ENERGETIC CONSIDERATIONS IN STRONGLY CORRELATED ELECTRON SYSTEMS

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Will mostly address problem of high-T superconductivity in cuprates and elsewhere (but considerations are more general)

1. Minimal reminders re superconductivity

2. Minimal reminders re cuprates

3. Can we say anything about high-temperature superconductivity without reliance on a specific microscopic model?

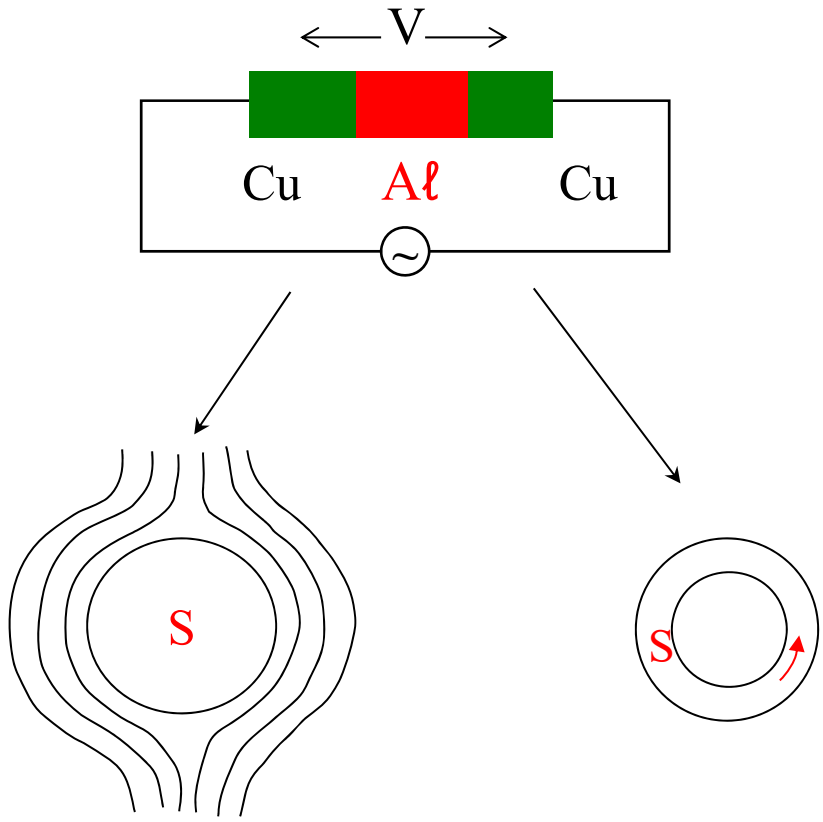
4. What (if anything) can we infer from general considerations (or experiment) on the $(\boldsymbol{q}, \omega)$ regimes in which energy is saved (or not)?

5. A specific conjecture about the regimes of $\boldsymbol{q}$ and ω in which saving takes place.

6. The current experimental situation.

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).

PHENOMENOLOGY OF SUPERCONDUCTIVITY

(London, Landau, Ginzburg, 1938-50)

Superconducting state characterized by

"macroscopic wave function" $\Psi(r)$ ← complex, Schr.-like

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

vector potential

electric current → $\mathrm{J}(\mathrm{r}) \propto |\Psi(\mathrm{r})|^2 \ (\nabla \varphi(\mathrm{r}) - \mathrm{e} * \underline{\mathrm{A}}(\mathrm{r}))$

(BCS: e* = 2e)

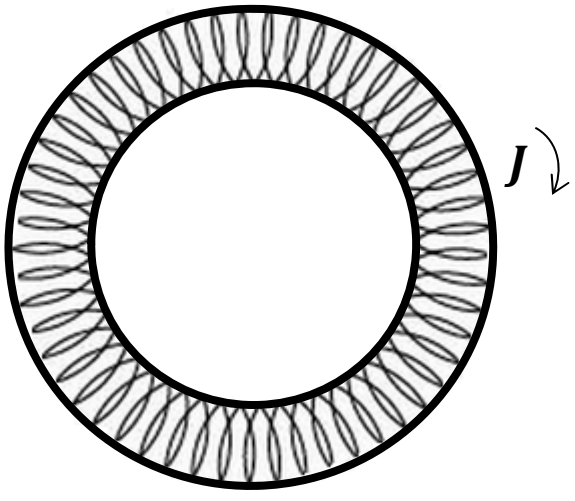
MEISSNER EFFECT: exact analog of atomic diamagnetism

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

$\Rightarrow \nabla^2 \underline{B} = \lambda_L^{-2} \underline{B} \Rightarrow B = B_0 e^{-\frac{z}{\lambda_L}}$ in atom, supr.

