} (symmetry group of square) with fundamental operations

(a) rotation through $\pi/2$ around $\boldsymbol{z}$ ($\perp$) axis ($\hat{R}_{\pi/2}$)

(b) reflection in crystal axis, e.g. (100) ($\hat{I}_{\text{axis}}$)

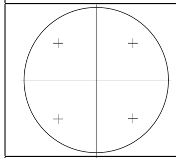
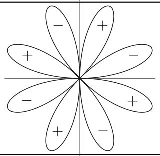
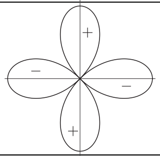
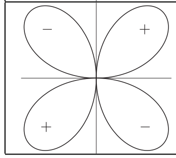
(c) reflection in a 45° axis, e.g. (110) ($\hat{I}_{\pi/4}$)

Note (a)-(c) are not independent:

$$\hat{I}_{\text{axis}}\hat{I}_{\pi/4}\hat{R}_{\pi/2} \equiv 1$$

Evidently $\hat{I}^2_{\text{axis}} \equiv \hat{I}^2_{\pi/4} \equiv 1$, and even parity $\Rightarrow \hat{R}^2_{\pi/2} = 1$.

$\Rightarrow$ only 4 possible irreps (irreducible representations), all 1-dimensional.

	Informal name	group theoretic notation	$\hat{R}_{\pi/2}$	$\hat{I}_{\text{axis}}$	Representative state
	s^+	A_{1g}	$+1$	$+1$	const
	s^- (‘g’)	A_{2g}	$+1$	-1	$xy(x^2 - y^2)$
	$d_{x^2-y^2}$	B_{1g}	-1	$+1$	$x^2 - y^2$
	d_{xy}	B_{2g}	-1	-1	xy

Are we sure order parameter belongs to a single irrep? In general, if i labels different irreps,

$$F(T) = \sum_{ij} \alpha_{ij}(T)\psi_i^*\psi_j + \frac{1}{2}\sum_{ijk\ell} \beta_{ijk\ell}(T)\psi_i^*\psi_j^*\psi_k\psi_\ell$$

Quite generally (for any symmetry group!) $\alpha_{ij} \sim \alpha_j\delta_{ij}$, but in general terms such as $|\psi_i|^2\psi_i^*\psi_j$ $(i \neq j)$ allowed (e.g. SO(3), $i = p$, $j = f$). However, for even-parity representation of C_{4v}, such terms are forbidden by symmetry: only allowed forms are $A_1 \sim |\psi_i|^2|\psi_j|^2$ and $A_2 \sim \psi_i^*\psi_i^*\psi_j\psi_j$. Thus most general form on F is

$$F(T) = \sum_{i=1}^{4} \alpha_i(T)|\psi_i|^2 + \frac{1}{2}\sum_{i,j=1}^{4} \beta_{ij}(T)|\psi_i|^2|\psi_j|^2 f(\varphi_{ij})$$

where φ_{ij} is the relative phase of ψ_i and ψ_j.

More than one $\psi_i \neq 0 \Rightarrow 2$ phase transitions. Not seen, so order parameter belongs to a single irrep.

SYMMETRY OF THE ORDER PARAMETER (cont.)

According to above argument, must be just one of

$$s \begin{bmatrix}\text{favored by some} \\ \text{types of theory}\end{bmatrix}, \quad d_{x^2-y^2} \begin{bmatrix}\text{favored by spin-} \\ \text{fluctuation theory}\end{bmatrix}, \quad d_{xy}, \quad s^-$$

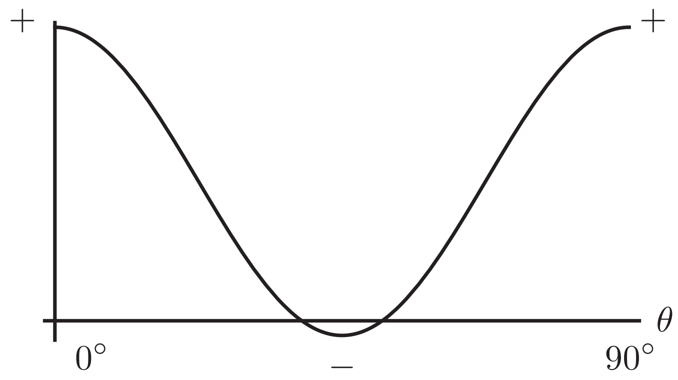
How to tell?

