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UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION
INTERNATIONAL CENTRE FOR SCIENCE AND HIGH TECHNOLOGY

SMR/543 - 3

EXPERIMENTAL WORKSHOP ON
HIGH TEMPERATURE SUPERCONDUCTORS AND RELATED MATERIALS
(BASIC ACTIVITIES)

(11 February - 1 March 1991)

" Introduction to High $T_c$ Theory "

presented by:

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# Introduction to High Tc Theory

1. Brief overview of ordinary SC, Fermi liquid theory and BCS theory

2. Main observations on high Tc superconductors: Normal state and SC properties

3. Theoretical models for high Tc SC

4. Various attempts to interpret the experimental observations

Superconductivity — one of the most profound phenomena in physics (at least for condensed matter).

1911 — Kamerlingh Onnes. Hg

1933 — Meissner effect

⋮

1937 London theory

1950 Ginsburg - Landau theory

1957 BCS pairing theory

$T_c$: Before 1986 $< 23.3K$ ($Nb_3Ge$)

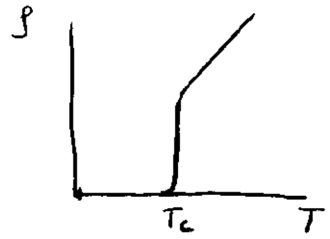
1986 G. Bednorz & K.A. Müller $La_{2-x}Sr_xCuO_4$ $\sim 40K$

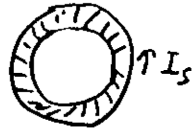
1987 K.M. Wu et al. $YBa_2Cu_3O_{7-\delta}$ $\sim 90K$

1988 - - - - .... $Tl_2Ba_2Ca_2Cu_3O_{10}$ $\sim 125K$

## Basic properties of LTSC

* zero-resistance — the defining property

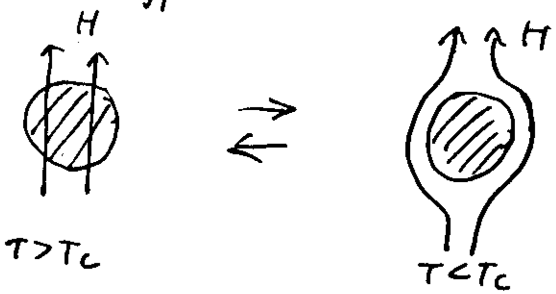



persistant current

$\rho_n/\rho_s \sim 10^{15}$ $\tau = \frac{L}{R} \sim 10^{7}$ s.

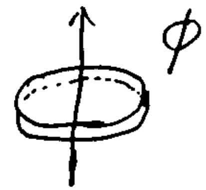
* Meissner effect — the deciding property




$\chi = -\frac{1}{4\pi}$

* Flux quantization

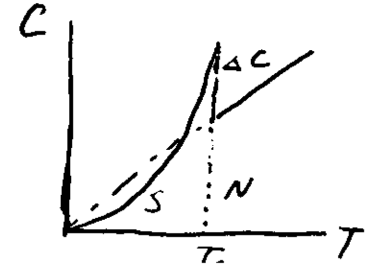
$$\Phi = n\,\frac{hc}{2e}$$




* 2nd order phase transition

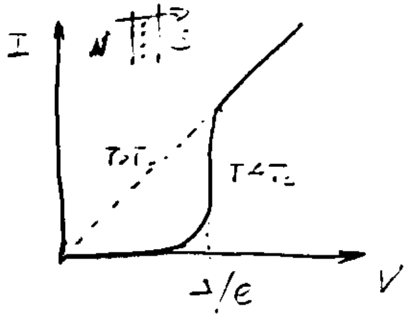
$$\frac{\Delta C}{\gamma T_c} \approx 1 \sim 2.6$$

BCS 1.43



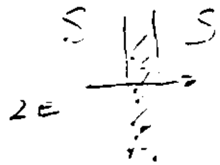
Gap in single-particle excitation

Tunneling.




Electron-pairing.

dc-Josephson effect



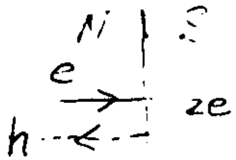

$I \neq 0$ for $V = 0$

ac-Josephson effect

$$2eV = \hbar\omega$$

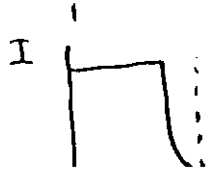
Generation of ac signal → Shapiro step

Andreev reflection

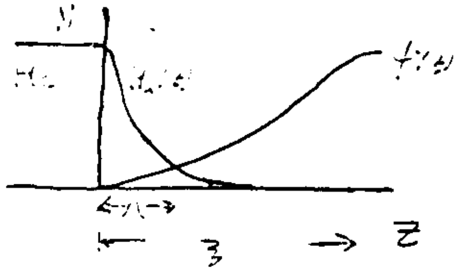


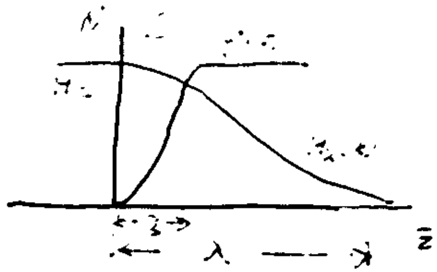

$E_k < \Delta$

Increase of the current



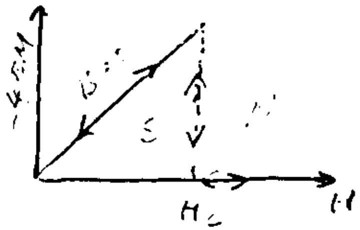

* Penetration depth λ and correlation length ξ

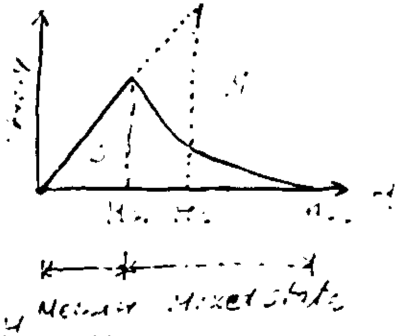


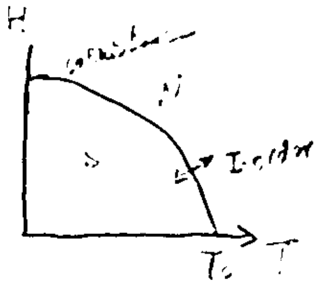



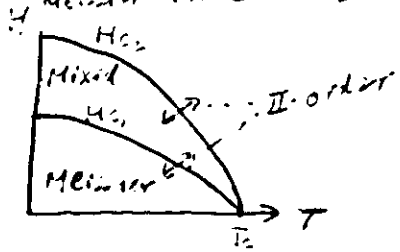

$\xi \gg \lambda$ $\lambda \gg \xi$

$$K = \lambda/\xi = \frac{1}{\sqrt{2}}$$






Type I SC

$\xi \sim 10^4$ Å

Interface energy > 0

Type II SC

$\xi \sim 10^2$ Å

Interface energy < 0

## SC as a macroscopic quantum phenomenon

London: "Rigid", macroscopic wave function

$$\psi_s(\vec{x}) = \sqrt{n_s}\, e^{i\theta},$$

"electron pair" condensation

$$e^* = 2e, \quad m^* = 2m$$

$$\vec{j}_s = \frac{-i e^* \hbar}{2m^*}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right] - \frac{e^{*2}}{m^* c}\vec{A}\psi^*\psi$$

For isolated, simply-connected, $\theta = 0$

$$\vec{j}_s = -\frac{e^{*2}}{m^* c}\vec{A}\,\psi^*\psi, \quad \nabla\cdot\vec{A} = 0$$

+ Maxwell eq.

$\Downarrow$

$$\nabla^2 \vec{h} = \frac{1}{\lambda^2}\vec{h}, \qquad \lambda^2 = \frac{m^* c^2}{4\pi n_s e^{*2}}$$

Two aspects of SC theory

* Symmetry-breaking — ordering — macroscopic quantum phenomenon — Ginsburg-Landau theory
* Microscopic theory — mechanism — model dependent

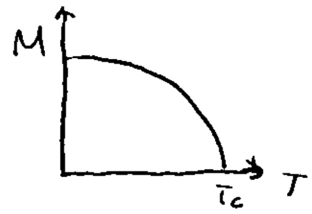
* Symmetry breaking

| | |
|---|---|
| Hamiltonian | Yes |
| State | No |

Heisenberg ferromagnet

$$\mathcal{H}_s = -\sum_{\langle ij\rangle} J_{ij}\,\vec{S}_i\cdot\vec{S}_j$$

$$\vec{M} = \sum_i \langle \vec{S}_i \rangle \neq 0$$




O(3) rotation

Gauge invariance in case of SC

$$H = \frac{\hbar^2}{2m}\sum_\sigma \int d\vec{x}\,\nabla\psi^*\nabla\psi + \frac{1}{2}\sum_{\sigma\sigma'}\int d\vec{x}\,d\vec{x}'\,\psi^\dagger_\sigma(x)\psi^\dagger_{-\sigma}(x')V(x-x')\psi_{-\sigma}(x')\psi_\sigma(x)$$

$$\psi_\sigma(x) \to e^{i\alpha}\psi_\sigma(x) = e^{-i\alpha N}\psi_\sigma(x)\,e^{i\alpha N}$$

$$N = \sum_\sigma \int dx\,\psi^\dagger_\sigma(x)\psi_\sigma(x)$$

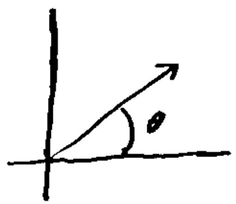
$N$, $\alpha$ canonical variable

Off-diagonal long-range order

$$\psi_s(x) = \langle \psi_\uparrow(x)\psi_\downarrow(x)\rangle$$

which breaks the gauge symmetry

$$\psi_s = \sqrt{n_s}\, e^{i\theta}$$



## Ginzburg - Landau order parameter theory

II-order phase transition. Taylor expansion

$\psi_s$: "small", "smooth"

$$F_{sh} = F_{n0} + a(T)|\psi_s|^2 + \frac{b}{2}|\psi_s|^4 + \frac{1}{2m^*}\left|(-i\hbar\vec{\nabla} - \frac{e^*}{c}\vec{A})\psi_s\right|^2 + \frac{h^2}{8\pi}$$

$$a(T) = \alpha(T_c - T)/T_c = \alpha\tau$$

$$\frac{\partial F_{sh}}{\partial \psi} = \frac{\partial F_{sh}}{\partial \vec{A}} = 0 \quad \Rightarrow \quad \text{GL equation}$$

$$\frac{1}{2m^*}(-i\hbar\vec{\nabla} - \frac{e^*}{c}\vec{A})^2\psi_s + b|\psi_s|^2\psi_s + a\psi_s = 0$$

$$\vec{J}_s = \frac{ie^*\hbar}{2m^*}(\psi_s\nabla\psi_s^* - \psi_s^*\nabla\psi_s) - \frac{e^{*2}}{m^*c}|\psi_s|^2\vec{A} = 0$$

$$\xi(T) = (\hbar^2/2m^*|a|)^{1/2} = \xi(0)\,\tau^{-1/2}$$

$$\lambda(T) = (m^*c^2 b/4\pi e^{*2}|a|)^{1/2} = \lambda(0)\,\tau^{-1/2}$$

As $\tau \to 0$, both $\xi(T)$ and $\lambda(T) \to \infty$,

$\kappa = \lambda(T)/\xi(T)$ is $T$ independent

GL theory "almost" explains "everything"

$$\psi_s = (|\alpha|/b)^{1/2}\,\tau^{1/2},$$

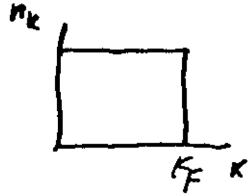
$$\frac{H_c^2(T)}{8\pi} = F_{n0} - F_{s0} = \frac{|\alpha|^2}{b}\tau^2$$

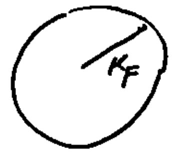
$$\Delta C = \frac{|\alpha|^2}{\ }, \quad \text{etc.}$$

## Theoretical basis of BCS theory:

Landau theory of Fermi Liquid

Ideal fermi gas:




$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

$$k_F = (3\pi^2 n)^{1/3}$$

$$N(0) = \frac{dn}{d\varepsilon} = \frac{\varepsilon_F}{\pi^2\hbar^3}\frac{2m}{v_F}$$

$$C_V = \frac{\pi^2}{3}k_B^2\,N(0)\,T$$

$$\chi = \frac{1}{2}\gamma^2\hbar^2\,N(0)$$

Interacting fermions — liquid state

particles — building blocks for matter

quasi-particles — " " for motion

Upon "adiabatic" switching on the interaction there is one-to-one correspondence between interacting and non-interacting systems.

$t$ slow enough, still eigenstate

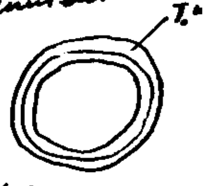
$t < \tau$ . livetime of the state

## Main features of Fermi-liquid behavior

1) Well-defined quasiparticles

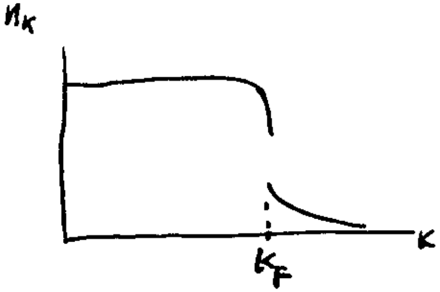
phase space argument

$$\underbrace{\mathrm{Re}\,\Sigma}_{T,\ \omega} \gg \underbrace{\mathrm{Im}\,\Sigma}_{T^2,\ \omega^2}$$



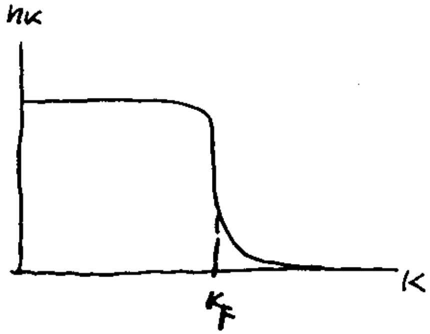

2) Charge $e$ and spin $1/2$ are associated with each other

3) Luttinger theorem
volume of Fermi-surface $\sim N$




FL. jump $\sim z$

$$G \sim \frac{z}{\omega - \varepsilon_k + i0\,\mathrm{sgn}\,\omega}$$




NFL, no jump

The difference is more subtle!

## Basic features of BCS theory

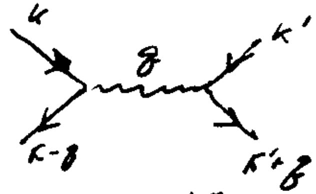
* Interaction, el-el or el-ph

isotope effect: $T_c \sim M^{-1/2}$

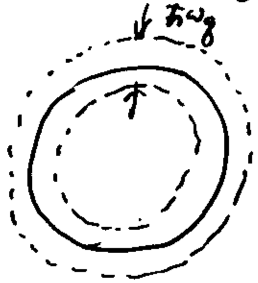
el-ph.

