CUPRATE SUPERCONDUCTIVITY:

THE CURRENT STATE OF PLAY

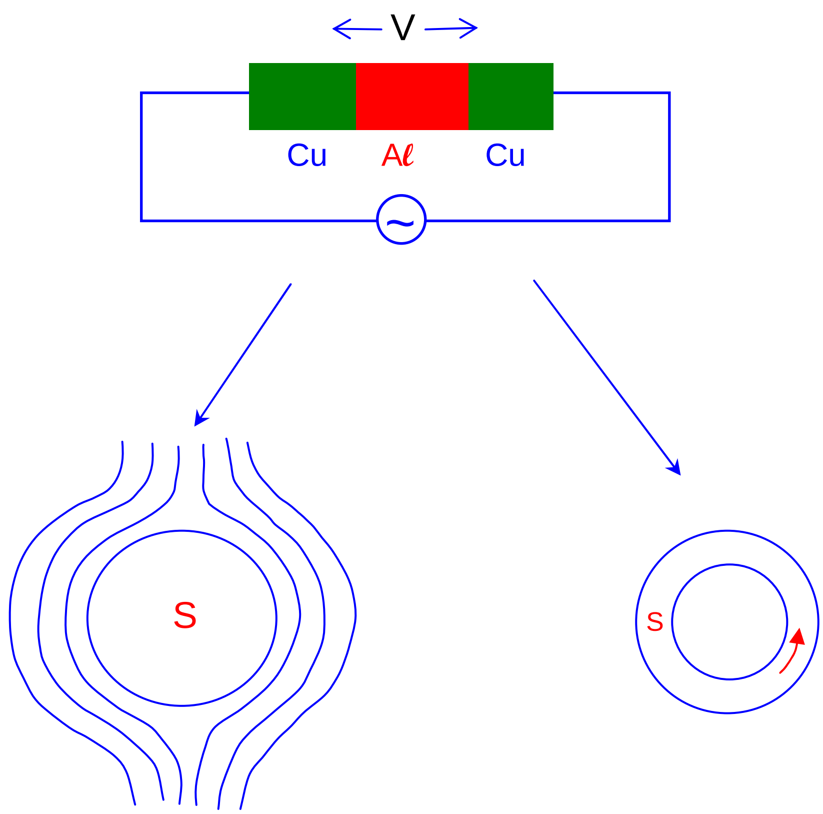
A. J. Leggett
Department of Physics
University of Illinois at
Urbana-Champaign

1. Brief overview of cuprate structure and properties
2. What do we know for sure about HTS in the cuprates?
3. Some existing "models"
4. Are we asking the right questions?

Support: NSF-DMR-99-86199 and 03-50842
Special thanks: D. van der Marel (Groningen)

What is Superconductivity?

Basic expt: (Onnes 1911)



perfect diamagnetism
(Meissner effect)
equilibrium effect

persistent currents,
astronomically stable
metastable effect

No a priori guarantee these two phenomena always go together!
(but in fact seem to, in all "superconductors" known to date).

CS 3

PHENOMENOLOGY OF SUPERCONDUCTIVITY

(London, Landau, Ginzburg, 1938–50)

Superconducting state characterized by
"macroscopic wave function" Ψ (r) ← complex, Schr.-like

$\Psi(r) \equiv |\Psi(r)| \exp i\varphi(r)$ ← must be single-valued mod. 2π

vector potential

electric current ⟶ $J(r) \propto |\Psi(r)|^2 (\underset{\sim}{\nabla} \varphi(r) - e^* \underset{\sim}{A}(r))$

(BCS: $e^*=2e$)

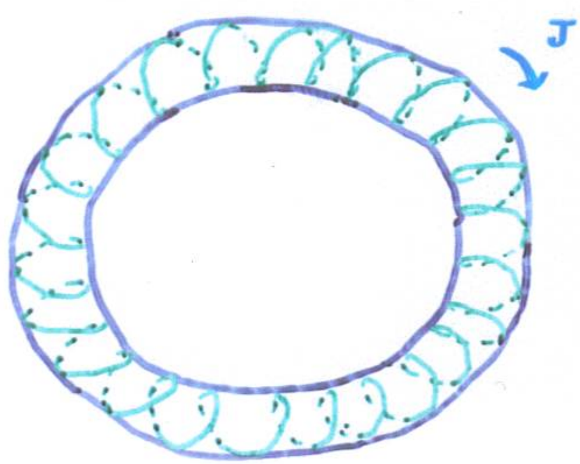
MEISSNER EFFECT: exact analog of atomic diamagnetism

$$(\int \nabla\varphi \cdot dl = 0 \Rightarrow J = -\underbrace{\frac{ne^2}{m}}_{\equiv\lambda_L^{-2}} A$$

$\Rightarrow \nabla^2 \underset{\sim}{B} = \lambda_L^{-2} \underset{\sim}{B} \Rightarrow B = B_o \exp - z/\lambda_L$ in atom, sup^r.