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

PERSISTENT CURRENTS



$$n \equiv \int \underline{\nabla}\phi \cdot d\underline{l}/2\pi$$

conserved unless $|\Psi(r)| \to 0$ across some X-section (highly unfavorable energetically)

$\Rightarrow J \sim n =$ conserved

STRUCTURE OF A TYPICAL CUPRATE

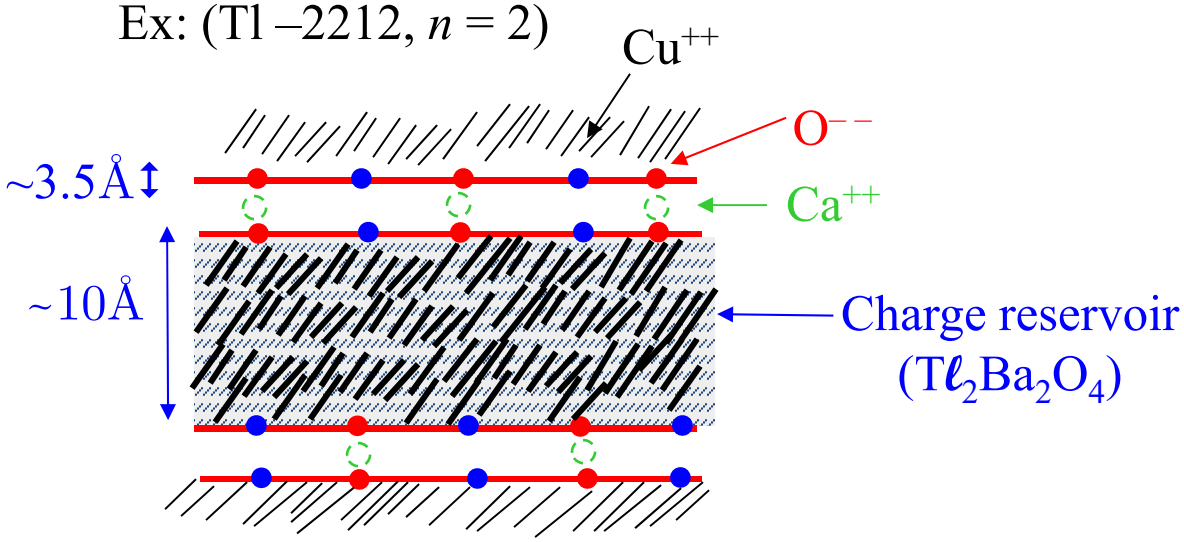
$XA_{n-1}(Cu)_2)_n$ ← copper oxide planes

"charge reservoir"

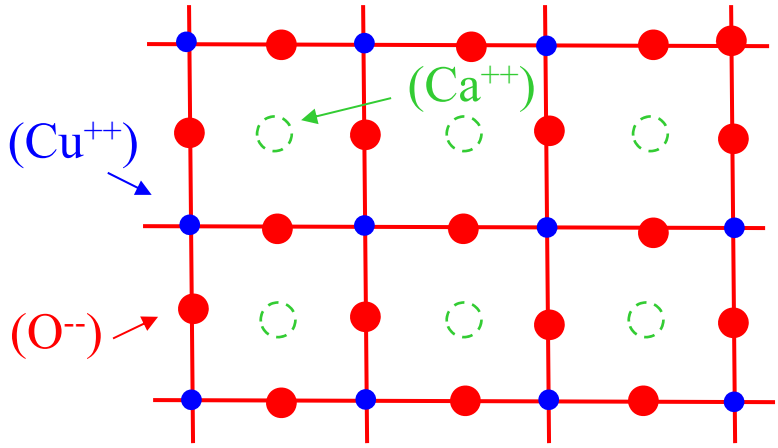
"spacer" (alk. earth, rare-earth, Y, La….)

n = 1, 2, 3… ("homologous series")

Ex: (Tl –2212, n = 2)