* Effective el-el. interaction due to exchange of virtual phonons

$$V_{kk'} \sim \frac{\hbar\omega_q}{(\varepsilon_k-\varepsilon_{k'})^2-(\hbar\omega_q)^2+i\delta}$$




$V<0, \quad |\varepsilon-\varepsilon'|<\hbar\omega_q$




* Coulomb interaction strong, but instantaneous
* el-ph. interaction weak, but retarded

* Cooper instability

Two electrons with attractive interaction at the Fermi surface form a bound state

$$E_b \sim -\hbar\omega_D\, e^{-\frac{2}{N_0 V}}$$

* BCS reduced Hamiltonian

$$H_{BCS} = \sum_{\sigma} (\varepsilon_k - \mu) c_{k\sigma}^{+} c_{k\sigma} + \sum_{k,k'} V_{kk'} b_k^{+} b_{k'}$$

$$b_k = c_{k\downarrow} c_{-k\uparrow}$$

$$V_{kk'} = \begin{cases} -V & \text{for } |\varepsilon_k|, |\varepsilon_{k'}| < \hbar\omega_D \\ 0 \end{cases}$$

MFT : pairing potential

$$-\Delta_k = \sum_{k'} V_{kk'} \langle b_{k'}^{+} \rangle$$

$$c_{k\uparrow} = u_k^{*} \alpha_{k\uparrow} + v_k \alpha_{-k\downarrow}^{+}$$
$$c_{-k\downarrow}^{+} = -v_k^{*} \alpha_{k\uparrow} + u_k \alpha_{-k\downarrow}^{+}$$

Gap equation

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

$$E_k = \left( (\varepsilon_k - \mu)^2 + \Delta_k^2 \right)^{1/2}$$

$$\Psi_{BCS} = \prod_k \left( u_k + v_k c_{k\uparrow}^{+} c_{-k\downarrow}^{+} \right) |0\rangle$$

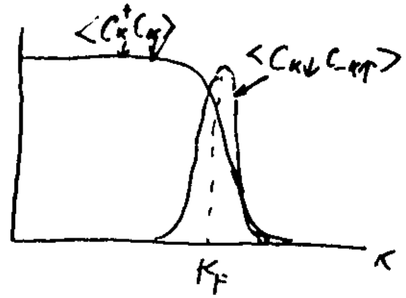
coherent superposition of $(k\uparrow, -k\downarrow)$ occupation takes advantage of attraction to lower the energy

$$k_B T_c = 1.13 \hbar\omega_D \, e^{-\frac{1}{N(0)V}}$$

$$\frac{2\Delta}{k_B T_c} = 3.5$$

$$\frac{\Delta C}{\gamma T_c} = 1.43$$

The particle distribution is modified near the Fermi surface within $\sim \Delta$




This is a very subtle effect!

$\varepsilon_F \sim 10$ eV

Correlation energy $\sim 1$ eV

Phonon energy $\sim 10^{-2}$ eV

gap parameter $\sim 10^{-3}$ eV

Condensation energy $(E_N - E_S)/N \sim 10^{-8}$ eV

Cooper pairs are not indepedent bosons

$\xi \sim 10^{-4}$ cm

average distance $\sim 10^{-6}$ cm

# Classes of Hi-Tc Superconductors

$La_{2-x}Sr_xCuO_4$ (214) $T_c \sim 40K$

$YBa_2Cu_3O_{7-y}$ (123) $T_c \sim 90K$

$X_mBa_2Ca_{n-1}Cu_nO_{2(n+1)+m}$

X = Bi, Tl. n = 1, 2, 3, m = 1 (Tl), 2

(2212) $T_c = 110K$

(2223) $T_c \approx 125K$

Others $Ln_{2-x}Ce_xCuO_{4-y}$ $T_c = 24K$

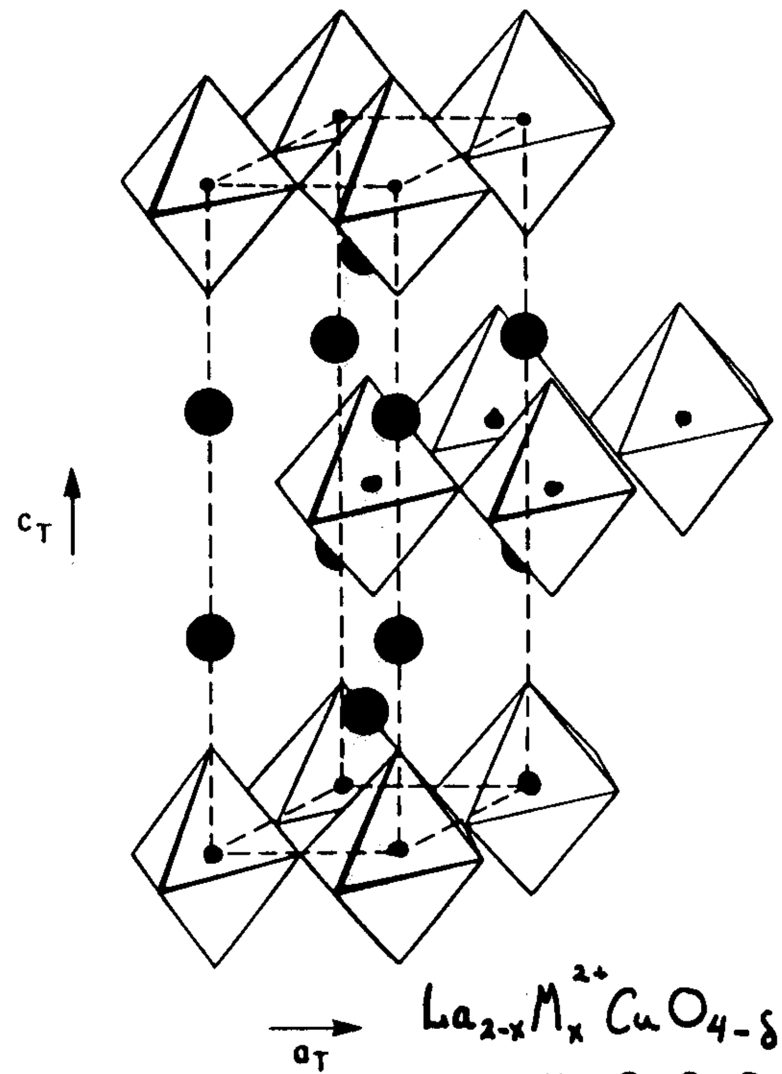
Ln = Nd, Pr. $x = 0.15$

Y. Tokura et al.

Cubic

$BaBiO_3$ —
- $BaPb_xBi_{1-x}O_3$ 13K
- $Ba_xK_{1-x}BiO_3$ 30K

DO NOT AFFIX OVERLAYS ALONG THIS SURFACE

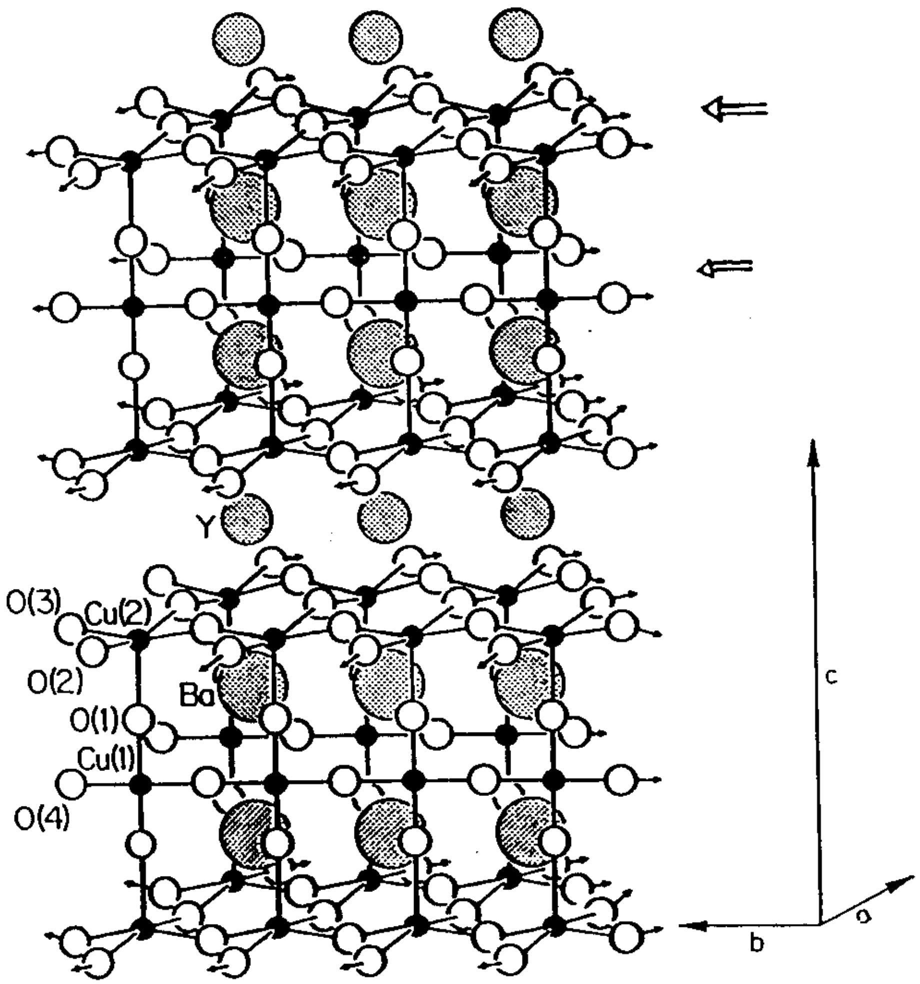


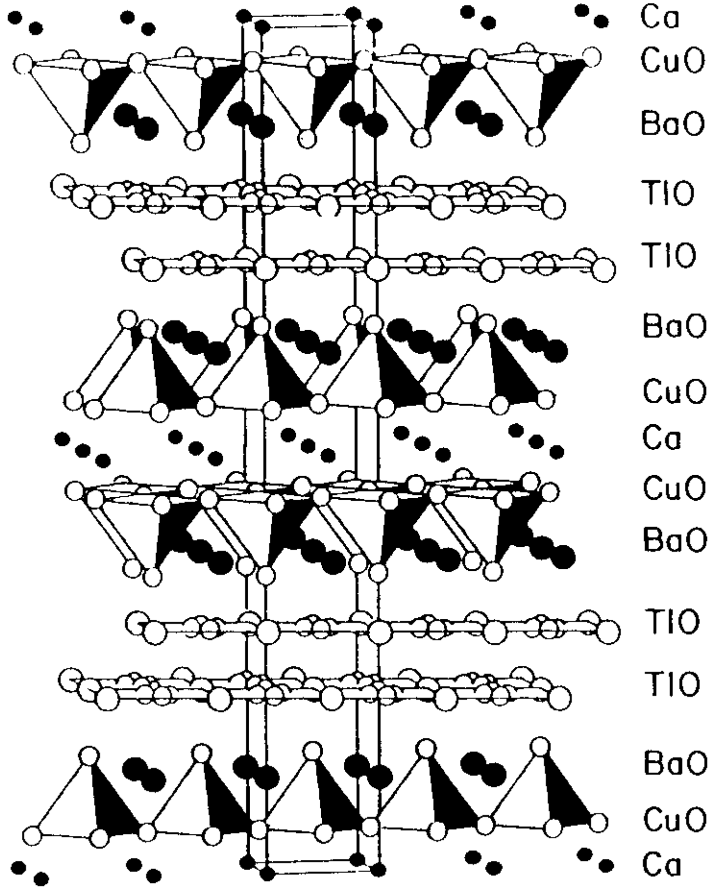

$La_{2-x}M^{2+}_xCuO_{4-\delta}$

M = Ca, Sr, Ba

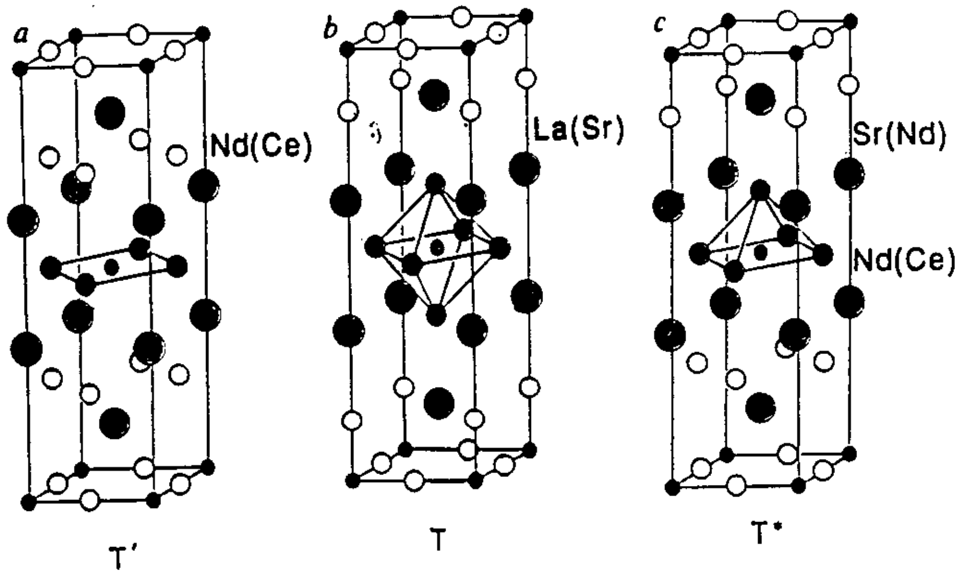
$K_2NiF_4$ structure

$Ba_2YCu_3O_{7-x}$




$Tl_2Ca_1Ba_2Cu_2O_8$




$Nd_{2-x}CeCuO_4$ $La_{2-x}Sr\,CuO_4$ $Nd_{2-x-z}Ce_xSr_zO_4$

Y. Tokura et al. Nature 337, 345 (89)

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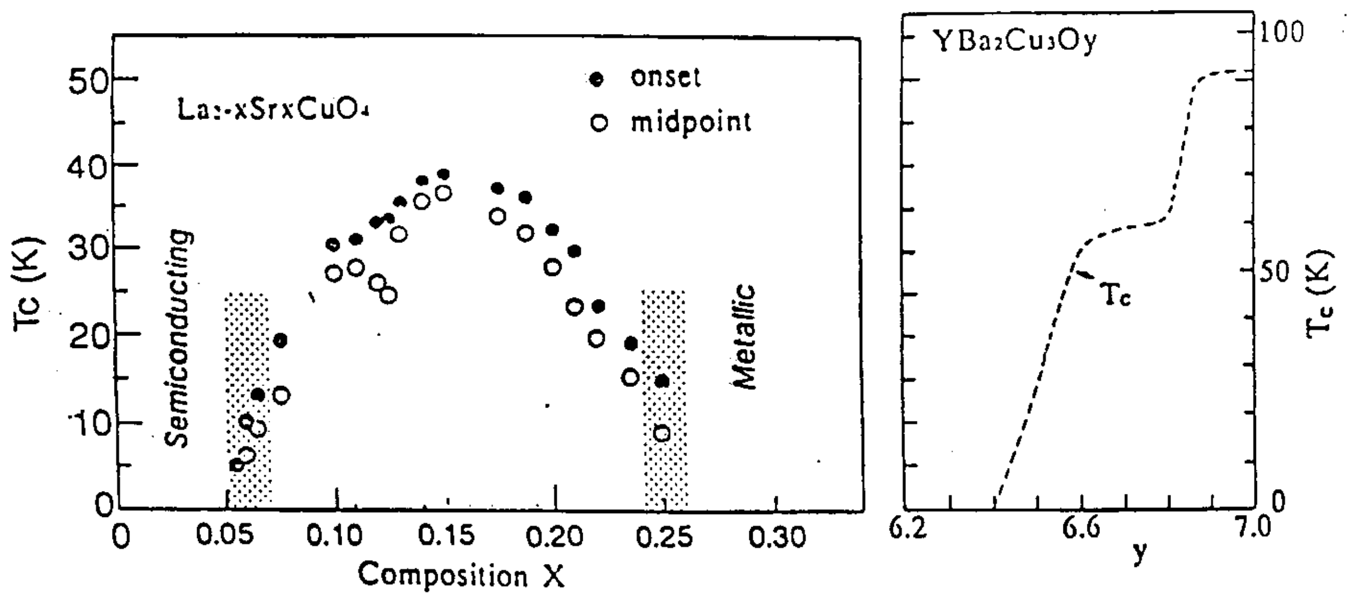



*Fig. 2 Composition dependence of $T_c$ for $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{6+x}$.*

# "Almost" BCS Behavior

- Meissner effect
- Zero resistance
- 2e flux quantization, Andreev reflection, ac & dc Josephson Tunneling
- Excitation gap ( Tunneling, IR, PE)

$$\frac{2\Delta}{k_B T_c} \simeq 2 \div \underline{\underline{8}}$$

- $\Delta C / \chi T_c$ roughly correct

- Ginzburg - Landau theory "works"

  $\Delta(T)$ , $H_c(T)$

  Anisotropy , short correlation length

  $\lambda_\perp / \lambda_\parallel \simeq 5$

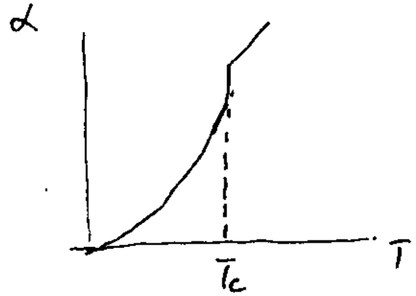
  $\xi_\parallel / \xi_\perp \simeq 10$ → even smaller ~2

- $m^*/m \simeq 3 \div 5$ determined from [illegible]tibility and optical [illegible]