But qualitative difference: $R_{at} << \lambda_L << R_{sup}$!

PERSISTENT CURRENTS



$n \equiv \int \underset{\sim}{\nabla}\varphi \cdot d\underset{\sim}{l} / 2\pi$

conserved unless $|\Psi(r)| \to O$ across some X-section (highly unfavorable energetically)

$\Rightarrow J \sim n =$ conserved

STRUCTURE OF A TYPICAL CUPRATE

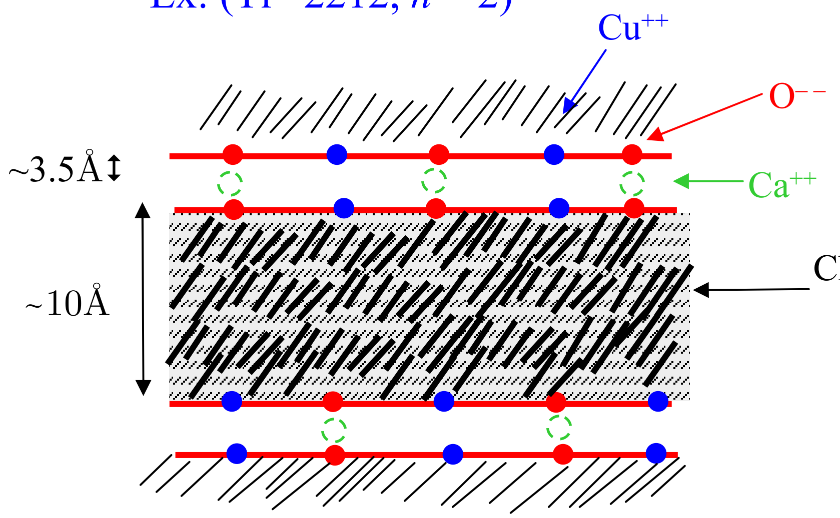
$$XA_{n-1}(CuO_2)_n \leftarrow \text{copper oxide planes}$$

"charge reservoir"

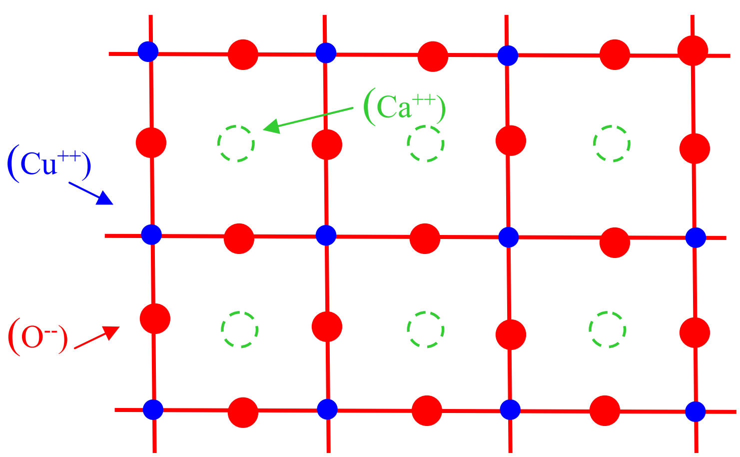
"spacer" (alk. earth, rare-earth, Y, La….)

n = 1, 2, 3… ("homologous series")

Ex: (Tl –2212, n = 2)