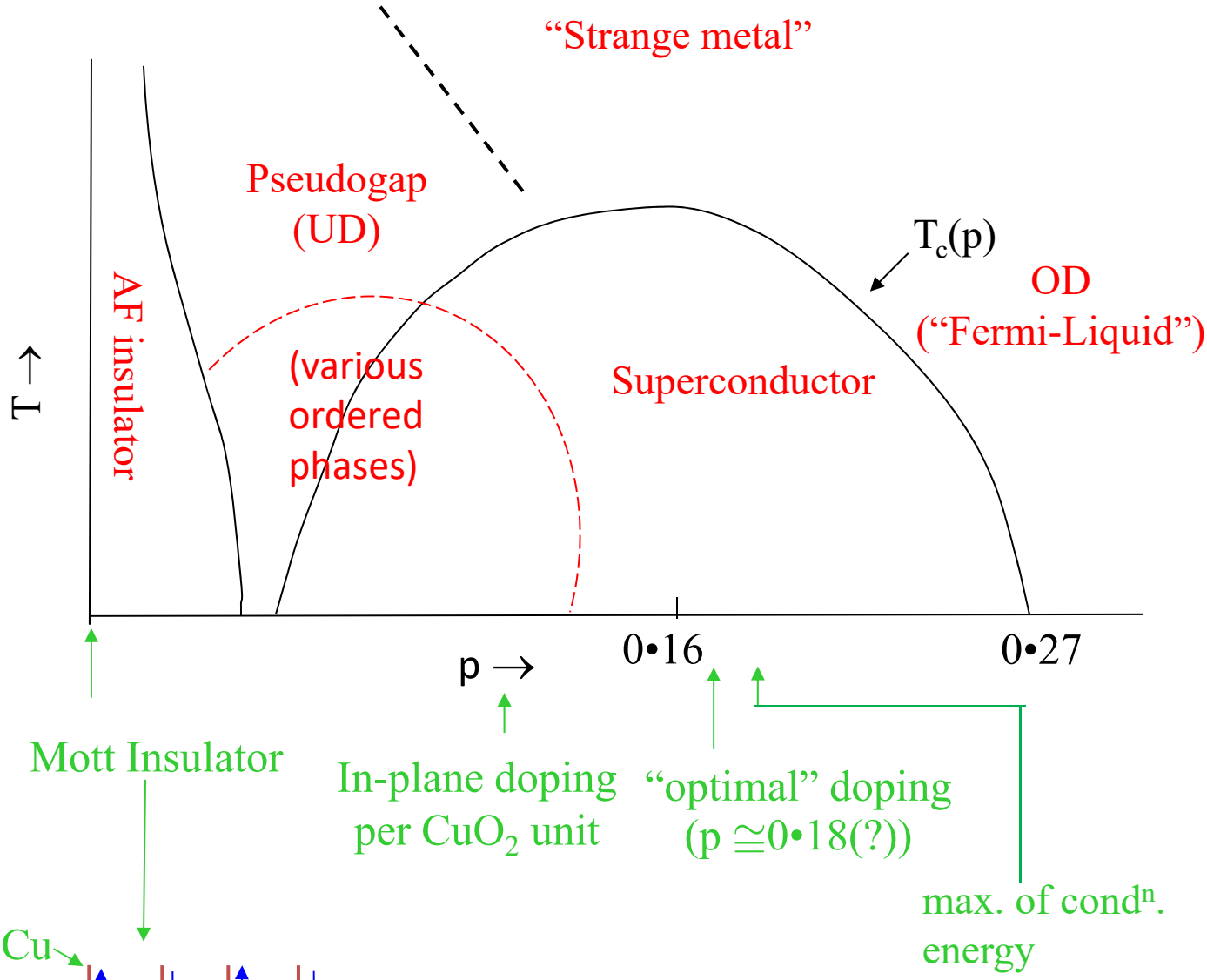


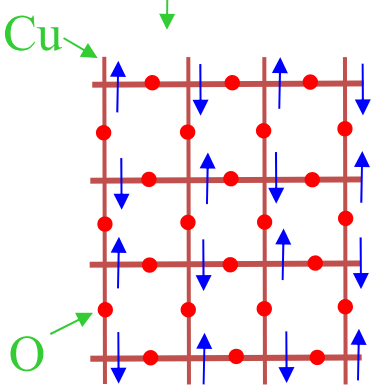
CuO_2 plane as viewed from above:



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.