(a) $d_{x^2-y^2}$, d_{xy}, s^- must have (at least) 4 nodes on Fermi surface. s need not. ⇒ exponential decrease of quasiparticle-associated quantities (χ, $T_1^{-1}, \Delta\lambda(T)$...) certainly ⇒ s-wave. Experimentally, all these quantities have power-law dependences consistent with 2D point node. Dose this inevitably ⇒ not s? Unfortunately not, because even s state may have nodes allowed by symmetry ("extended s-wave").

(b) More specifically, $d_{x^2-y^2}$ (and s^-) must have nodes at (π, π), s (and d_{xy}) would have them there only by pathology. ⇒ observation of node favors $d_{x^2-y^2}$. ARPES data indeed indicates such a node. But...

i) "gap" seen in ARPES may not simply be superconducting gap (cf. pseudo gap regime.)

ii) "extended s-wave" state of form $F(\theta) = A + B\cos 4\theta$ $(0 < B - A \ll A)$ may be difficult in practice to distinguish from $d_{x^2-y^2}$.



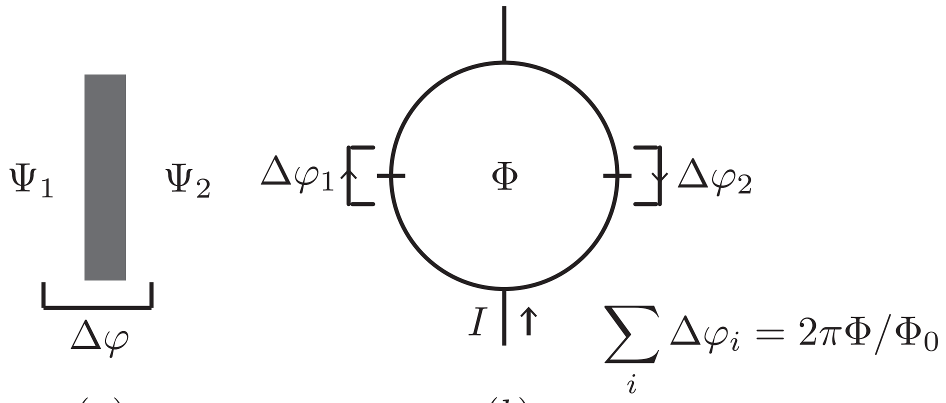
So: need experiment which is directly sensitive to sign (or more generally phase) of order parameter $\Rightarrow$ Josephson ("phase-sensitive") experiments.

Reminder: for simple s-wave case, to lowest order in Ψ's

$$E_J \propto -\text{const.}(\Psi_1^* \Psi_2 + \text{c.c.}) \sim -\text{const.} \cos \Delta\varphi$$

(a) Josephson effect occurs for any geometry.

(b) in SQUID geometry, critical current max. at $\Phi = n\Phi_0$, and min. at $\Phi = (n + 1/2)\Phi_0$



(a) (b)

Principles of Josephson experiment in cuprate (and other exotic) superconductor

(a) If bulk superconductor + junction described by Hamiltonian $\hat{H}$ invariant under symmetry group G, then Josephson coupling energy must be similarly invariant under G.