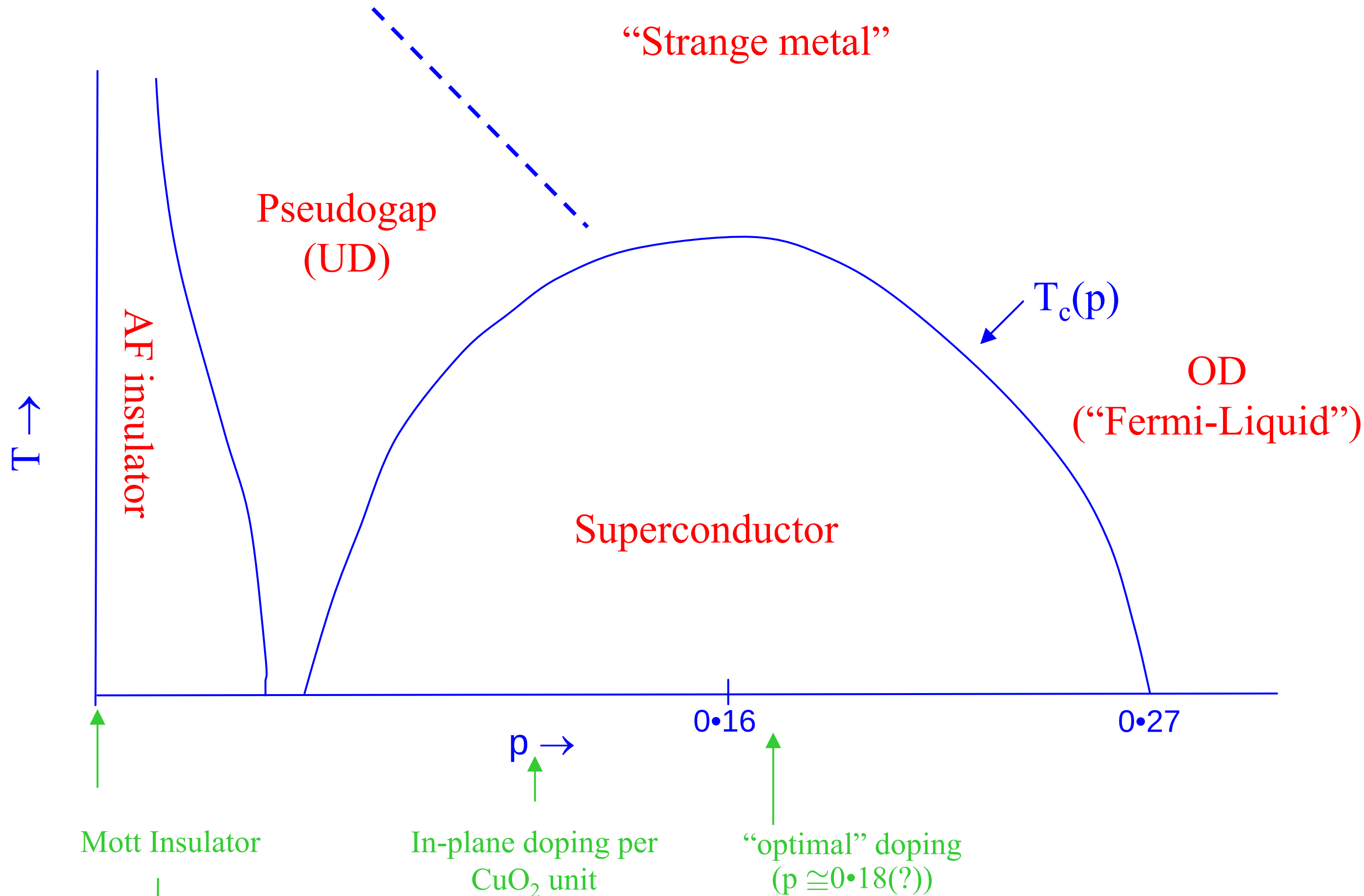


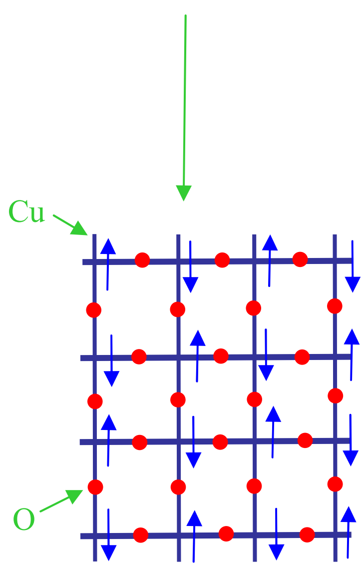
CuO$_2$ plane as viewed from above:



Note:
Each CuO$_2$ plane has valency—2e per formula unit, hence homologous series require spacer with +2e (i.e., typically alkaline earth (Ca^{++}, Sr^{++} . . .)

"CANONICAL" PHASE DIAGRAM OF CUPRATES AS FUNCTION OF T AND DOPING (COMPOSITE):





Doping: e.g.