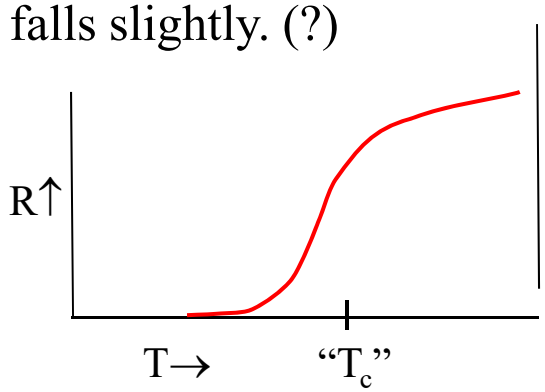
$Y\,Ba_2\,Cu_3\,O_{6+x}$, $La_{2-x}\,Sr_x\,CuO_4$

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 and properties "per plane" approx. "universal," ↑: but difficult to check directly.

SOME BASIC EXPERIMENTAL FACTS ABOUT CUPRATES

1. Until 2014, unique in showing (reproducible) sup^y at T> 60 K. (>200 different materials). (2014: metal hydrides, T ~ 200K!).
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 = 95 – 120 K)

   Atm. 20 GPa
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 ⇒ 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

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

antisymmetrizer

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

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

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

"pair wave function" (anomalous average)

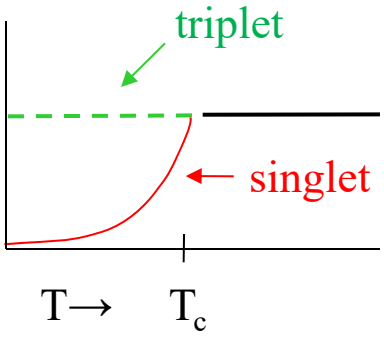
Note: "Macroscopic wave function" of Ginzburg and Landau, $\Psi(\underline{R})$, is just $F(\mathbf{r}_1 \mathbf{r}_2 \sigma_1 \sigma_2)$ for $\sigma_1 = -\sigma_2 = +1$, $\underline{r}_1 = \underline{r}_2 = \underline{R}$, i.e. wave function of COM of Cooper pairs.

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. $\chi_{s\uparrow}$



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

4. Absence of substantial FIR absorption above gap edge ⇒
   pairs formed from time-reversed states

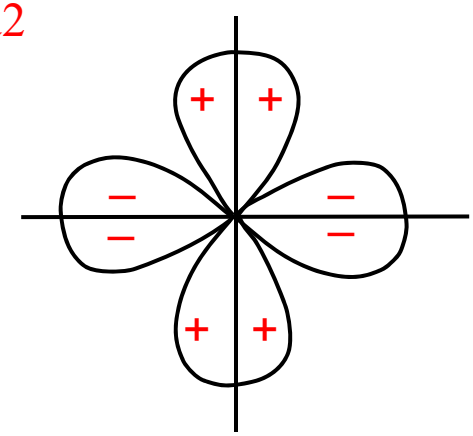
5. Order-of-magnitude (BCS-based) estimate from (a) T_c and (b) H_c ⇒ (in-plane) "radius" of Cooper pairs ~ a few lattice spacings.
   (thus, ξ_o / a ~ 3-10: contrast ~ 10^4 for Aℓ

pair radius inter-cond. electron spacing

⇒ fluctuations much more important than in e.g. Aℓ

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?)

7. c-axis resistivity ⇒ hopping time between unit cells along c-axis » $\hbar/k_BT$⇒
   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.

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.

Is there more we can say without a microscopic model?

HIGH-TEMPERATURE AND "QUASI-HIGH-TEMPERATURE" SUPERCONDUCTORS

Compound	(quasi-) 2D?	proximity to AF?	MIR peak?
cuprates	✓	✓	✓
ferropnictides	✓	✓	✓
β-FeSe	✓	✓	✓
organics (including doped PAH*)	✓	✓	✓
$PuMGa_5$	✓	(✓)	?

(exceptions: doped fullerenes, (H_2S) – BCS-like?)

On the other hand:
band structures very different
order parameter symmetry probably very different ...

What does this suggest?

Answer: Common factor related to above commonalities, but insensitive to details of band structure and OP symmetry

*polycyclic aromatic hydrocarbons

WHICH ENERGY IS SAVED IN THE SUPERCONDUCTING* PHASE TRANSITION?