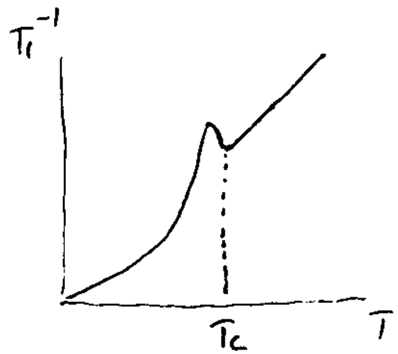
More subtle coherence effects

$$\alpha_{k\uparrow} = u_k a_{k\uparrow} + v_k a^+_{-k\downarrow}$$

"Destructive effect"
e.g. Acoustic absorption




"constructive" effect
e.g.
NMR relaxation

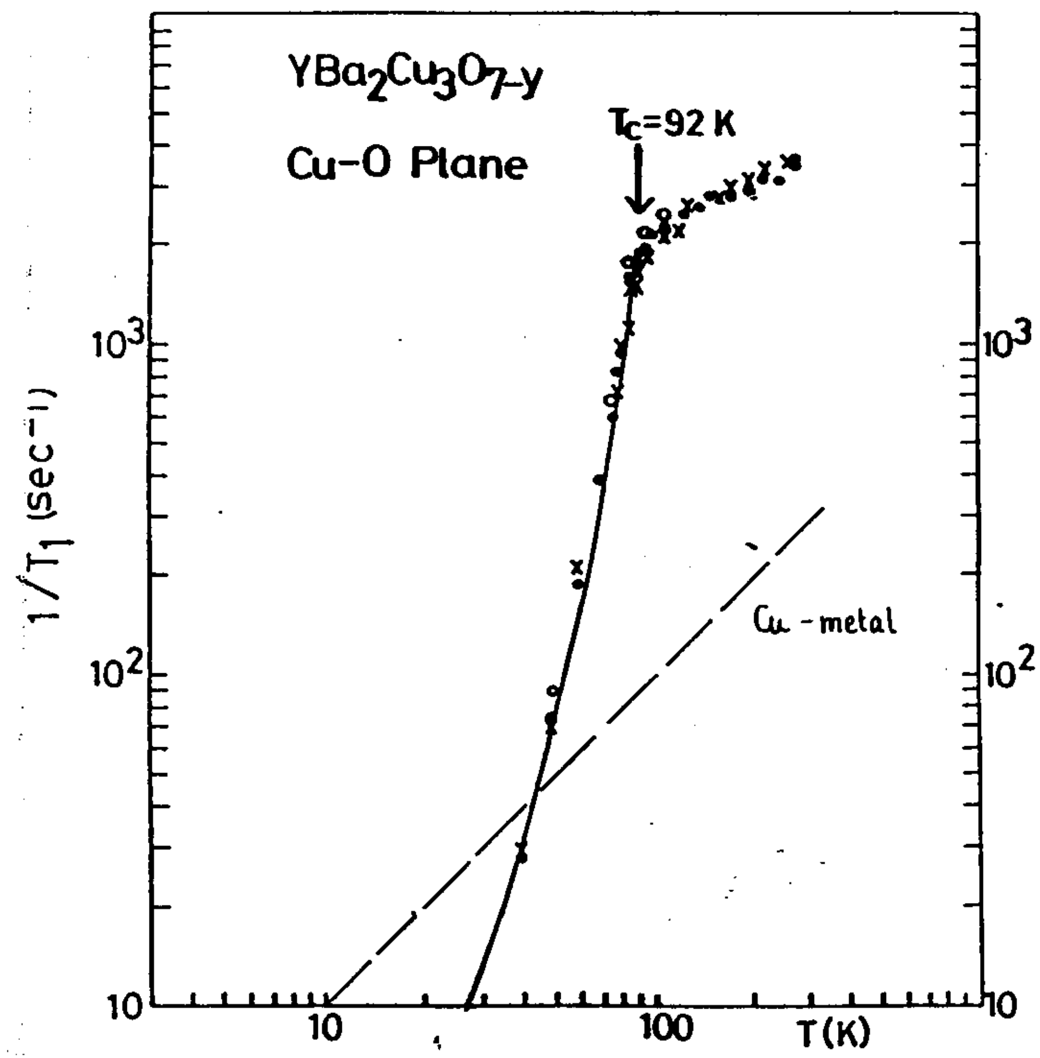


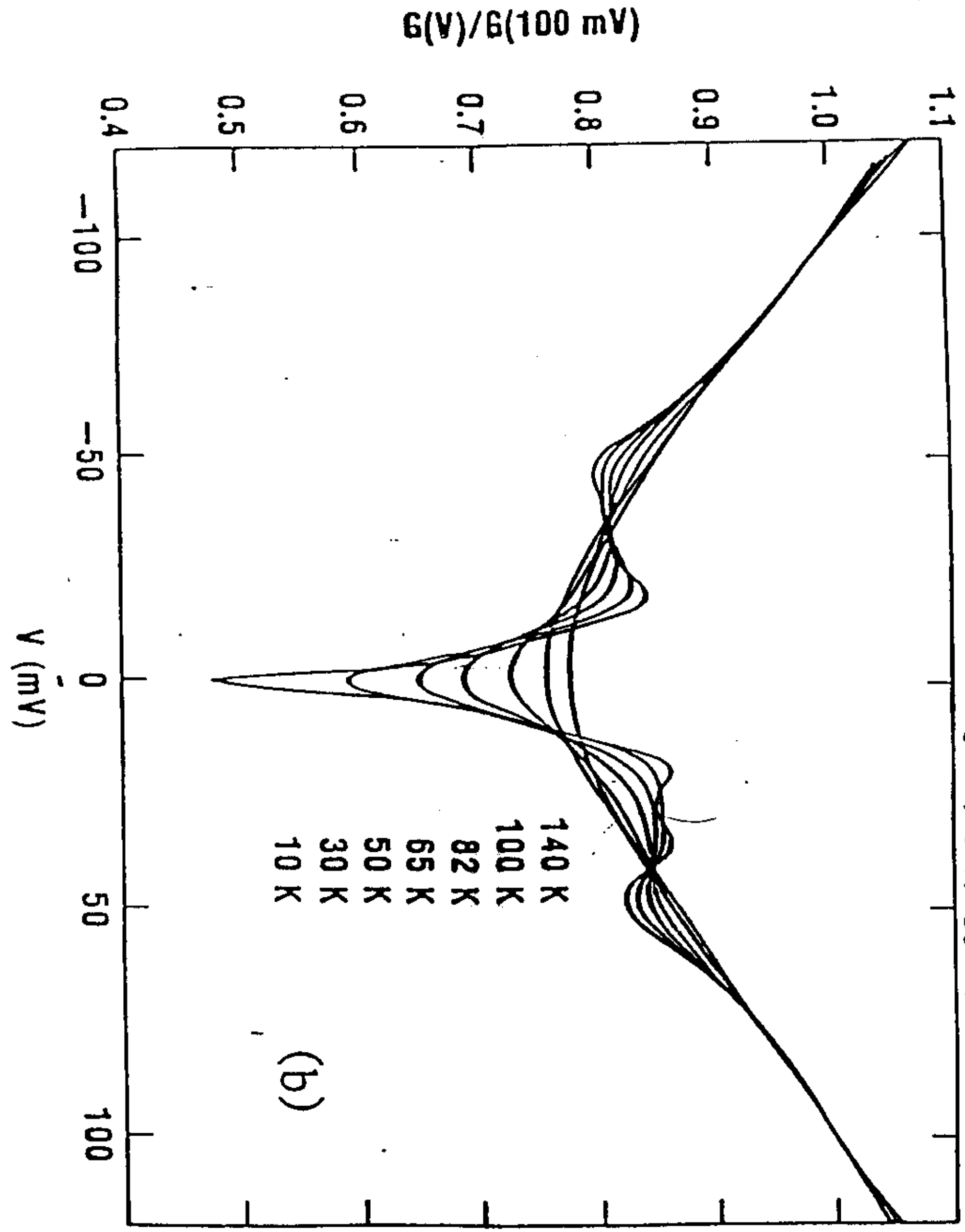

Hebel-Slichter resonance

It has not been observed.

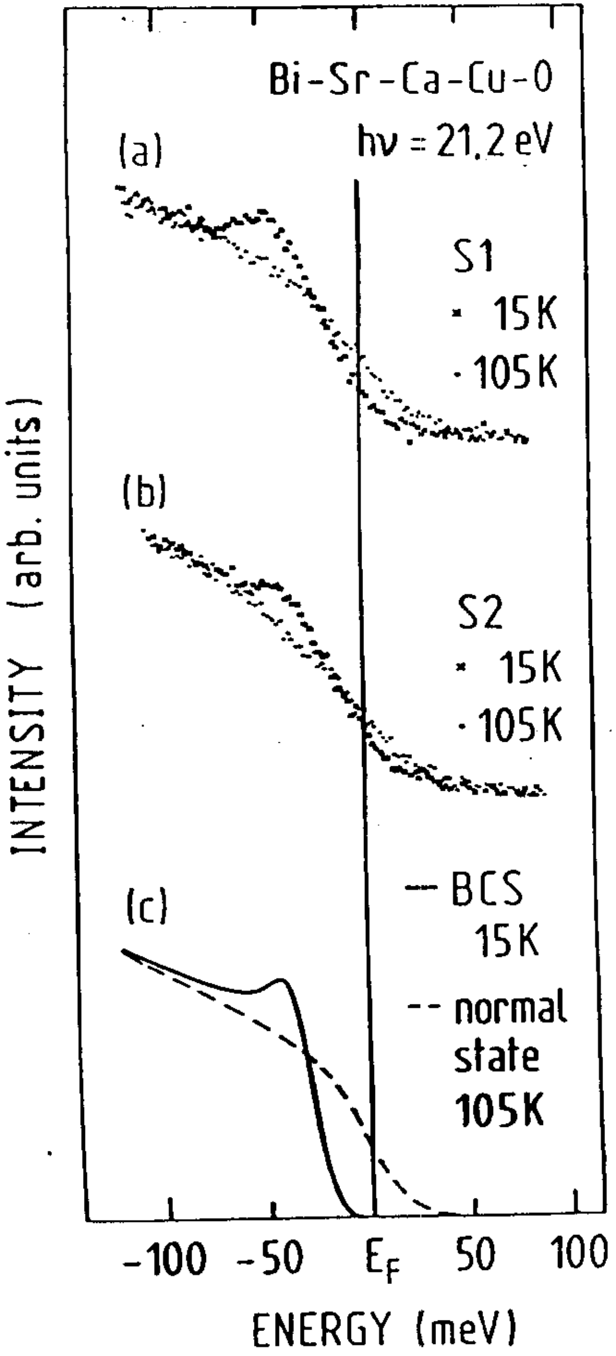
damping effect?

Kitaoka et al.




Gurvitch et al.




Imer et al.

Anomalous "normal state" Properties

* Resistivity

$$\rho_{\parallel} \sim T$$

$$\rho_{\perp} \sim \frac{1}{T} \quad ?$$

* Optical absorption

Drude component + Strong background $\sim \omega^{-1}$

$$\sigma(\omega) = \frac{ne^2\tau^*}{m^*} \frac{1}{1 - i\omega\tau^*}$$

From the width $(\tau^*)^{-1} \sim 2kT$

$\therefore$ the $T$ dependence is lifetime effect, not due to $n/m^*$

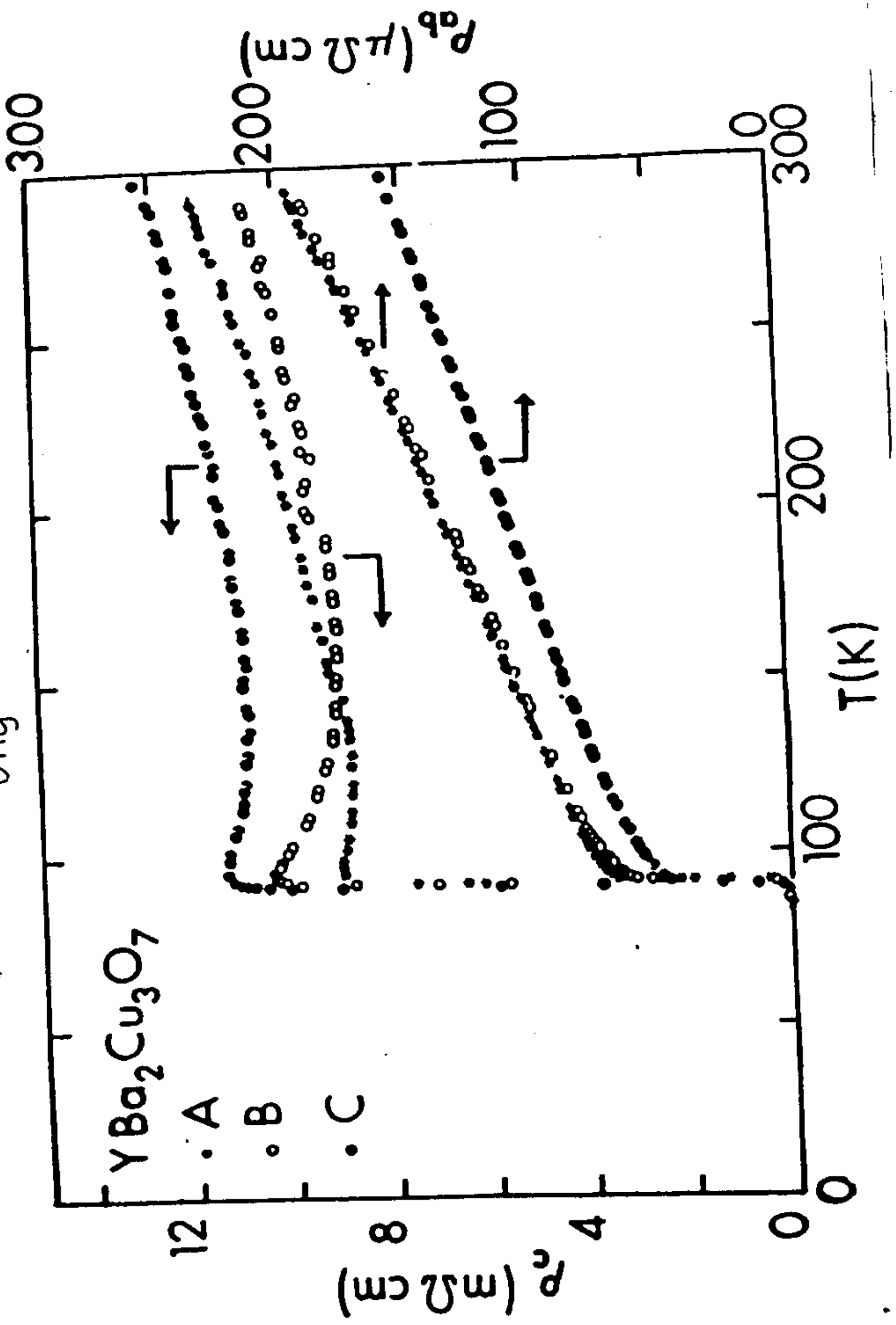
also, $\frac{n}{m^*} \sim \delta/m^*$ not $(1-\delta)/m^*$

* Strong background in Raman scattering up to $4000\,cm^{-1}$

metals: $\sim 20\ cm^{-1}$ particle-hole

* Tunneling conductivity $G = g_0 + g_1 |V|$

Ong et al.