$Y\,Ba_2\,Cu_3\,O_{6+x}$, $La_{2-x}\,Sr_x\,CuO_4$

For any given compound, can find mapping from x (chemical stoichiometry) to p (no. of holes per CuO_2 unit in plane) which makes phase diagram <u>and</u> properties "per plane" <u>approx</u>. "universal," ↑: but difficult to check directly.

SOME BASIC FACTS ABOUT CUPRATES

1. Until 2008, unique in showing (reproducible) sup^y at T> 50 K. (>200 different materials). (2008: FeAs compounds, T~55K).

2. However, ∃ some cuprates which can never be made superconducting (multilayers spaced by Sr or Ba).

3. Both N– and S– state props. highly anisotropic (e.g., in Bi 2212, $\rho_c/\rho_{ab} \sim 10^5$)

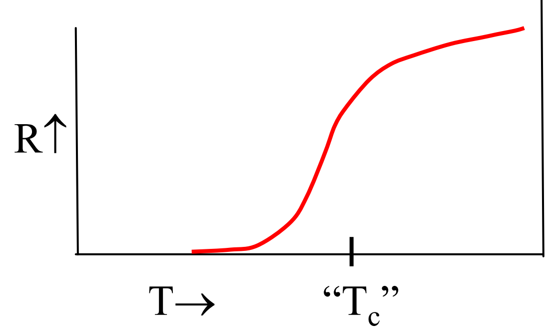
4. Many N-state props. very anomalous (e.g., $\rho_{ab} \sim T$, $\theta_H \sim a + bT^2$). (S: rather "normal"!)

5. Most N- (and S-) state props. approximately consistent with hypothesis that at given doping, properties of CuO_2 phase are universal. (⇧: transport properties prob. sensitive to near-plane disorder, e.g. $La_{2-x}Sr_xCuO_4$.)

6. When S state occurs, v. sensitive to doping and pressure, (e.g., Hg–1201: $T_c = \underset{\text{Atm.}}{95} - \underset{\text{20 GPa}}{120}$ K)

7. For Ca-spaced homologous series, T_c always rises with layer multiplicity n up to $n = 3$, thereafter falls slightly. (?)

8. Macroscopic EM props of S state show large fluctuations, esp. in high magnetic fields (extreme type-II)



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

$$\Psi \sim \mathcal{A}\{\varphi(r_1 r_2 \sigma_1 \sigma_2)\varphi(r_3 r_4 \sigma_3 \sigma_4)\ldots.\varphi(r_{N-1} r_N \sigma_{N-1} \sigma_N)\}$$

antisymmetric

Same "molecular" wave function
for all pairs (quasi-BEC!)

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

$$F(\mathbf{r}_1\mathbf{r}_2\sigma_1\sigma_2) \equiv \left\langle \psi^+_{\sigma_1}(\underline{r}_1)\psi^+_{\sigma_2}(\underline{r}_2) \right\rangle$$

"pair wave function" (anomalous average)

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

CS 8

WHAT DO WE KNOW FOR SURE . . . . ? (CONT.)

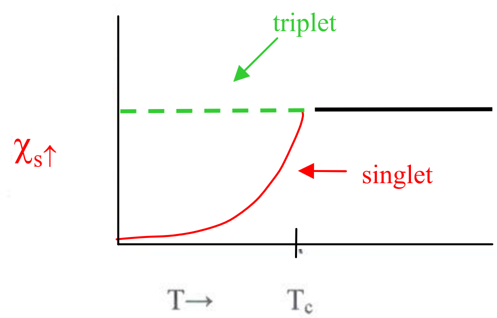
2. "Universality" of HTS in cuprates with very different chemical compositions, etc. ⇒

   Main actors in superconductivity are electrons in CuO_2 planes.

3. NMR (χ_s, T_1 . . .)

   ⇒spin wave function of

   Cooper pairs singlet not triplet, i.e.



$$\varphi(\boldsymbol{r}_1\boldsymbol{r}_2\sigma_1\sigma_2) \sim \frac{1}{\sqrt{2}}\uparrow\downarrow - \downarrow\uparrow)\bullet\varphi(\underline{r}_1, \underline{r}_2)$$

4. Absence of substantial FIR absorption above gap edge ⇒ pairs formed from time-reversed states (but cf. J. Tahir-Kheli)