A. DIRAC HAMILTONIAN (NR LIMIT):

$$\hat{H} = \underbrace{\sum_i \hat{p}_i^2 / 2m + \sum_\alpha \hat{P}_\alpha^2 / 2M}_{\hat{K}} + \frac{1}{2} \cdot \frac{1}{4\pi\varepsilon_o} \left\{ \sum_{ij} \frac{e^2}{|\boldsymbol{r} - \boldsymbol{r}_j|} + \underbrace{\sum_{\alpha\beta} \frac{(Ze)^2}{|\boldsymbol{R}_\alpha - \boldsymbol{R}_\beta|} - 2\sum_{i\alpha} \frac{Ze^2}{|\boldsymbol{r}_i - \boldsymbol{R}_\alpha|}}_{\hat{V}} \right\}$$

Consider competition between "best" normal GS and superconducting GS:

Chester, Phys. Rev. 103, 1693 (1956): at zero pressure,

$$\langle \hat{H} \rangle = \langle \hat{K} \rangle + \langle \hat{V} \rangle$$

$$\langle \hat{K} \rangle = -\frac{1}{2} \langle \hat{V} \rangle \quad \leftarrow \text{ virial theorem}$$

$$\rightarrow \langle \hat{H} \rangle = \frac{1}{2} \langle \hat{V} \rangle$$

Since $E_{cond} \equiv \langle \hat{H} \rangle_N - \langle \hat{H} \rangle_S > 0$,

$$\langle V \rangle_S < \langle V \rangle_N$$

i.e. total Coulomb energy must be saved in S transⁿ.

($e-e$, $e-n$, $n-n$) (and total kinetic energy must increase)

*or any other.

B. INTERMEDIATE-LEVEL DESCRIPTION:

partition electrons into "core" + "conduction", ignore phonons. Then, eff. Hamiltonian for cond^n electrons is

$$\hat{H} = \underbrace{\hat{K} + \sum_i \hat{U}(r_i)}_{\hat{K}_{eff}} + \frac{1}{2}\,\frac{1}{4\pi\varepsilon_o}\sum_{ij}\frac{e^2}{\varepsilon\left|\mathbf{r}_i - \mathbf{r}_j\right|} \leftarrow \hat{V}$$

high-freq. diel. const. (from ionic cores)

with $U(\mathbf{r}_i)$ independent of ε (?).

If this is right, can compare 2 systems with same form of $U(\mathbf{r})$ and carrier density but different ε.

Hellman-Feynman:

$$\frac{\partial\langle H\rangle}{\partial\varepsilon} = \left\langle\frac{\partial\hat{V}}{\partial\varepsilon}\right\rangle = -\frac{\hat{V}}{\varepsilon}$$

Hence provided $\langle\hat{V}\rangle$ decreases in N → S trans^n, (assumption!)

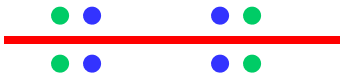
$\frac{\partial E_{cond}}{\partial\varepsilon} < 0$, i.e. "other things" ($U(\mathbf{r})$, n) being equal,

advantageous to have as strong a Coulomb repulsion as possible ("more to save"!)

Ex: Hg-1201 vs (central plane of) Hg - 1223

$\Rightarrow \varepsilon \gg 1$

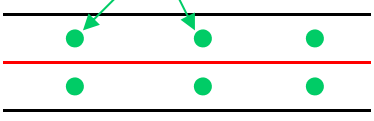
BaO_2, α large



Hg - 1201

$\Rightarrow \varepsilon \cong 1$

Ca^{++}, $\alpha \cong 0$



Hg - 1223

ENERGY CONSIDERATIONS IN "ALL-ELECTRONIC" QUASI-2D SUPERCONDUCTORS

(neglect phonons, inter-cell tunnelling)

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

- $\hat{T}_{(\|)}$: in-plane e^- KE
- $\hat{U}$: potential energy of conduction e^-'s in field of static lattice
- $\hat{V}_c$: inter-conduction e^- Coulomb energy (intraplane & interplane)

AND THAT'S ALL

(DO NOT add spin fluctuations, 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:

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

$$\left[3D :\equiv \int dq\int d\omega\left(\underbrace{\mathrm{Im}\frac{1}{\varepsilon(q\omega)}}_{\text{loss function}}\right)\right]$$

- 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?