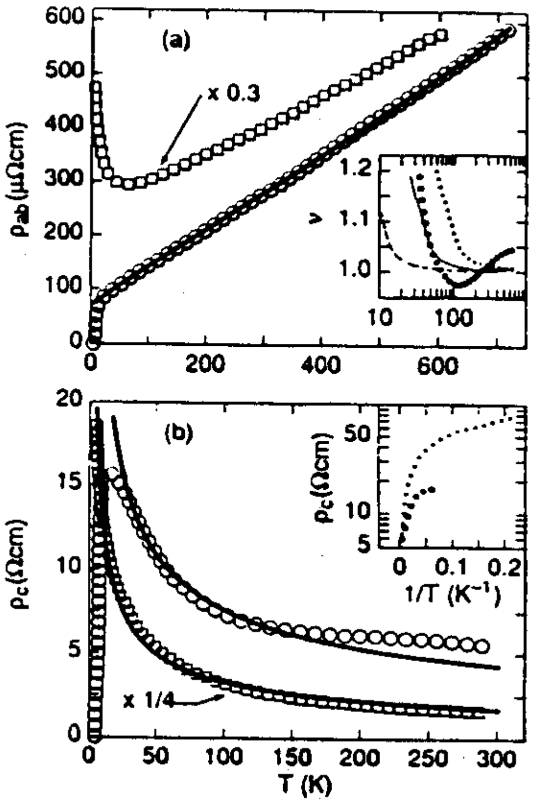
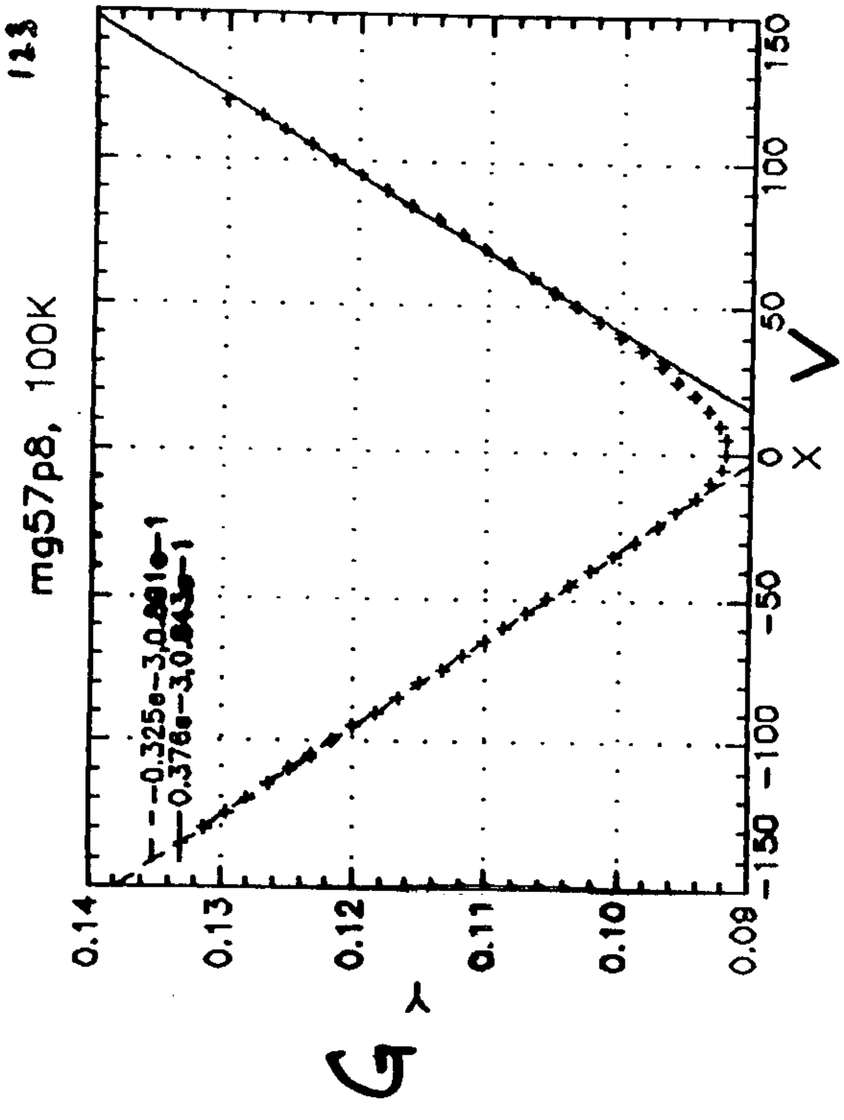




FIG. 1. In-plane (a) and out-of-plane (b) resistivities measured in 2:2:0:1 crystals: a nonsuperconductor (□) grown with Sr/Bi = 1.22 and $P_{O_2}$ = 20%, and a superconductor (○), with Sr/Bi = 1.0 and $P_{O_2}$ = 4%. Curve in (a) is a fit assuming BG; curves in (b) are power-law fits. Inset (a) shows $\nu = d[\ln(\rho_{ab} - \rho_0)]/d[\ln T]$ vs $T$ for the superconducting sample (●) as compared with BG fits with $\Theta_D^* = 10$ K (dashed), 35 K (solid), and 80 K (dotted). Inset (b) illustrates $\rho_c$ is non-Arrhenius.

S. Martin et al. P.R. B41, 846 (90)

01




J. Valles, M. Gurvitch, R. Dynes, A. Cucolo, L. Schneemeyer,

Beasley, Kapitulnik et al.

$G \approx G_0 + G_1|V|$

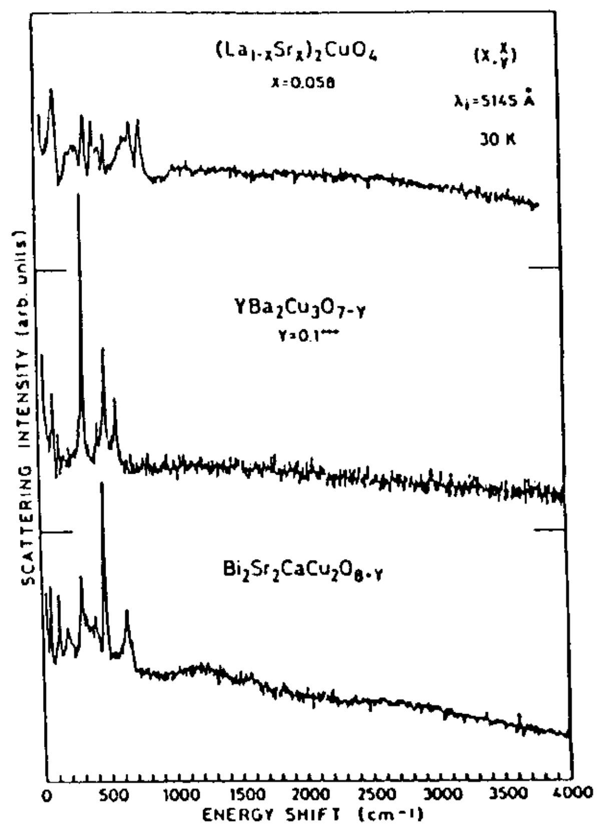



Fig. (9): Raman scattering intensity for various superconducting Cu-O compounds. From Ref. (14), Sugai et al.

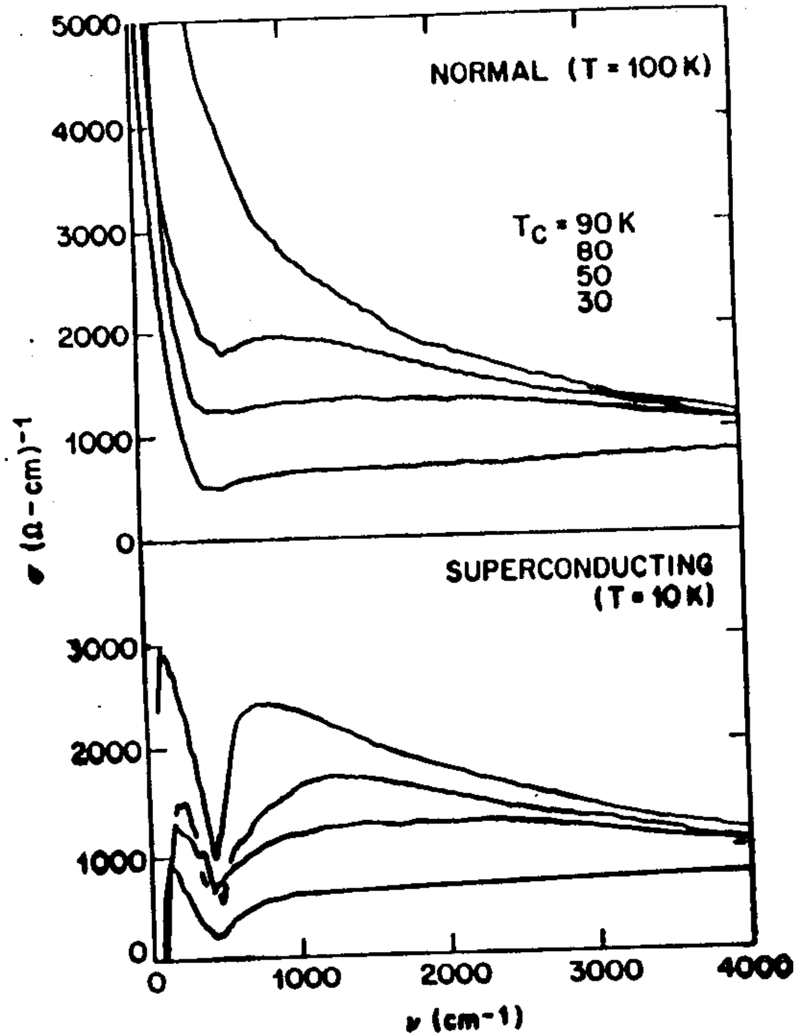
hypothesis:

$\mathrm{Im}\,\chi(\omega) < \begin{cases} S_0\, \omega/T & \text{for } \omega < T \\ S_0 & \text{for } \omega > T \end{cases}$

· Klein et al.

due to continuum excitations

Optical Conductivity:
Orenstein, Thomas et. al.




3 Anomalous features in the Normal state.

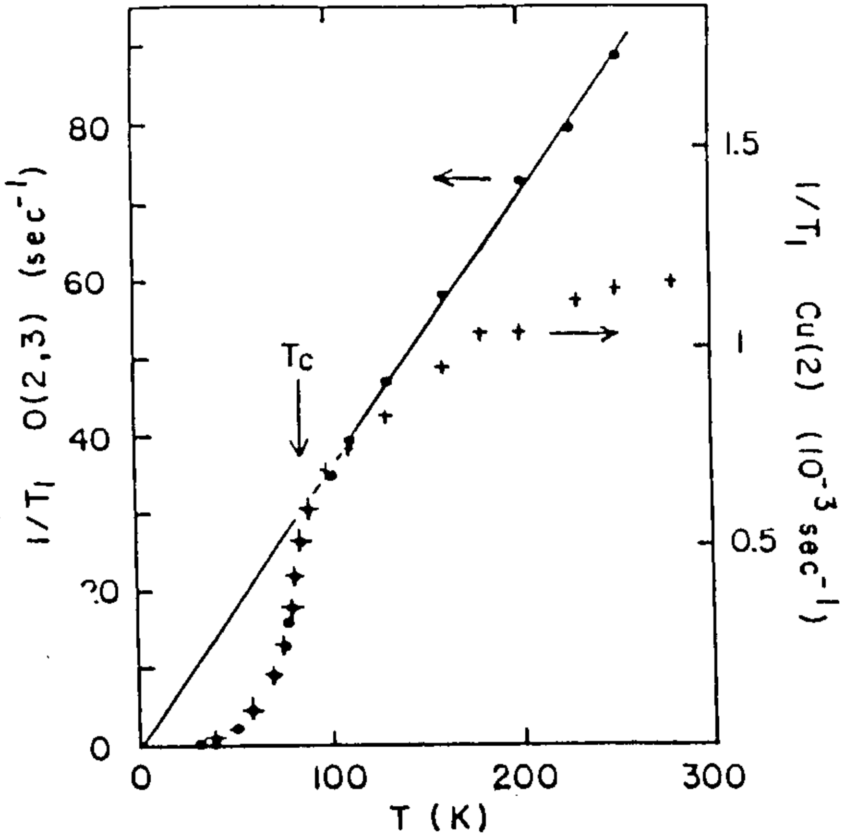



Figure 3. Temperature dependence of $1/T_1$ at the O(2,3) (solid dots) and the Cu(2) (crosses) sites.

Normal state: $^{17}O$ $\frac{1}{T_1} \sim T$, Korringa

$^{63}Cu$ much larger, ~~not Korringa~~

Superconducting State.

No Hebel-Slichter resonance

\# NMR relaxation

$^{89}Y$, $^{17}O$ Korringa like

$T_1^{-1} \sim T$, [illegible]

$T_1^{-1} \sim$ # of excitation

$^{63}Cu$ the same plane

not Korringa like

much faster

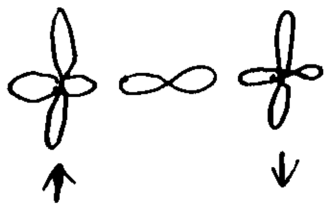
Millis et al. $\chi(\frac{\pi}{a}, \frac{\pi}{a})$ enhanced