5. Order-of-magnitude estimates from (a) T_c and (b) H_c ⇒ (in-plane) "radius" of Cooper pairs ~ a few lattice spacings.

   (thus, ξ_o / a ~ 3–10 :contrast ~ 10^4 for $A\ell$

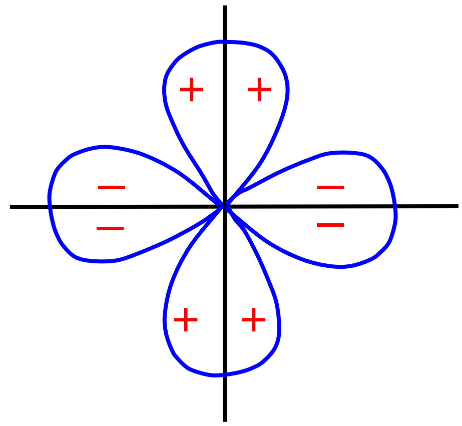
   pair radius inter-cond. electron spacing

   ⇒ fluctuations much more important than in e.g. $A\ell$

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

6. Josephson (phase-sensitive) experiments ⇒ at least in YBCO, Tℓ-2201, NCCO. . . .
   symmetry of pair wave function is $d_{x^2-y^2}$

   i.e. odd under $\pi/2$ rot^n in ab-plane,
   even under refl^n in a- or b-axis
   (in bulk: near (110) surface, d + is?)



[↑: Li et al.]

7. c-axis resistivity ⇒ hopping time between unit cells along c-axis » $\hbar/k_B T$ ⇒
   pairs in different multilayers effectively independent
   (but cf. Anderson Interlayer Tunneling theory)

8. Absence of substantial isotope effect (in higher –T_c cuprates) + "folk-theorems" on T_c ⇒
   phonons do not play major role in cuprate superconductivity.
   (↑: Newns and Tsuei)

NOTE: AT LEAST 95% OF LITERATURE MAKES
ALL OF ABOVE ASSUMPTIONS AND A LOT MORE
e.g. 2d Hubbard, t-J, gauge field … all special cases of generic
Hamiltonians based on these features.

HOW WILL WE KNOW WHEN WE HAVE A "SATISFACTORY" THEORY OF HTS 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) RT 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 HTS?

(2) If so, what is special about them? (e.g. band structure, 2-dimensionality, AF …)

(3) Should we think of HTS 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 LT ("pseudogap") phase?

(5) If yes to (4), is this relevant to HTS or a completely unconnected phenomenon?

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

SOME REPRESENTATIVE CLASSES OF "MODELS" OF COOPER PAIRING IN THE CUPRATES (conservative $\Longrightarrow$ exotic):

1. Phonon-induced attraction ("BCS mechanism")
   problems: N-state $\rho_{ab}(T) \propto T$ down to T~10 K (Bi-2201 T_c)
   no isotope effect in higher $-T_c$ HTS
   folk-theorems on T_c (but ↑: 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:*

$$\hat{H} = -t \sum_{i,j=\varepsilon nn} \underbrace{(c^{+}_{i\sigma} c_{j\sigma} + H.c.)}_{\text{hopping}} + U \sum_{i} \underbrace{n_{i\uparrow} n_{i\downarrow}}_{\text{on-site repulsion}}$$

   a. Attempts at direct solution, computational or analytic

   b. Theories based on postulate of "exotic ordering" in groundstate (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 ….")

---

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

Energy Considerations in the Cuprates (neglect phonons, inter-cell tunnelling)

$$\hat{H} = \hat{T}_{(\parallel)} + \hat{U} + \hat{V}_c$$

in-plane e^- *KE*

potential ex. of cond.^{n} e^-'s in field of static lattice

inter-conduction $-e^-$ Coulomb energy (intraplane & interplane)

AND THAT'S ALL

(DO NOT add spin fluct^{ns}, excitons, anyons….)

At least one of $\langle T \rangle, \langle U \rangle, \langle V_c \rangle$ must be decreased by formation of Cooper pairs. Default option: $\langle V_c \rangle$

Rigorous sum rule:

$$\langle V_C \rangle \sim - \int d\boldsymbol{q} \int d\omega \ \mathrm{Im} \left\{ \frac{1}{1 + V_q \chi_o(q\omega)} \right\}$$

$$\left[3D :\equiv \int dq \int d\omega \left(-\mathrm{Im} \frac{1}{\varepsilon(qw)} \right) \right]$$

Coulomb interaction (repulsive)

bare density response function

WHERE IN THE SPACE OF (q, ω) IS THE COULOMB ENERGY SAVED (OR NOT)?