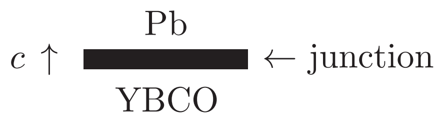
(b) For a circuit, the fundamental equation

$$\sum_i \Delta\varphi_i \;=\; 2\pi\Phi/\Phi_0$$

[taken in same sense around circuit] [flux trapped in circuit]

must hold provided the Φ's (hence the $\Delta\varphi_i$) consistently defined. Assume lowest-order Josephson effect (testable via Fraunhofer diffraction pattern etc), i.e.

$$E_J \sim -\text{const.}(\Psi_1^*\Psi_2 + \text{c.c.})$$

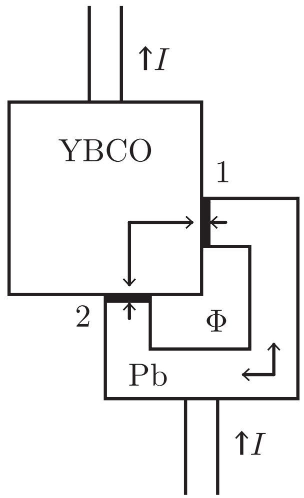


Application (a) alone:

consider $\pi/2$ rotation around z-axis. $\Psi_{\text{Pb}} \to +\Psi_{\text{Pb}}$.

For YBCO, if s-wave (s or s^-) $\Psi_{\text{YBCO}} \to +\Psi_{\text{YBCO}} \Rightarrow$ lowest-order Josephson effect allowed.

But if d-wave ($d_{x^2-y^2}$ or d_{xy}) then $\Psi_{\text{YBCO}} \to -\Psi_{\text{YBCO}} \Rightarrow$ lowest-order Josephson effect forbidden.



Application (b) alone:

Pb order parameter invariant under $\pi/2$ rotation $\Rightarrow$ "Ψ_1" identical at junctions 1 and 2. If YBCO is s-wave, same situation as in conventional dc SQUID. $\Rightarrow I_c(\Psi)$ is maximum at $\Psi = n\Psi_0$, min at $\Psi = (n+1/2)\Psi_0$. If YBCO is d-wave, sign of "Ψ_2" changes between 1 and 2, so effectively adds π to LHS of $(*)$ $\Rightarrow I_c$ max at $\Psi = (n+1/2)\Psi_0$.

[Application of (a) and (b) e.g. "tricrystal ring" experiment]

Conclusion from ∼ 20 phase-sensitive experiment:

order parameter of cuprates is $d_{x^2-y^2}$.

How will we know when we have a "satisfactory" theory of high-T_c superconductors in the cuprates?

Thesis :

We should (at least) be able to :

(A) give a blueprint for building a robust room-temperature superconductor,

OR (B) assert with confidence that we will never be able to build a (cuprate-related) room temperature superconductor

OR (C) say exactly why we cannot do either (A) or (B)

In the meantime, a few more specific questions:

(1) Are the cuprates unique in showing high-T_c superconductors?

(2) If so, what is special about them?

(e.g. band structure, 2-dimensionality, AF ....)

(3) Should we think of high-T_c superconductors as a consequence of the anomalous N-state properties, or vice versa?

(4) Is there a second phase transition associated with the T^*-line ? If so, what is the nature of the low temperature ("pseudogap") phase?

(5) If yes to (4), is this relevant to high-T_c superconductors or a completely unconnected phenomenon?

(6) Why does T_c depends systematically on n in homologous series?

Some representative classes of "models" of Cooper pairing in the cuprates (conservative $\Rightarrow$ exotic)

1. Phonon-induced attraction ("BCS mechanism")
problems : N-state $\rho_{ab}(T) \propto T$ down to $T \sim 10$ K (Bi-2201 T_c)
no isotope effect in higher-T_c high-T_c superconductors
folk-theorems on T_c (but $\uparrow$: FeAs compounds)
2. Attraction induced by exchange of some other boson :
— spin fluctuations
— excitons
— fluctuations of "stripes"
— more exotic objects
3. Theories starting from single-band Hubbard model*:

$$\hat{H} - t \sum_{ij\sigma} (c^\dagger_{i\sigma} c^\dagger_{j\sigma} + H.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

a. Attempt at direct solution, computational or analytic
b. Theories based on postulate of "exotic ordering" in ground state (e.g. spin-charge separation)

Problems : — to date, no direct evidence for exotic order
— T^*-line appears to be unrelated to T_c

(and "Nature has no duty ....")

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* See e.g. P. A. Lee, Reps. Prog. Phys. **71**, 012501 (2008)