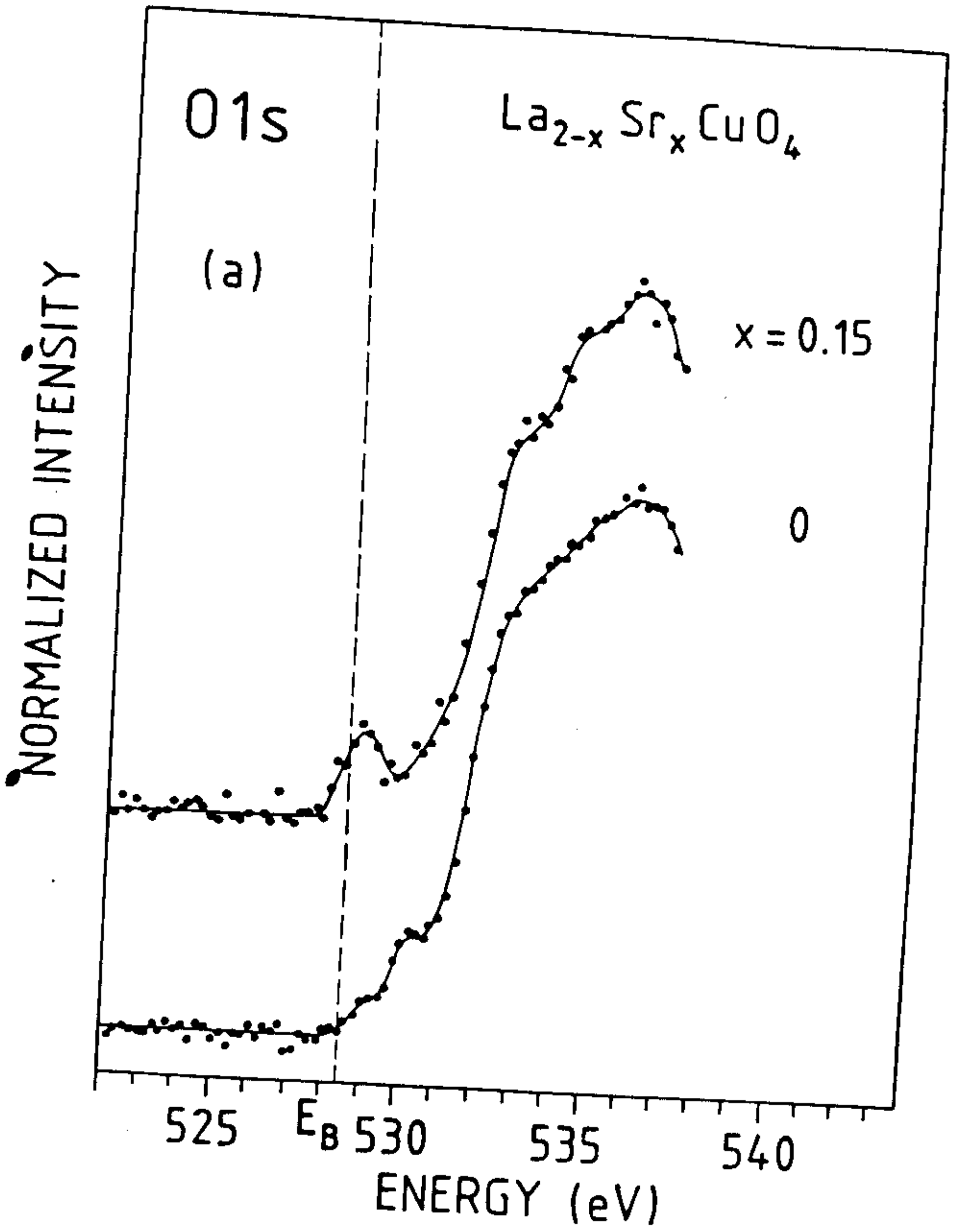
AF correlation

$^{63}Cu$ is sensitive to this part

$^{17}O$, $^{89}Y$ - not . due to symmetry

one component spin system





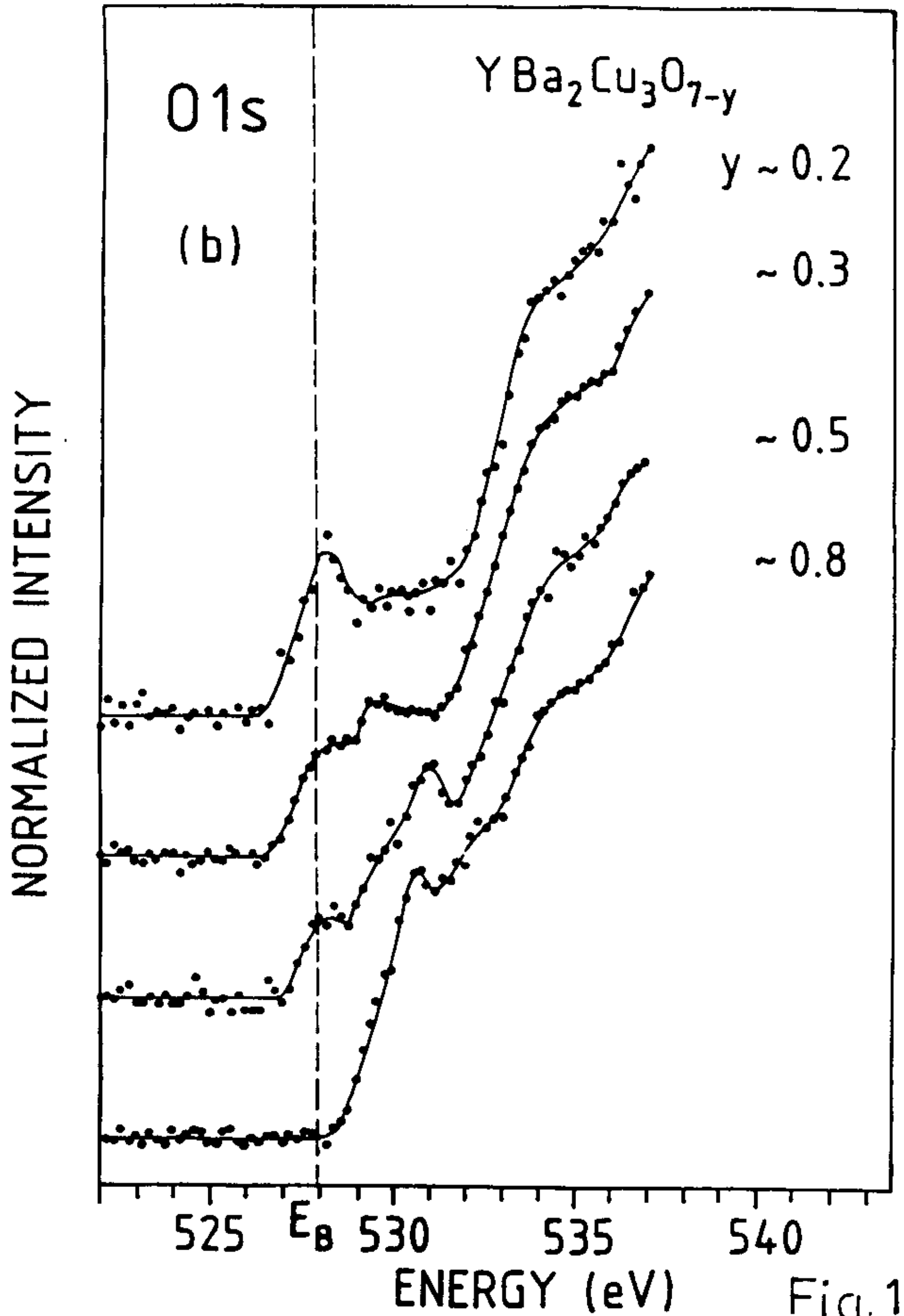



Fig. 1b

N. Nücker et al. EELS

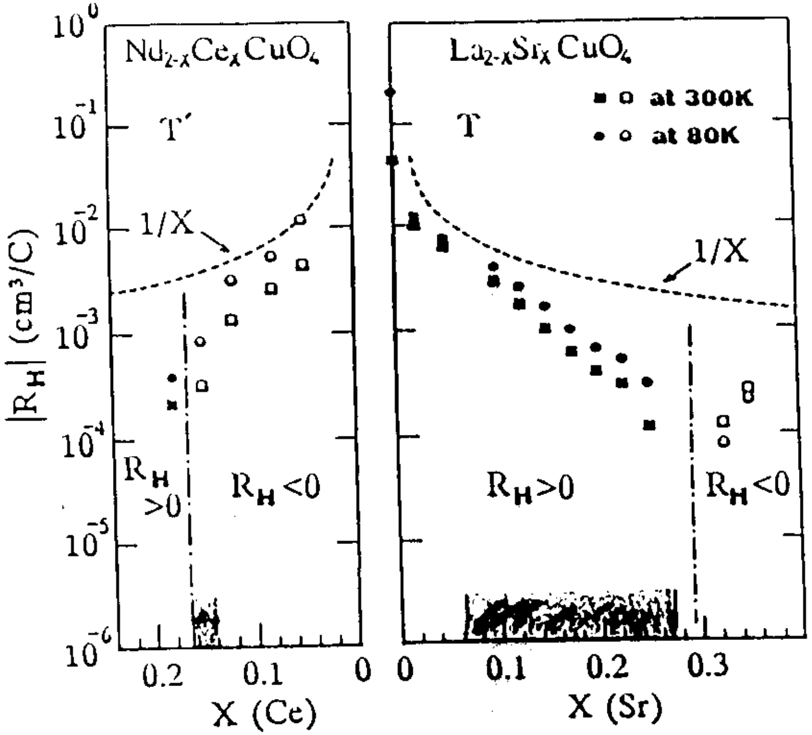


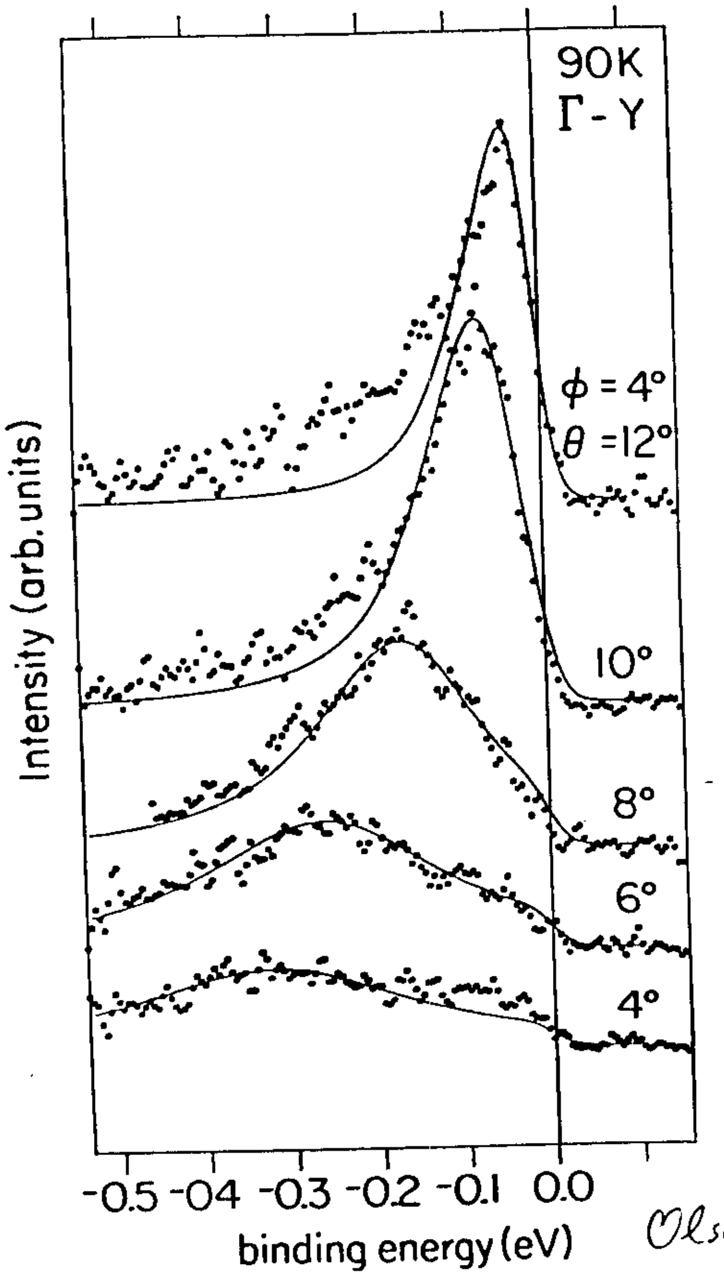

Fig. 8 The absolute value of the Hall coefficient as a function of Ce composition for reduced $Nd_{2-x}Ce_xCuO_{4-y}$. The same ploted for $La_{2-x}Sr_xCuO_4$ are show for composition. The shaded are a indicates composition region where superconductivity is observed.

~~$R_H \sim \frac{1}{nec}$~~

1) consistent with Mott - Hubbard pict

2) deviation from 1/X

3) consistent with disappearance of lin law and magn. correlations




Olson et al.

Fig. 5

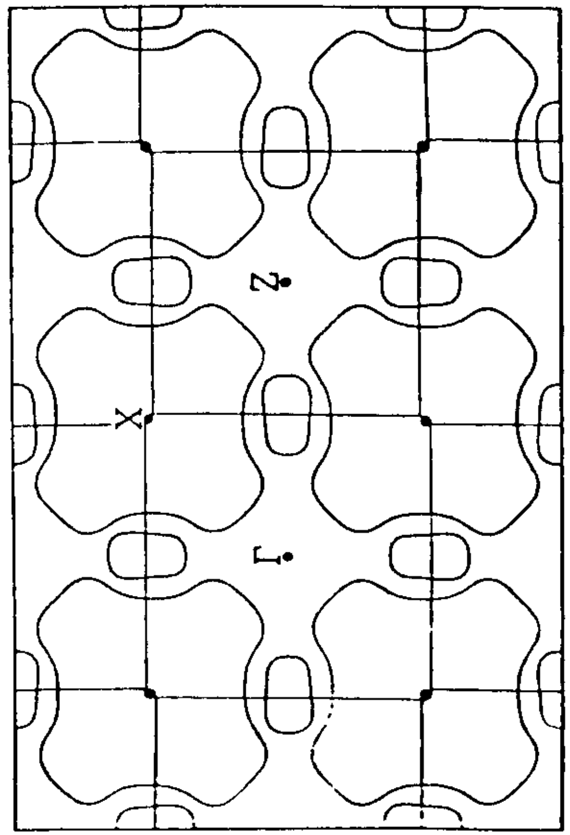
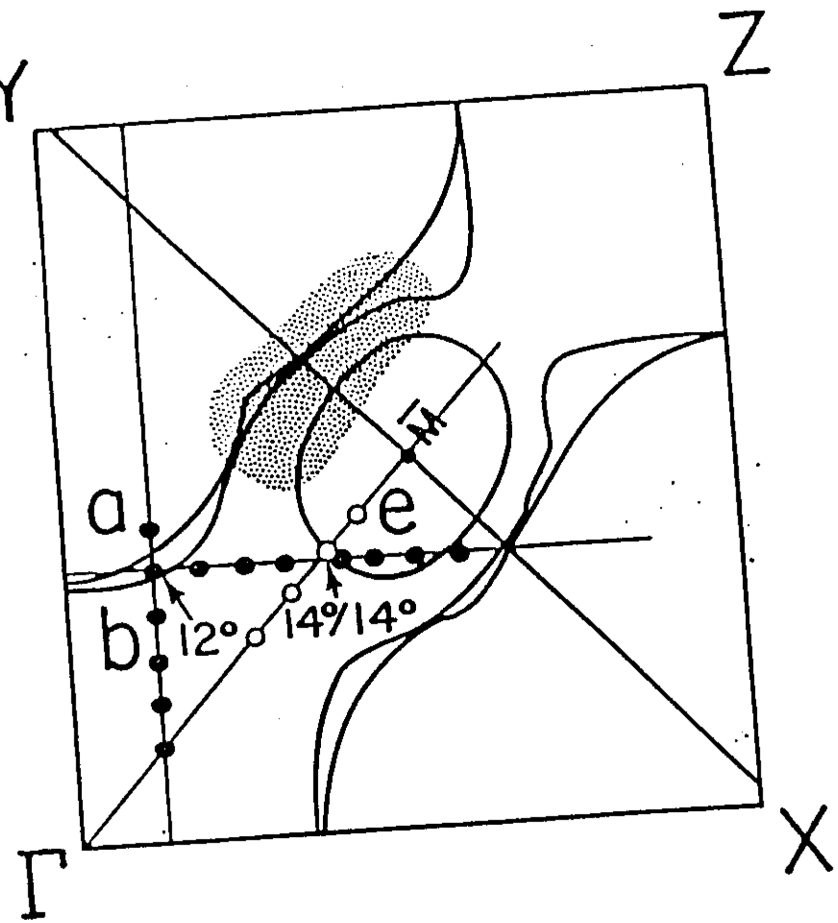
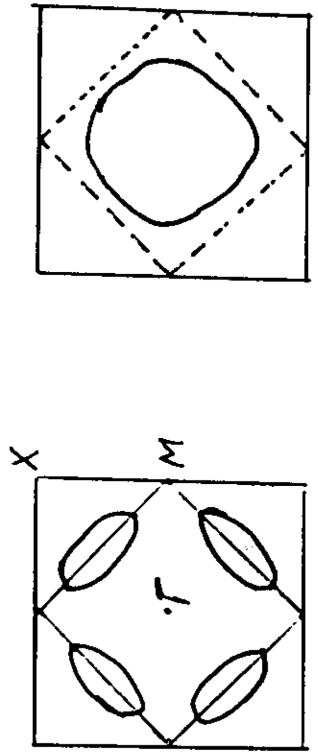


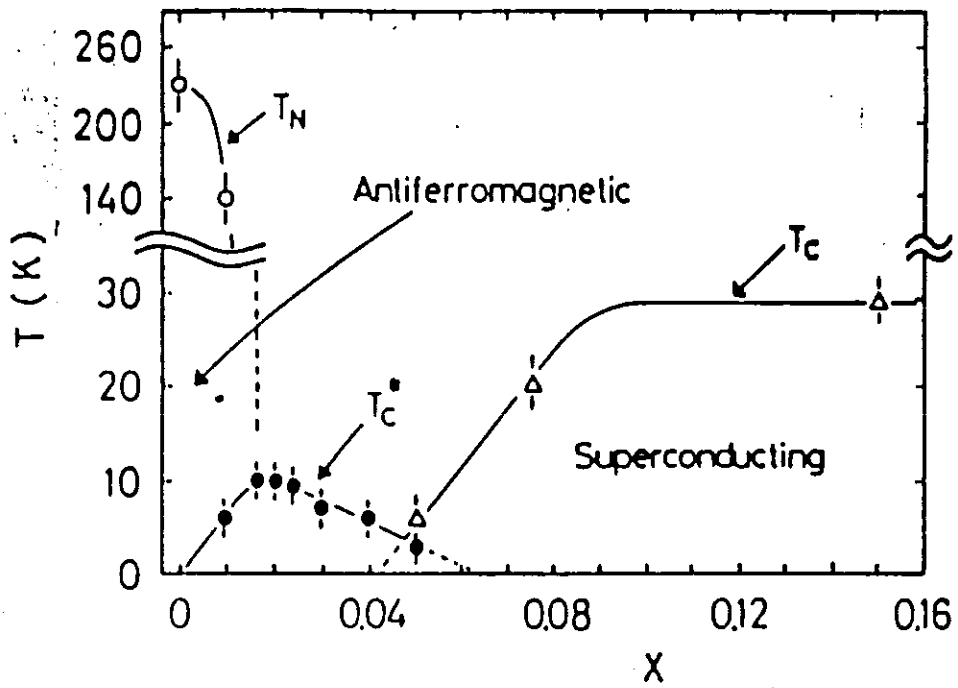

FIG. 3. Calculated Fermi surfaces in the (001) plane. For clarity, we show only one of the two large, nearly degenerate X-centered sheets arising from the Cu-O bonds. The small rounded rectangular electron pockets midway between Γ and Z arise from Bi-O states.