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

[exact]

Coulomb interaction (repulsive)

bare density response function

$\sim \min(k_F, k_{FT}) - 1\text{Å}^{-1}$

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

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

perturbation—theoretic result

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

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

$\Rightarrow$ gap should change sign $\left(d_{x^2-y^2}, s_{\pm} \ldots\right)$

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

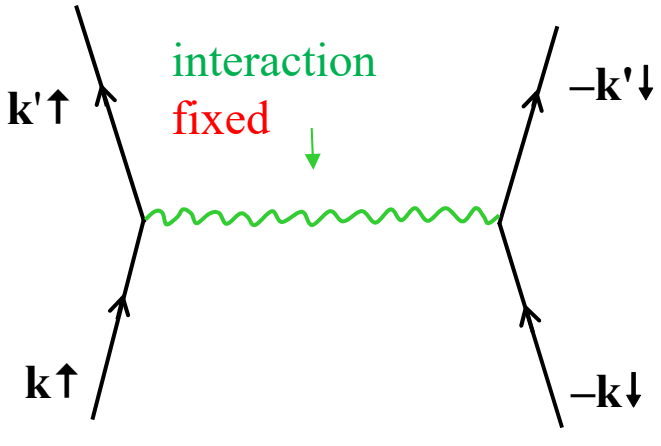
$$\langle V_c \rangle_q \cong \frac{1}{V_q}\left(-\mathrm{Im}\frac{1}{\chi_o(q\omega)}\right)$$

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

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

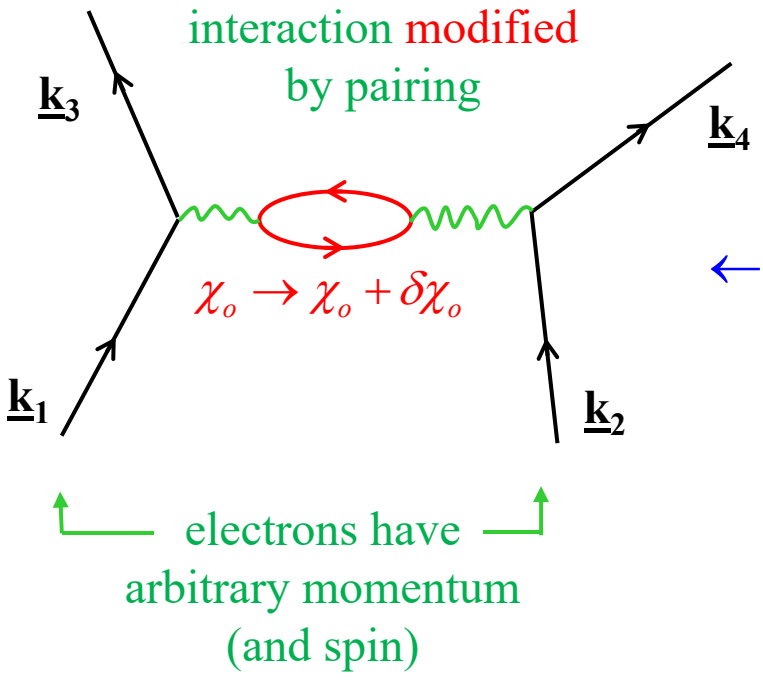
increased correlations $\Rightarrow$ increased screening $\Rightarrow$ decrease of Coulomb energy!

ELIASHBERG VS. OVERSCREENING



← ELIASHBERG

REQUIRES ATTRACTION IN NORMAL PHASE



← OVERSCREENING

NO ATTRACTION REQUIRED IN NORMAL PHASE

THE ROLE OF 2-DIMENSIONALITY

As above,

$$\langle V \rangle = -\frac{1}{2} \cdot \sum_{q} \int_{o}^{\infty} \frac{d\omega}{2\pi} \, \mathrm{Im} \left\{ \frac{1}{1 + V_q \chi_o(q\omega)} \right\}$$

$$= -\frac{1}{2} \cdot \frac{1}{(2\pi)^{d+1}} \int_{o}^{\infty} d^d q \, \mathrm{Im} \left\{ \frac{1}{1 + V_q \chi_o(q\omega)} \right\}$$