THIS QUESTION CAN BE ANSWERED BY EXPERIMENT!

(EELS, OPTICS, X-RAYS)

How Can Pairing Save Coulomb Energy?

$$\langle V_c \rangle \sim -\int d\underline{q} \int d\omega \ \mathrm{Im}\left\{ \frac{1}{1+V_q \chi_o(q\omega)} \right\}$$

[exact]

Coulomb interaction (repulsive)

bare density response function

$\sim$ min $(k_F, k_{T\uparrow}) \sim 1\dot{A}^{-1}$

A. $V_q \chi_o(q\omega) \ll 1$ (typical for $q \gg q_{FT}^{(eff)}$)

pert^n-theoretic result

$$\langle V_c \rangle_q \cong +V_q \int d\omega \ \mathrm{Im}\, \chi_o(q\omega) = V_q \langle \rho_q \rho_{-q} \rangle_o$$

$\Rightarrow$to decrease $\langle V_c \rangle_q$, must decrease $\langle \rho_q \rho_{-q} \rangle_o$

but $\underbrace{\delta \langle \rho_q \rho_{-q} \rangle}_{\text{pairing}} \sim \sum_p \Delta_{p+q/2} \Delta^*_{p-q/2}$

$\Rightarrow$ gap should change sign (d-wave?)

B. $V_q \chi_o(q\omega) \gg 1$ (typical for $q \ll q_{FT}^{(eff)}$)

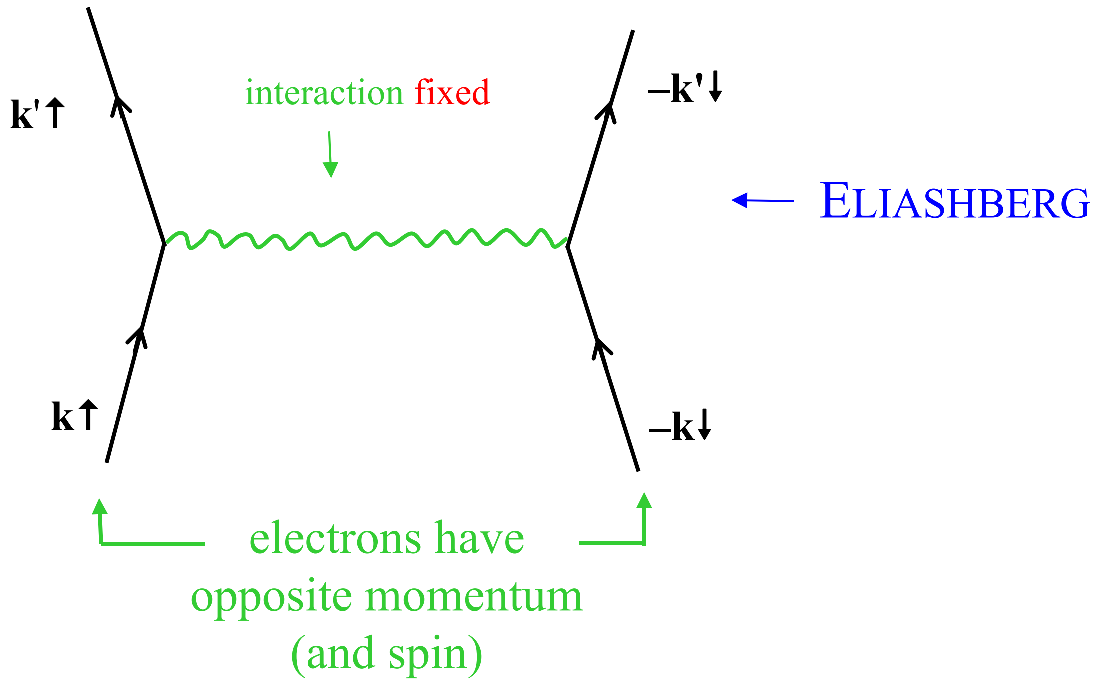
$$\langle V_c \rangle_q \cong \frac{1}{V_q}\left(-\mathrm{Im}\frac{1}{\chi_o(q\omega)}\right) \leftarrow \text{note inversely proportional to } V_q.$$

$\Rightarrow$ to decrease $\langle V_c \rangle_q$, (may) increase $\mathrm{Im}\, \chi_o(q\omega)$