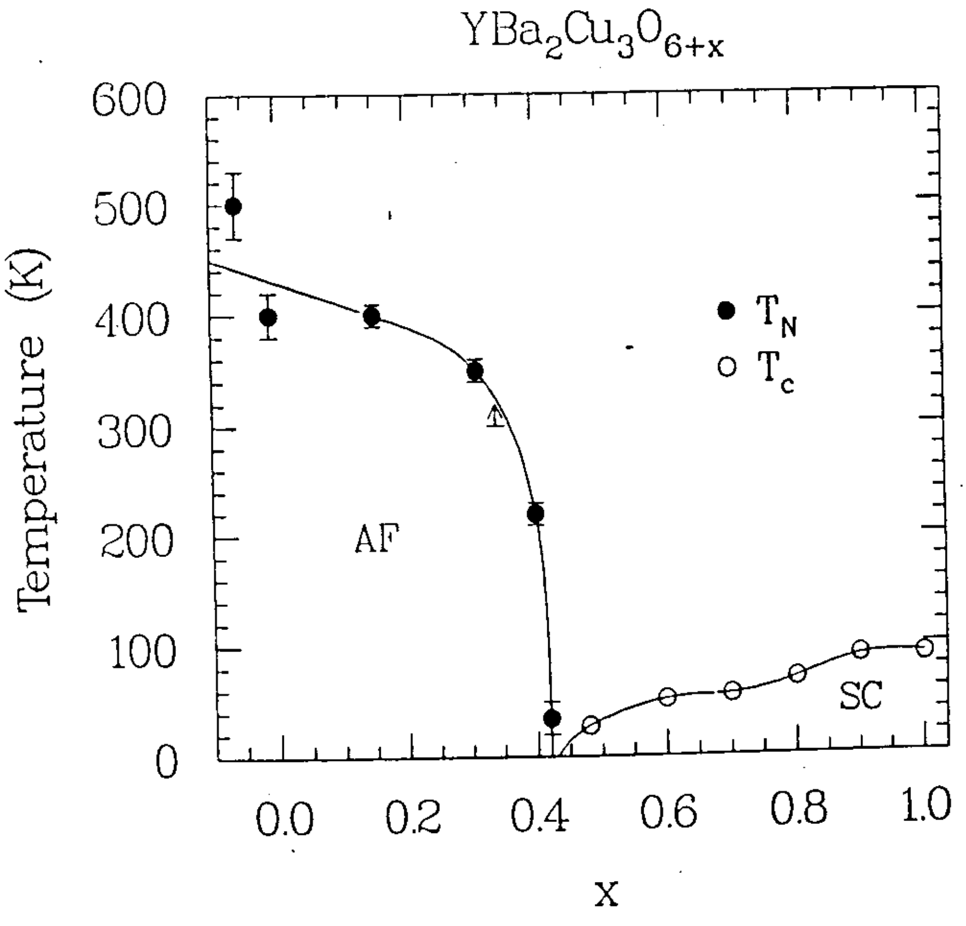



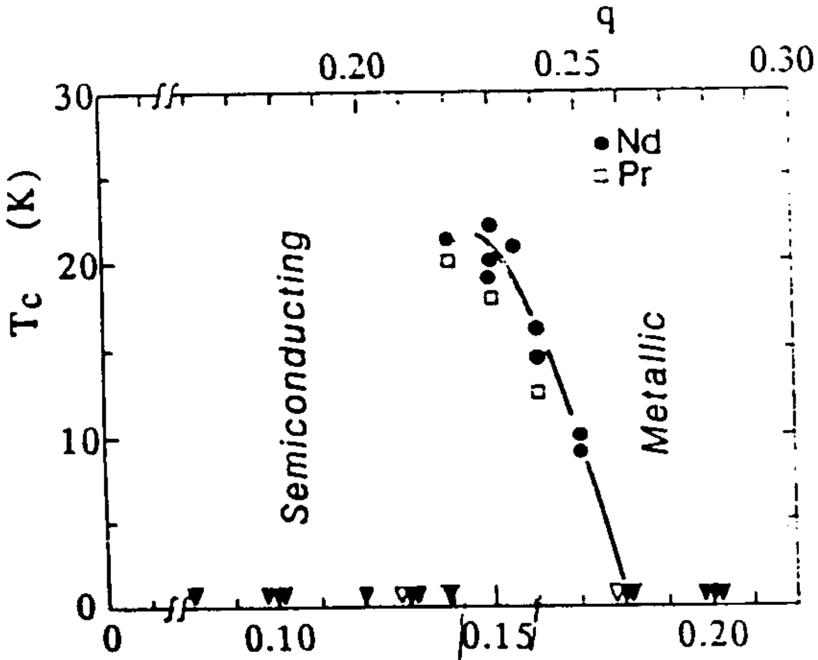

(b)

(a)




*Low Temp. Phase diagram for $(La_{1-x}Ba_x)_2CuO_4$*
*Kitagawa et al. Physica 151-153, 12, 1964*






$T_N = 300K$ 240K

Not magnetic above 4K

$Ln_{2-x}Ce_x\,CuO_{4-y}$

H. Takagi et al. PRL 62, 1197(89)

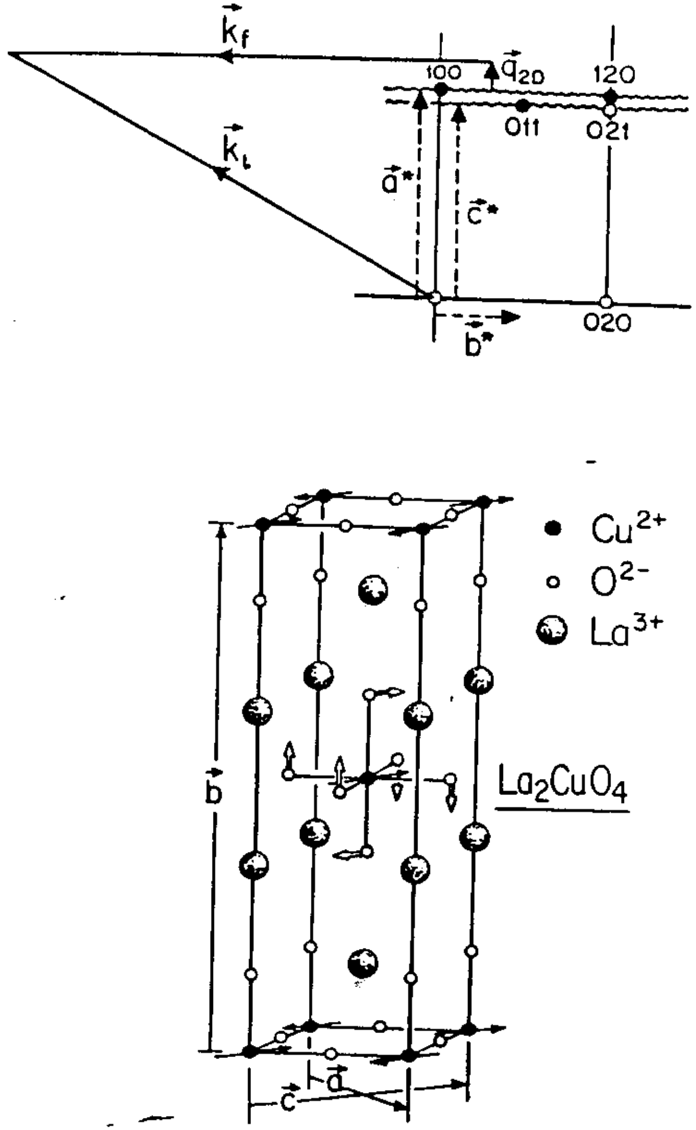



FIGURE 1

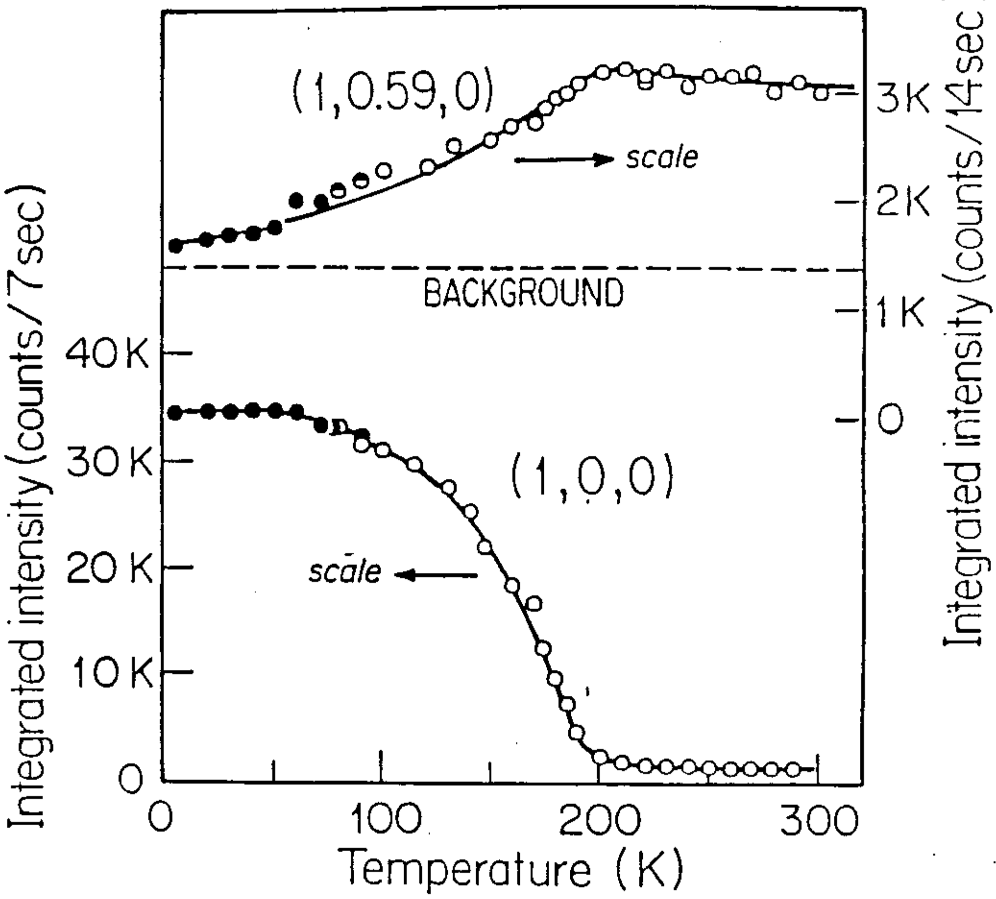
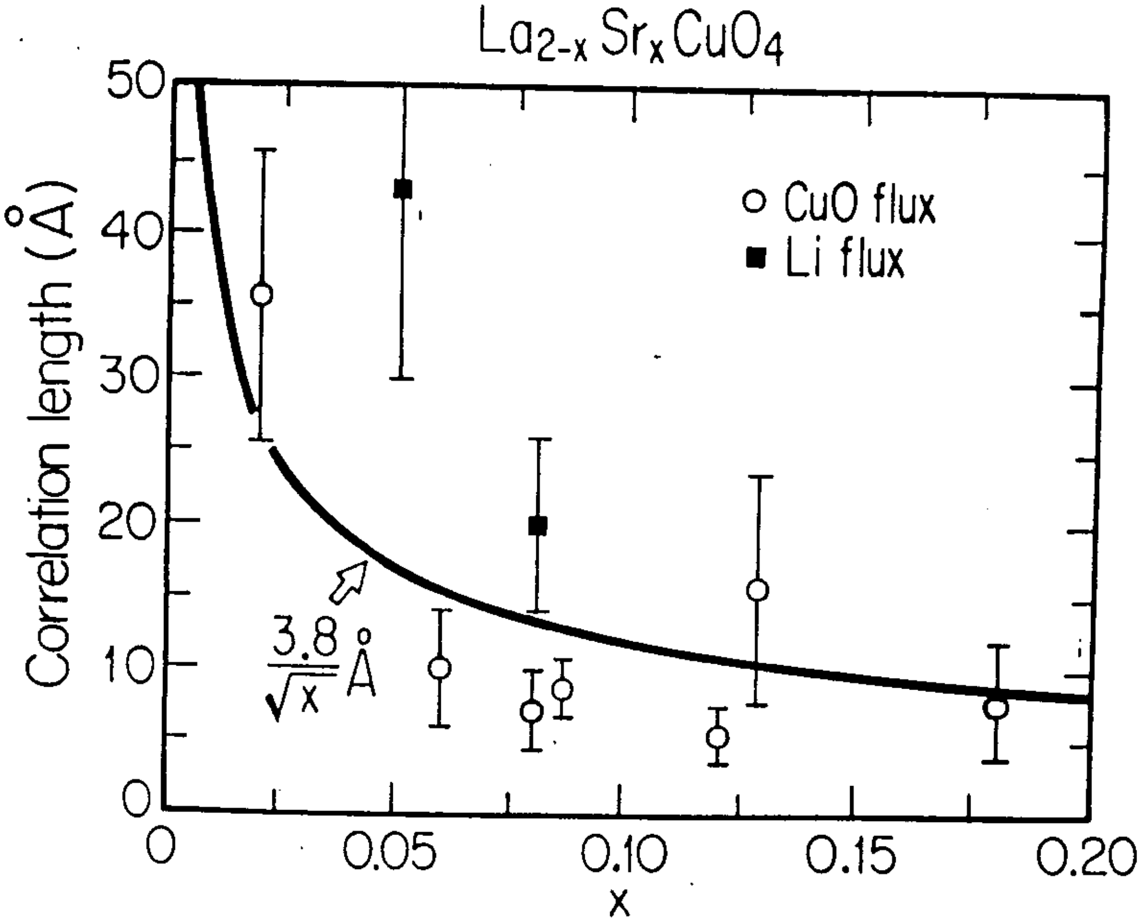

(1,0.59,0)
scale
BACKGROUND
(1,0,0)
scale
Integrated intensity (counts/7sec)
Integrated intensity (counts/14sec)
Temperature (K)
0
100
200
300
0
10K
20K
30K
40K
1K
2K
3K

FIGURE 2


$La_{2-x}Sr_xCuO_4$
○ CuO flux
■ Li flux
$\frac{3.8}{\sqrt{x}}$ Å
Correlation length (Å)
x
0
0.05
0.10
0.15
0.20
10
20
30
40
50

Summary of Experiments

Superconducting properties

BCS like

Normal state properties

Abnormal

Non-FL behavior

Angle-resolved photoemission

Well-defined Fermi surface

Strong interplay between Magnetism and SC.



## Questions to be answered

1. Scenario for SC

BCS pairing? Bose condensation? Bipolarons? Something entirely new?

2. What is the interaction responsible for SC?

Electron-phonon? Coulomb interaction in terms of charge or magnetic fluctuations

3. What is the appropriate model?

Charge transfer? Hubbard? one, two, or three bands?

4. What is the theoretical basis?

Weak-coupling theory based on Landau Fermi-Liquid theory

or

Strong-coupling theory with entirely new concepts?