In 3D, $V_q \sim q^{-2}$,

$1 + V_q \chi_o(q\omega) \equiv \varepsilon_{\|}(q\omega)$, so

$$\langle V \rangle \sim \int q^2 dq \int d\omega \left\{ -Im \frac{1}{\varepsilon_{\|}(q\omega)} \right\} \quad \leftarrow \text{loss function}$$

so "small" q strongly suppressed in integral

In 2D, $V_q \sim q^{-1}$, ← interplane spacing

$$V_q \chi_o(q\omega) \sim q \frac{d}{2} \left(\varepsilon_{3D}(q\omega) - 1 \right)$$

$$\Rightarrow \langle V \rangle \sim \int q \, dq \left\{ -\mathrm{Im} \frac{1}{1 + q\frac{d}{2}\left(\varepsilon_{\|}(q\omega) - 1\right)} \right\}$$

$(qd \gtrsim 1)$

$$\sim \frac{1}{d} \int dq \left\{ -\mathrm{Im} \frac{1}{\varepsilon_{3D}(q\omega)} \right\} \qquad (\uparrow: \text{at given } \omega)$$

at least at first sight, small q as important as large q.

Hence, $64K question:

In 2D-like HTS (cuprates, ferropnictides, organics…)

is saving of Coulomb energy mainly at small q?

(might explain insensitivity to band structure, OP symmetry...)

CONSTRAINTS ON SAVING OF COULOMB ENERGY AT SMALL q*

$$\langle V \rangle_q = V_q \langle \rho_q \rho_{-q} \rangle = V_q \cdot \frac{1}{2\pi} \int_o^\infty \mathrm{Im}\ \chi(q\omega) d\omega$$

Sum rules for "full" density response χ(qω) (any d)

$$J_{-1} \equiv \frac{2}{\pi} \int_o^\infty \frac{\mathrm{Im}\ \chi(q\omega)}{\omega} d\omega = \chi(qo) \qquad \text{KK}$$

$$J_1 \equiv \frac{2}{\pi} \int_o^\infty \omega\ \mathrm{Im}\ \chi(\mathrm{q}\omega)\ \mathrm{d}\omega = \frac{nq^2}{m} \qquad \text{f-sum}$$

$$J_3 \equiv \frac{2}{\pi} \int_o^\infty \omega^3\ \mathrm{Im}\ \chi(\mathrm{q}\omega)\ \mathrm{d}\omega = \frac{q^2}{m^2}\langle A \rangle + q^4 \frac{n^2}{m^2}\ V_q + o(q^4)$$

(generalized Mihara-Puff)

where:

$$\langle A \rangle \equiv -\frac{1}{\pi} \sum_{\boldsymbol{\kappa}} (\hat{\kappa} \cdot \hat{\boldsymbol{q}})^2 U_{-\kappa} \rho_\kappa > 0$$

reciprocal lattice vector

Note in 2D, term in $\langle A \rangle$ is dominant at small q.

General CS inequalities (any d):

Cauchy-Schwarz

$$\frac{1}{2}\left(V_q^2 J_{-1} J_1\right)^{1/2} \geq \langle V \rangle_q \geq \frac{1}{2}\left(V_q^2 J_1^3 / J_3\right)^{1/2}$$

or

*M. Turlakov and AJL, Phys. Rev. B **67**, 94517 (2003)
(do not go via band theory!)

$$\frac{\hbar\omega_p}{2} + o\left(q^2\right) \geq \left\langle V \right\rangle_q \geq \frac{\hbar\omega_p}{2} \frac{1}{\left(1 + \left\langle A \right\rangle / nm\omega_p^2\right)^{1/2}} + o\left(q^2\right)$$

notional "plasma frequency,"

$$\left(nq^2 V_q / m\right)^{1/2}$$

Implications for saving of Coulomb energy at small q by N→S transition:

(a) order of magnitude of $\left\langle V_c \right\rangle_q$ is $\hbar\omega_p(q)$.

(b) for $\left\langle A \right\rangle \to 0$ ("jellium" model), no saving (for any d). Lattice is crucial! ("umklapp")

↑ dimension

(c) in 3D $\left(\omega_p^2 \sim const.\right)$ can save at most a fraction of N-state Coulomb energy, while in 2D $\left(\omega_p^2 \sim q\right)$ can in principle save all of it.

(d) Thus, total contribution from $q < q_0 \left(\ll k_F\right)$:

3D: q_0^3, of which only part can be saved

2D: $q_0^{5/2}$, of which all can be saved

(e) "other things being equal", lower limit $\propto n^{5/2} \Rightarrow$ might favor low e^- density

Q: How much needs to be saved?