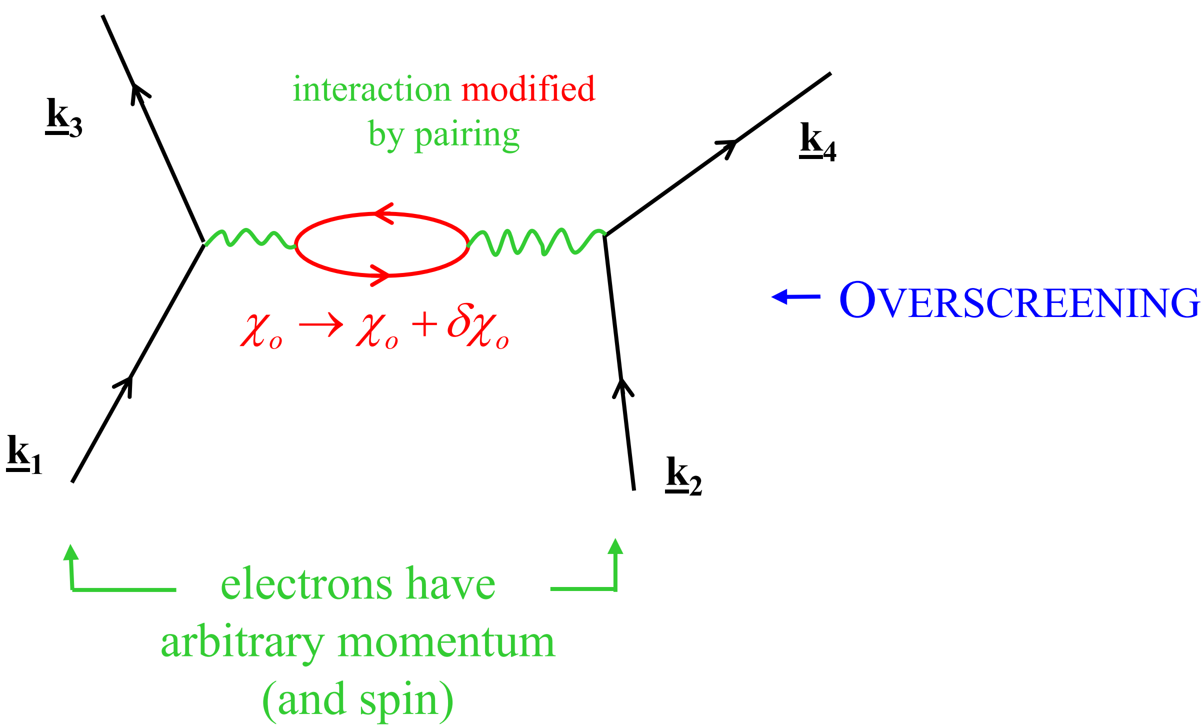
and thus (possibly) $\langle \rho_q \rho_{-q} \rangle_o$

increased correlations $\Rightarrow$ increased screening $\Rightarrow$ decrease of Coulomb energy!

ELIASHBERG vs. OVERSCREENING



REQUIRES ATTRACTION IN NORMAL PHASE



NO ATTRACTION REQUIRED IN NORMAL PHASE

$$\langle V_c \rangle_S - \langle V_c \rangle_N \sim +\int d^2q \int d\omega\, V_q\; Im \left\{ \frac{\delta\chi(q,\omega)}{\left(1+V_q\chi_o(q\omega)\right)^2} \right\}$$

* WHERE in the space of q and ω is the Coulomb energy saved (or not)?

* WHY does T_c depend on n?

In <u>Ca-spaced</u> homologous series, T_c rises with n at least up to $n=3$ (noncontroversial). This rise <u>may</u> be fitted by the formula (for "not too large" n)

$$T_c^{(n)} - T_c^{(1)} \sim \text{const}\left(1-\frac{1}{n}\right) \qquad \text{(controversial)}$$

<u>Possible explanations</u>:

A. ("boring"): Superconductivity is a single-plane phenomenon, but multi-layering affects properties of individual planes (doping, band structure, screening by off-plane ions…)

B. ("interesting"): Inter-plane effects essential

1. Anderson inter-layer tunnelling model
2. Kosterlitz-Thouless
3. Inter-plane Coulomb interactions ← WE KNOW THEY'RE THERE!

in-plane wave vector

$$V_{\text{int}}(q) \sim q^{-1}\exp - qd \leftarrow \text{intra-multilayer spacing}$$

(~3 · 5Å)