# Attempts in constructing Hi-Tc theory

- Phonon
  - Strong coupling
  - Bipolaron
  - Jahn-Teller
- Electronic
  - charge fluctuations
    - charge transfer exciton $[Cu^{2+}O^{2-}] \to [Cu^{+}O^{-}]$
    - plasmon
    - two band (localized vs extended) mode
  - Magnetic fluctuations
    - weak coupling SDW
    - strong coupling two (three) band models
    - One-band Hubbard model $\Rightarrow$ $\boxed{\text{RVB}}$
    - t-J model $\Rightarrow$ $\boxed{\text{Spin wave theory}}$

## $CuO_2$ plane is responsible for SC

1) "Common" structure, not CuO chains

2) Anisotropy

Normal state: $\rho_\perp / \rho_\parallel \div 10^{-2} \div 10^{-1}$, $\rho_\parallel \sim T$, $\rho_\perp \sim 1/T$

Superconducting state: $\xi_\perp / \xi_\parallel \sim 10^{-1}$

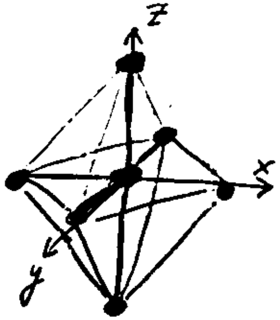
3) Strong correlation of $T_c$ with distance between $CuO_2$ layers


Correlation of $T_c$ with number of $CuO_2$ layers

4) 2D nature of band structure

5) Interplay between 2D magnetism and SC

$\overset{6+}{La_2}\,\overset{2+}{Cu}\,\overset{8-}{O_4}$




● Cu
• O

$Cu^{2+}$, $3d^9$

Cubic harmonics

$T_{2g}$, $xy$, $xz$, $yz$

$E_g$, $x^2-y^2$, $3z^2-r^2$ ✓

Jahn-Teller splitting

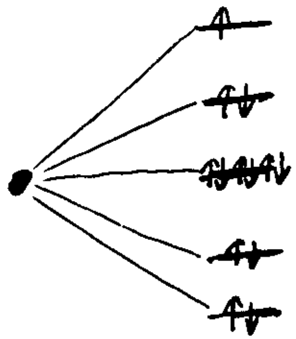
Cu-O 2.4 Å ∥z

1.9 Å xy plan

Cu-O hybridization

$Cu^{2+}$

$3d^9$



$E_g^*$(antibonding) $x^2-y^2 \Leftrightarrow O_{2p}$

$3z^2-r^2 \Leftrightarrow O_{2p}$

$T_{2g}$(nonbonding) $xy$, $xz$, $yz$

$E_g$(bonding) $O_{2p} \Leftrightarrow 3z^2-r^2$

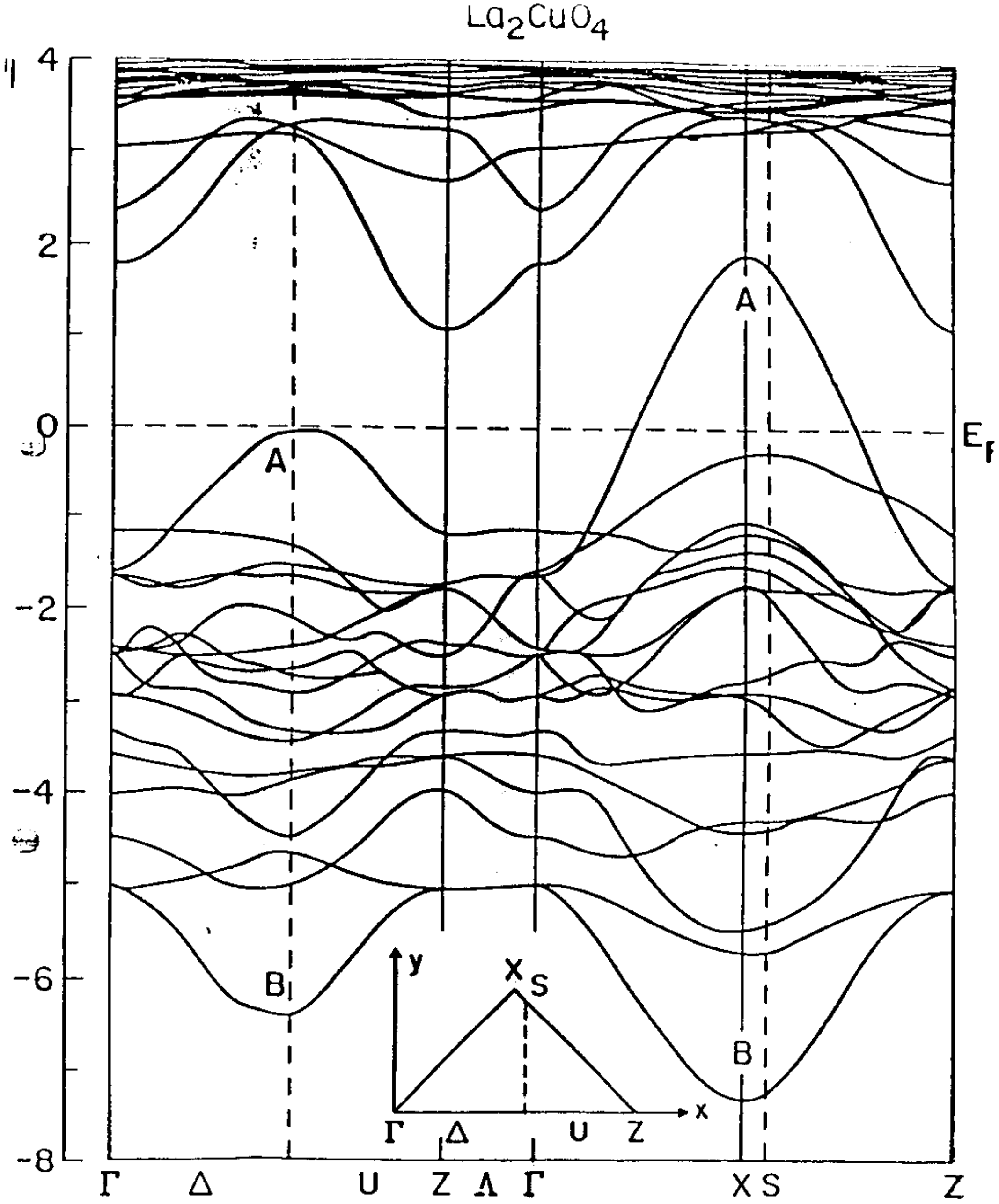
$O_{2p} \Leftrightarrow x^2-y^2$

Half-filled, should be a <u>METAL</u>

but it is not !

Lower symmetry? AF order? Mott insulator

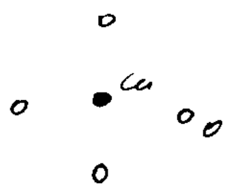
Mattheiss. Phys. Rev. Lett. <u>58</u>, 1028 (1987)




25

Model Hamiltonian for $CuO_2$ plane

$$H = -\sum_{\langle i l\rangle \sigma} t_{il} \left( d_{i\sigma}^{+} p_{l\sigma} + c.c. \right)$$




$$- \sum_{\langle l l'\rangle \sigma} t'_{ll'} \left( p_{l\sigma}^{+} p_{l'\sigma} + c.c. \right)$$

$$+ \epsilon_d \sum_{i,\sigma} d_{i\sigma}^{+} d_{i\sigma} + \epsilon_p \sum_{l,\sigma} p_{l\sigma}^{+} p_{l\sigma}$$

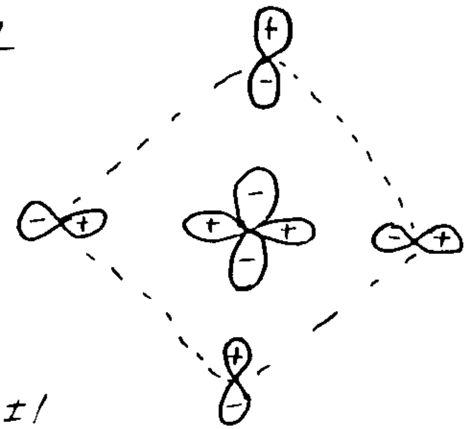
$$+ U_d \sum_i n_{di\uparrow} n_{di\downarrow} + U_p \sum_l n_{pl\uparrow} n_{pl\downarrow}$$

$$+ V \sum_{\langle i l\rangle, \sigma, \sigma'} n_{di\sigma} n_{pl\sigma'}$$

| | | |
|---|---|---|
| $\epsilon_p - \epsilon_d$ | $= 3.6$ eV | $2.75 \div 3.75$ eV |
| $t$ | 1.5 eV | 1.5 eV |
| $t'$ | 0.65 eV | 0.65 eV |
| $U_d$ | 10.5 eV | 8.8 eV |
| $U_p$ | 4 eV | 6 eV |
| $V$ | 1.2 eV | $< 1$ eV |
| | ...ertsen et al | Fischer & Sawatzky |

Effective one-band model

Zhang & Rice




$$\hat{P}_i = \frac{1}{2} \sum_l \zeta_{il} P_l$$

$$\zeta_{il} = \pm 1$$

$$\phi_i^{s,t} = \frac{1}{\sqrt{2}} \left( \hat{P}_{i\uparrow} d_{i\downarrow} \mp \hat{P}_{i\downarrow} d_{i\uparrow} \right)$$

$$E^t - E^s \simeq 16 \cdot \frac{t_{pd}^2}{\Delta}$$

Wannier state of singlet

* Emery & Reiter . objection
  Exact solution on FM background
  Different from singlet, $\langle S \rangle \neq 0$

* Pang, Xiang, Su, Yu
  "Exact" solution can be reproduced by combining singlet & triplet states

* NMR seems to show one
  ...tation

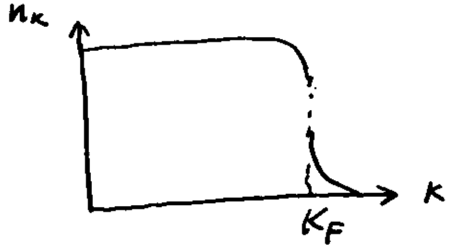
Two different schools of thoughts

$U=0$ fixed point, weak coupling BCS theory

* Landau Fermi-Liquid Theory is valid

well-defined quasiparticles

Luttinger theorem - jump in the momentum distribution at Fermi Level



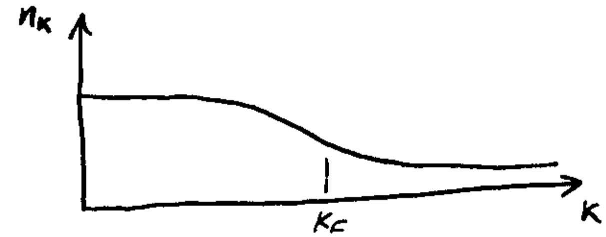

$U=\infty$ fixed point, strong coupling Mott insulator

* Fermi-liquid behavior break down

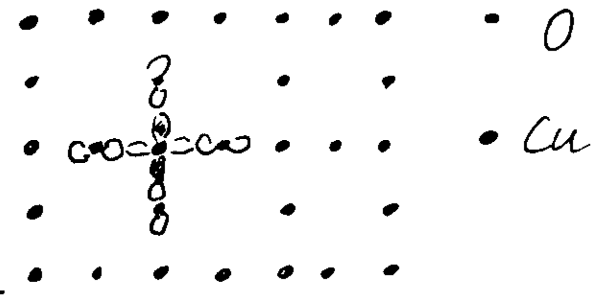
No well-defined quasiparticles

No jump in the momentum distribution

Essentially new physics




## $CuO_2$ layers




½ filled n.n.

tight binding band

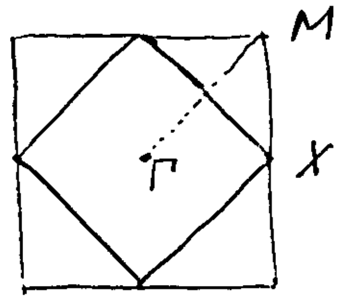
$$\varepsilon(\vec{k}) = 2t(\cos k_x a + \cos k_y a)$$

$t \simeq 0.5$ eV

## Fermi Surface

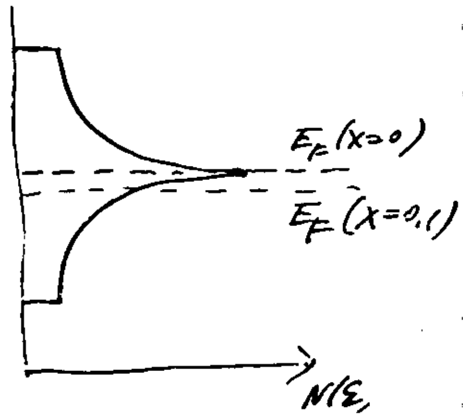
a) Saddle Points

b) Perfect Nesting



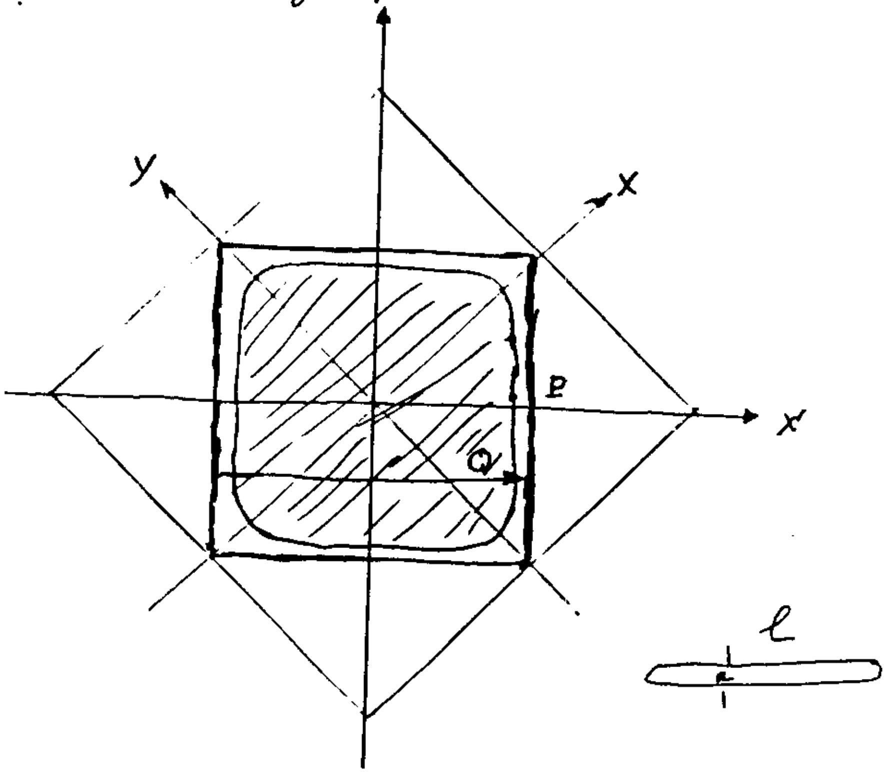

favor distortion with wavevector ΓM

Saddle-points give a van Hove Logar. Singularity at $\varepsilon = E_F$



"Spin Bag" model of J.R. Schrieffer, X.G. Wen, S.C. Zhang

1. SDW background, $\Delta_{SDW}$
2. Nesting vector is fixed
3. Doping reduces local gap $\Delta_B$
4. "Sharing Bag" lowers energy




$\ell \sim \xi_{SDW} = \frac{\hbar v_F}{\pi \Delta_{SDW}}$, $\quad \Delta_0 \approx \Delta_{SDW}\, e^{-\frac{t}{\alpha' j}}$

Effective Hamiltonian in strong coupling limit

$U \gg t$, $\quad \delta = 1 - n \ll 1$

Canon. transform. $H_H \to H_{eff} = e^{iS} H_H e^{-iS}$

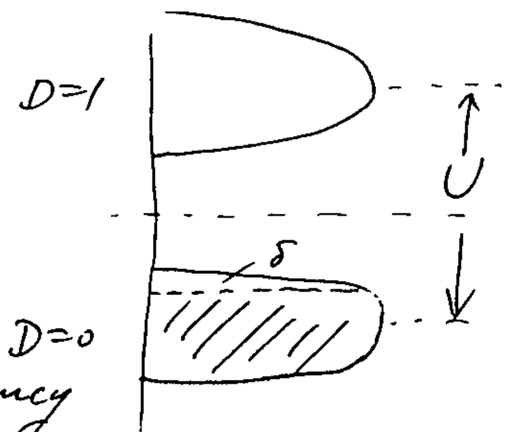
$T \to T_{hole} + \underset{0}{\underset{\shortparallel}{T_{mix}}} + \underset{\text{project out}}{\underset{\shortparallel}{T_{double\ occ.}}}$

$$\boxed{\begin{aligned} H_{eff} = \; & P_{D=0}\,(-t)\sum_{\substack{\langle ij\rangle \\ \sigma}} c_{i\sigma}^{+} c_{j\sigma}\, P_{D=0} + h.c. \\ & + J\sum_{\langle ij\rangle}\left(\vec{S}_i\cdot\vec{S}_j - \tfrac{1}{4}\right) \\ & + O\left(\delta^2,\ t^2/U^2,\ \delta t/U\right) \end{aligned}}$$

t – J model

$J = 4t^2/U$

$H_{eff}$ operates in Hilbert subspace without double occupancy



# Ground State of Hubbard or $t$-$J$ models.

## 1D Lieb-Wu Bethe Ansatz solution

$n=1$, singlet state, no LRO

$n \neq 1$ non-FL behavior

Excitations: spin ½ fermion
no gap

Inspiration for RVB

## 2D No exact solution

$T=0$ LRO ? yes, probably

$n=1$ Neél order + Quantum FL.
RVB

$\langle S_{iz} \rangle$ , $\langle C_{i\uparrow}^{+} C_{j\downarrow}^{+} - C_{i\downarrow}^{+} C_{j\uparrow}^{+} \rangle$

AF singlet pairing

$n \neq 1$ their coexistence



## Resonant Valence Bond RVB

P.W. Anderson
1973, 1987

No (or very few) $S=\frac{1}{2}$ AF

Maybe Neel state is not the ground state

Heisenberg AF

$$\mathcal{H} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \quad , \quad J > 0$$

1D case:

Néel state: ↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓

$$\langle \mathcal{H} \rangle = -\frac{1}{4} NJ$$

Singlet pairs: (↑↓)(↑↓)(↑↓)(↑↓)

$$| \rangle = \frac{1}{\sqrt{2}} (\alpha_i \beta_j - \alpha_j \beta_i)$$

$$\langle | \mathcal{H} | \rangle = -\frac{3J}{4} \cdot \frac{N}{2} = -\frac{3}{8} NJ$$