A: Not much! (~1K/CuO_2 unit for Tl 2201, for Tl-2223 ~2.5K/ CuO_2 unit)

Are there independent reasons for suspecting small q may be important? Apparently totally unrelated question:

* WHY, in homologous series, does T_c depend on n?

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

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

Possible explanations:

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

$V_{int}(q) \sim q^{-1} \exp -qd$ ← intra-multilayer spacing ($\sim 3 \cdot 5$)

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…)

CONJECTURED "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. why HTS insensitive to band structure + OP symmetry
   d. trends of T_c with layering structure in Ca-spaced cuprates
   e. absence of superconductivity in bilayer Ba/Sr-spaced cuprates.
   f. "huge" (~100 × BCS) effects of superconductivity on optical properties in 1–3 eV range.
3. Unambiguously falsifiable in EELS experiments.

CONS (as of May, 2019):

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 experiments indicate falsified for UD regime (but OK for OD).

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

TO TEST MIR SCENARIO:

Ideally, would like to measure

Changes in loss function $\leftarrow -Im\frac{1}{\varepsilon_{\parallel}(q\omega)}$

across superconducting transition, for

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

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

Possible Probes:

1) Optics (ellipsometry) "transverse," arb. ω but q ≪ $0 \cdot 3$ Å^{-1}
2) Transmission EELS
3) Inelastic X-ray SC'G

} "long'l," arb. q, ω

Existing experiment:

Optics*: small (~1 – 2%) change on crossing T_c in loss function integrated across MIR region: positive in underdoped regime, negative in overdoped regime.

EELS: recent Abbamonte group data shows doping-dependence similar to optics, but with onset substantially above T_c.

*Levallois et al. (inc. AJL), Phys. Rev. X **6**, 031027 (2016)

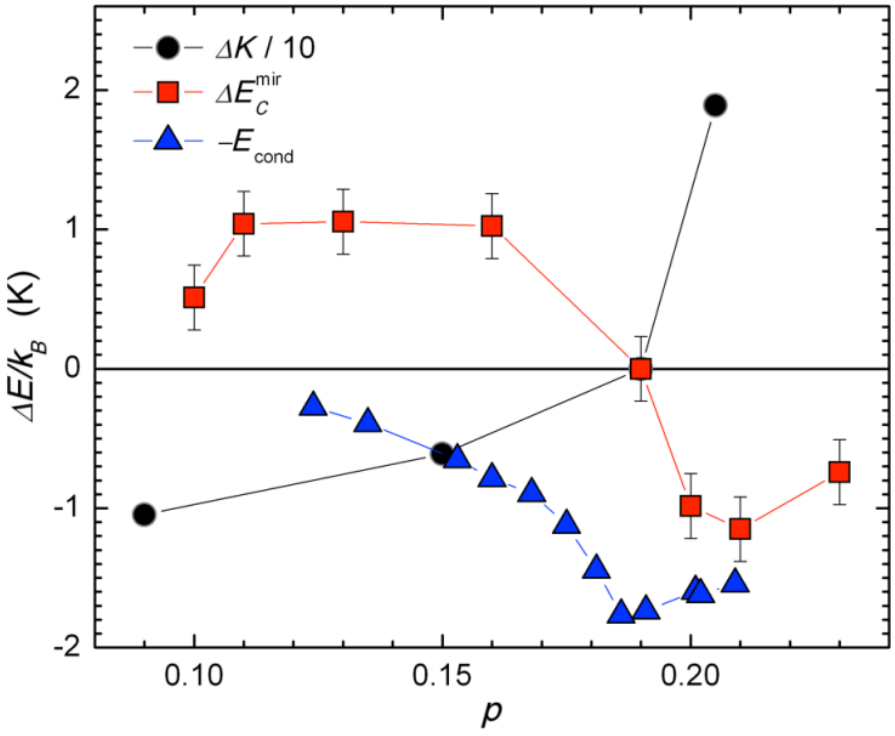


FIG. 5. The S–N difference of the **q**-integrated Coulomb energy $\Delta E_C^{\mathrm{mir}}$, together with the total energy difference $-E_{\mathrm{cond}}$ (data reproduced from Ref. [44], with original units converted to the present ones for the sake of comparison) and band-energy difference ΔK [33].