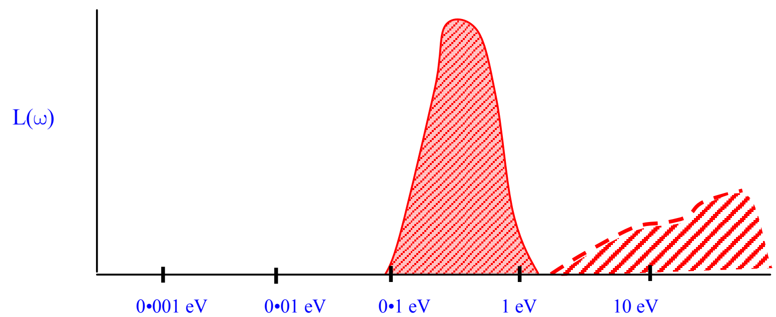
If (3) is right, then even in single-plane materials dominant region of q is $q < d^{-1}$!!

Where in ω is energy saved? (REMEMBER WILLIE SUTTON….)

N STATE

MIR OPTICAL + EELS SPECTRA OF THE CUPRATES

A. OPTICS. Plot in terms of loss function $L(\omega) \equiv -Im\, \varepsilon^{-1}(\omega)$:



ω (logarithmic scale) $\longrightarrow$

B. EELS

Confirms $q \rightarrow 0$ shape of the loss function, and verifies that (roughly) same shape persists for finite q. (at least up to ~0·3 Å^{-1})

SO THAT'S WHERE THE MONEY IS!

Digression:

This strong peaking of the loss function in the MIR appears to be a necessary condition for HTS. Is it also a sufficient condition? No! Counter examples:

(a) BKBO (not layered)

(b) $\begin{cases} La_{4-x}Ba_{1+x}Cu_5O_{13} \\ La_{2-x}\,Sr_{1+x}Cu_2O_6 \end{cases}$ layered (2D) materials!

TO TEST MIR SCENARIO:

IDEALLY, WOULD LIKE TO MEASURE

CHANGES IN LOSS FUNCTION $\leftarrow -Im\dfrac{1}{\varepsilon_{\|}(q\omega)}$

ACROSS SUPERCONDUCTING TRANSITION, FOR

$100\ \text{meV} < \omega < 2\text{eV}$, AND ALL $q < d^{-1}$ ($\approx 0 \cdot 3$ Å^{-1})

NB: for $q > d^{-1}$, no simple relation between quantity $-\text{Im}\,(1 + V_q\,\chi_o\,(q\omega))$ and loss function.

POSSIBLE PROBES:

1) TRANSMISSION EELS
2) INELASTIC X-RAY SC'G

} "long'l", arb. q, ω

3) OPTICS (ELLIPSOMETRY)

"transverse", arb. ω
but $q \ll 0 \cdot 3$ Å^{-1}

EXISTING ELLIPSEMETRIC EXPTS. (v.d. MAREL, RÜBHAUSEN) INDICATE THAT IN LIMIT $q\rightarrow 0$, MIR LOSS FUNCTION INCREASES!

↑: (1) TRANSVERSE

(2) $q_{opt} \ll \xi_O^{-1} \ll d^{-1}$

↑

Cooper pair radius

HENCE, ESSENTIAL TO DO EELS/X-RAY EXPERIMENTS.

(P. Abbamonte)

THE "MIDINFRARED" SCENARIO FOR CUPRATE SUPERCONDUCTIVITY:

Superconductivity is driven by a saving in Coulomb energy resulting from the increased screening due to formation of Cooper pairs. This saving takes place predominantly at long wavelengths and midinfrared frequencies.

PROS:

1. No specific "model" of low-energy behavior required
2. Natural explanation of
   a. why all known HTS systems are strongly 2D
   b. why all known HTS systems show strong and wide MIR peak
   c. trends of T_c with layering structure in Ca-spaced cuprates
   d. absence of superconductivity in bilayer Ba/Sr-spaced cuprates.
   e. "huge" (~100 × BCS) effects of superconductivity on optical properties in 1–3 eV range.
3. Unambiguously falsifiable in EELS experiments.

CONS (as of Jan '09):

1. No explicit gap equation constructed: KE cost too great?
2. No explanation of origin of MIR spectrum
3. Connection (if any) to low-energy phenomenologies unclear.
4. *optical expts.

CONSEQUENCES IF TRUE:

All 2D Hubbard, t-J models etc. unviable

Crucial property of normal state is MIR spectrum (most other properties are "incidental"

May suggest HTS candidates other than cuprates

····