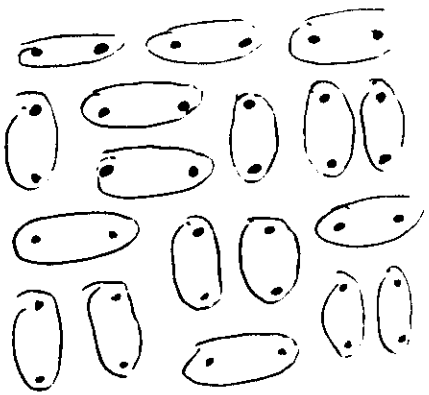
Exact Bethe Ansatz solution

$$\boxed{E_g = -0.443 \ NJ}$$

15% better

Linear combination of all possible singlet pairs

$|\psi\rangle = \sum_{p} (ij)(kl)(mn) \cdots$



No spontaneous magnetization

All possible (including well-separated) pairs

Quantum Spin Liquid as opposed to "spin crystal" – Neel state

Triangular lattice. Yes

Square lattice. ? frustration

What happens upon doping

Excitations:

SPINON, $S = 1/2$, $Q = 0$

Holon, $S = 0$, $Q = e$

Hole = spinon + holon

2) Quantum Antiferromagnetic State

Finite size calculation

AF LRO $\langle S_z \rangle \sim 0.3$ instead of $1/2$

Neel state + Quantum Fluctuations

SPIN WAVE THEORY

$1/S$ expansion

Nonlinear $\sigma$-model

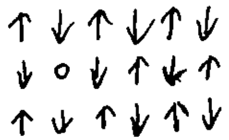
$\langle \vec{S}_i \cdot \vec{S}_j \rangle$ correlation function

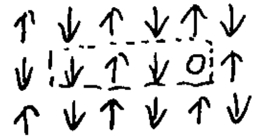
Chakravarty, Halperin, Nelson

$\langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle \simeq -0.334$

## Single hole on a QAFM

* Frustration





"wrong" bonds, energy $\propto l J$

* Major physical effects

① Distortion of spin background short and long range

② Quantum spin fluctuations

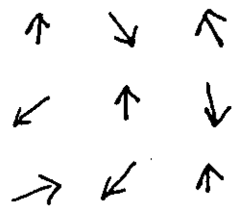
③ Renormalization due to emitting and reabsorbing spin waves

$t \to J$

Spin polaron effect

## Possible ground states at finite doping

* spiral phase

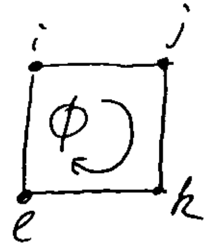


$\langle \vec{S}_i \vec{S}_j \rangle \propto \cos \vec{Q}(\vec{r}_i - \vec{r}_j)$

$\vec{Q} \sim (1,1)$

* Flux phase

$\chi_{ij} = \langle \sum_\sigma c^+_{i\sigma} c_{j\sigma} \rangle$



$\langle \chi_{ij} \chi_{jk} \chi_{kl} \chi_{li} \rangle = |\chi|^4 e^{i\phi}$

Chiral phase

$\phi \neq n\pi$

* Phase separation

AF + hole-rich region

Coulomb repulsion prevents

* Dimerized phase ?

* Phenomenological approach

Marginal FL behavior

C.M. Varma et al.

Ansatz: Polarization of charge or spin fluctuations

$$\mathrm{Im}\,\tilde{P}(\vec{q},\omega) \sim \begin{cases} -N(0)\,\omega/T, & \text{for } |\omega| < T \\ -N(0)\,\mathrm{sgn}\,\omega, & \text{for } |\omega| > T \end{cases}$$

independently of $\vec{q}$. generalization from Raman experiments

Self-energy:

$$\Sigma(\vec{k},\omega) \approx g^2 N(0)^2 \left(\omega \ln \frac{x}{\omega_c} - i\frac{\pi}{2}x\right)$$

$x = \max(T, |\omega|)$ , $\omega_c$ cut-off

$$G(\vec{k},\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(\vec{k},\omega)} = \frac{Z_k}{\omega - E_k + i\Gamma_k} + G_{inc}$$

$$Z_k^{-1} = \left(1 - \frac{\partial \mathrm{Re}\,\Sigma}{\partial \omega}\right)_{\omega = E_k} \sim \ln|\omega_c/E_k|$$

$E_k \to 0$, $Z_k^{-1} \to \infty$

Marginal Fermi liquid !!

FL: $\mathrm{Re}\,\Sigma \sim \omega$

$\mathrm{Im}\,\Sigma \sim \omega^2$

Marginal FL $\mathrm{Re}\,\Sigma \sim \omega \ln \frac{\omega}{\omega_c}$

$\mathrm{Im}\,\Sigma \sim \omega$

Difference is measurable

* Explains "ALL" anomalies

* Linear dependence $\rho \sim T$

* Background in Raman

* Tunneling

$$G \sim g_0 + g_1 |V|$$

assuming

$$N(\omega) \sim \sum_{k} A(\vec{k},\omega) \sim N_0 + N_1|\omega|$$

To get $g_1 > 0$, additional elastic scattering

* NMR

$T_1^{-1} \sim aT + b$

why the difference for $^{17}O$ and $^{63}Cu$

* Optical absorption

$\sigma(\omega) = \sigma_1(\omega) + \sigma_2(\omega)$

$\sigma_1(\omega) \propto \mathrm{Im}\,\frac{\omega_{pl}^2}{\omega + i\Sigma(\omega)}$ Drude

$\sigma_2(\omega) \sim -\omega\, \mathrm{Im}\, \tilde{P}(0,\omega)$

Good fit

* Photoemission
more sensitive to angular average

* Superconducting properties
S-wave
$2\Delta/kT \sim 8$
No Hebel-Slichter resonance
Life-time effects

Microscopic origin ??

Dogmas and Dictats of Anderson

F.C. Crick The central dogmas or the "secret of Life"

1. $CuO_2$ planes are responsible, both for charge and spin carriers
$O_{2p} - d_{x^2-y^2}$ orbits
2. Magnetism and SC are related
the Same electrons are responsible
3. One band Hubbard model with fairly large $U$
4. Luttinger Liquid (Haldane 1D) is the prototype
5. This state is strictly two-dimensional
6. SC due to interlayer tunneling

* 1 D Hubbard model

Typical Non-FL behavior

at the same time - very similar to experimental observations

Bethe Ansatz solution

* Ogata & Shiba — cluster calc.
* Sorella, Parola, Parrinello, Tosatti: $U/t \gg 1$
* Separation of charge and spin

holons, charge e, spinless fermion

$2K_F$

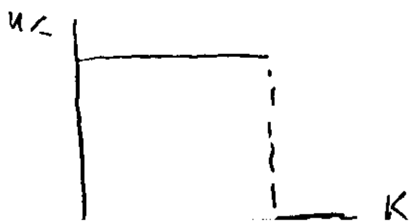
Spinons, $S=1/2$, $Q=0$

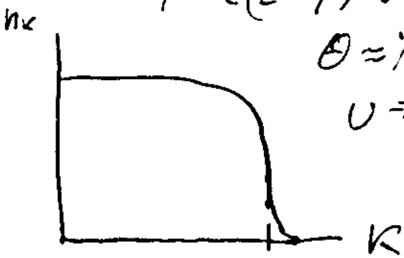
$K_F$

* $n_k$ — $1-\mathrm{sgn}(\varepsilon-\varepsilon_F)$ — $1-C(\varepsilon-\varepsilon_F)^{\theta}\,\mathrm{sgn}(k-k_F)$

$\theta \approx 1/8$

$U \to \infty$




No singularity at $2K_F$

Weak singularity at $3K_F$

$Z_k \to 0$ at $K_F$, no charge

$$\langle C^{\dagger}(0)\,C(r)\rangle \sim \frac{\sin k_F r}{r^{1+\theta}}$$

Continuity from $U<t \to U>t$

$$\langle \rho(0)\rho(r)\rangle \to K_2\, r^{-\alpha}\cos 2k_F r + K_4\, r^{-\beta}\cos 4k_F r + \dots$$

$$\langle \vec{S}(0)\cdot\vec{S}(r)\rangle \to H_2\, r^{-\gamma}\cos 2k_F r + \dots$$

$U=0$, $\alpha=\gamma=2$, $K_4=0$

$U\to\infty$, $\alpha=\gamma=3/2$, $\beta=2$, $\theta=1/8$

Anderson's conjecture: Two different fixed points. FL vs LL

This is true also for 2D and higher dimensions. Luttinger Liquid vs Fermi Liquid

Orthogonality Catastrophe
Anderson 1973

Noninteracting Fermions $N$
Scattering potential $V$

$$\langle VAC(V) | VAC(0) \rangle \propto e^{-\frac{1}{2}\left(\frac{\delta}{\pi}\right)^2 \ln N} \ominus V$$

$\Rightarrow 0$ $\delta$ phase shift

X-ray edge problem

In higher dimension, adding one electron

$$\sqrt{Z} = \langle C_{k\sigma}^{+} \Psi_G(N) | \Psi_{k\sigma}(N+1) \rangle > 0$$

However, in 1D

$\sqrt{Z} \Rightarrow 0$, all states are phase shifted do not carry charge

Anderson's conjecture:

This is also true for 2D !!

"Gedanken theory"



* Fermi Liquid Theory

1) "Genuine" FL

BCS pairing. spin fluctuation
Schrieffer, Wen, Zhang, spin bag
Kampf, Schrieffer, pseudo gap

No problem with FS
Normal State properties ?
Optical sum rule

$$\left(\frac{N}{m}\right)^{*} \sim \frac{x}{m_1}, \text{ not } \frac{1-x}{m^*}$$

2) Heavy fermion version

P.A. Lee et al. ...
Newns et al. ...
Anderson lattice model → slave boson
Anderson lattice → renormalization of Cu level, etc.
No problem with FS
Not so heavy ! $m^*/m \simeq 2$
concentration dependence of $\chi$, $\sigma$

$\chi \sim 1/x$ but ↑

# Anyon Superconductivity

Laughlin

Fetter, Hanna, Laughlin

Fradkin

Lee, Fisher

Canright

Wen, Zee

Chen, Wilczek, Witten, Halperin

Banks,

Mele, Voit

- - - -

"anyon gauge", multivalued wave function

$$\psi \to \psi e^{i\theta}$$

Generically $e^{i\theta} \neq e^{-i\theta}$

depends on the presence of other particles

* Single-valued wave function as for bosons or fermions

Fermions + flux tubes

$$H = \sum_{\alpha=1}^{N} \frac{|\vec{p}_\alpha - \vec{a}_\alpha|^2}{2m^*} + V$$

$$\vec{a}_\alpha = \left(\frac{\pi-\theta}{\pi}\right) \sum_{\beta\neq\alpha} \frac{\hat{z}\times\vec{r}_{\alpha\beta}}{|r_{\alpha\beta}|^2}$$

$$\vec{r}_{\alpha\beta} \equiv \vec{r}_\alpha - \vec{r}_\beta$$

$$\therefore \quad \vec{\nabla}_\alpha \times \vec{a}_\alpha = \left(\frac{\pi-\theta}{\pi}\right) \sum_{\beta\neq\alpha} \delta(\vec{r}_\alpha - \vec{r}_\beta)$$

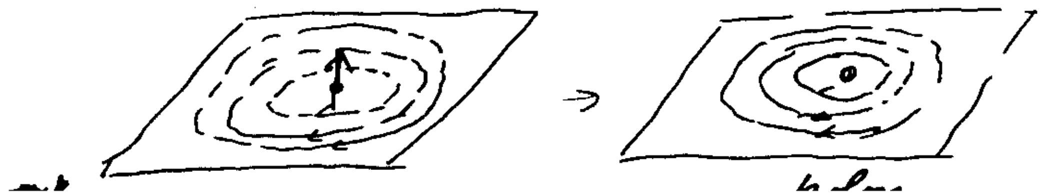
$\vec{H}_{eff} = 0$, except for positions of other particles

Where to find?

1. Fractional Quantum Hall Effect
   Laughlin, Halperin - - - direct measurement
2. Vortices in thin films of $^3He$-A
   Volovik + Yakovenko
3. Models of High $T_c$ SC
   Laughlin -- analogy with FQHE

Chiral Spin liquid

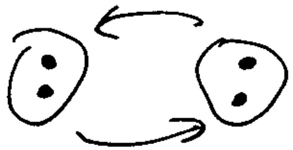
$\theta = \pm\frac{\pi}{2}$, P, T, sym. broken but PT conserved



There is an effective long-range gauge force $\Rightarrow$ pairing

Pair of half-fermions $\Rightarrow$ boson

$$e^{i4\theta} = 1$$



Dilute anyon gas

$$\theta = \pi\left(1 - \frac{1}{n}\right) \qquad n: \text{integer}$$

RPA.

1) Ground state is SC. with Meissner effect...
2) Quasiparticle excitations — charged vortices. with gap
3) Long-wave length collective mode - sound
4) At least two species of anyons



Experimental Consequences of Broken T. P symmetry

Single layer

1. Intrinsic orbital magnetic moment

   $\approx \frac{1}{4}\mu_B \frac{m}{m^*}$ per carrier

   $\mu$SR ?

2. Optical Rotation at $\vec{B}=0$

   Wen & Zee

   absent in effective mass approx.

3. Righi-Leduc effect at $\vec{B}=0$

   (= Hall effect in thermal conductivity tensor

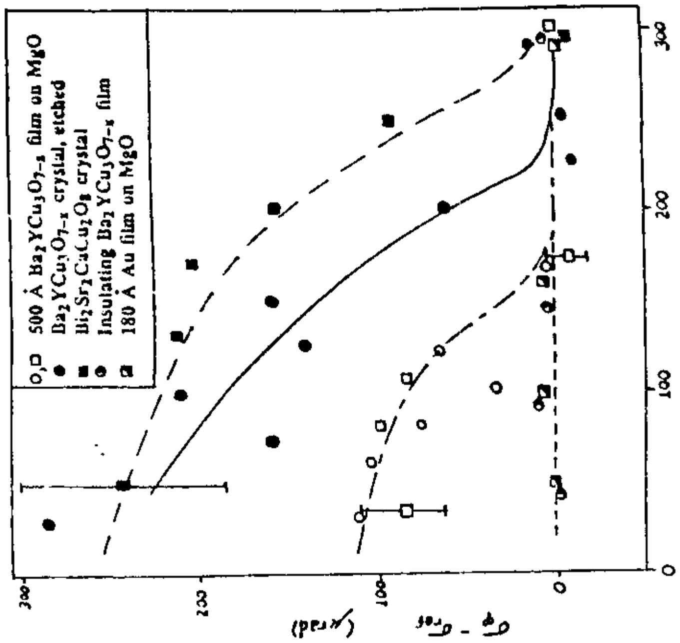
4. Spontaneous Hall effect at $\vec{B}=0$ in the normal state (CSL)

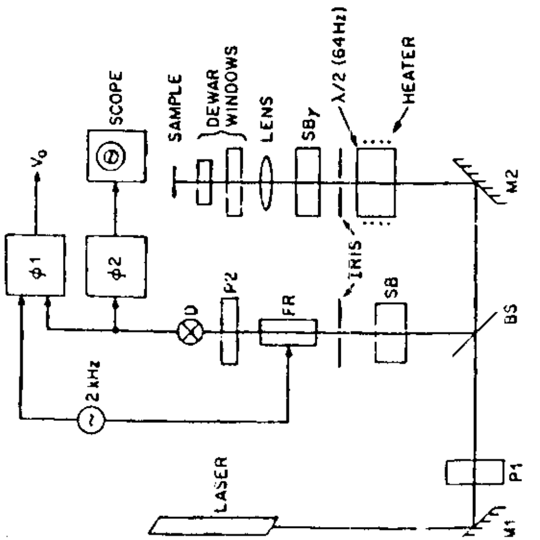
3D Ferromagn. or AF coupling

Bulk or surface effect.

Local probe_ magnetic fiel

~10 Gauss




$\frac{R_\pm}{R_{av}} = e^{\pm\psi}$

# Concluding Remarks

* Constraints set by experiments

S-Wave pairing ...

Fermi Surface ...

Normal state anomalies

Optical sum rules ----

* All theoretical approaches have "successes" and "troubles"

Weak coupling

Strong coupling ⟨ slave boson / slave fermion

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Heavy fermions

phenomenology – useful, but

... difficulties