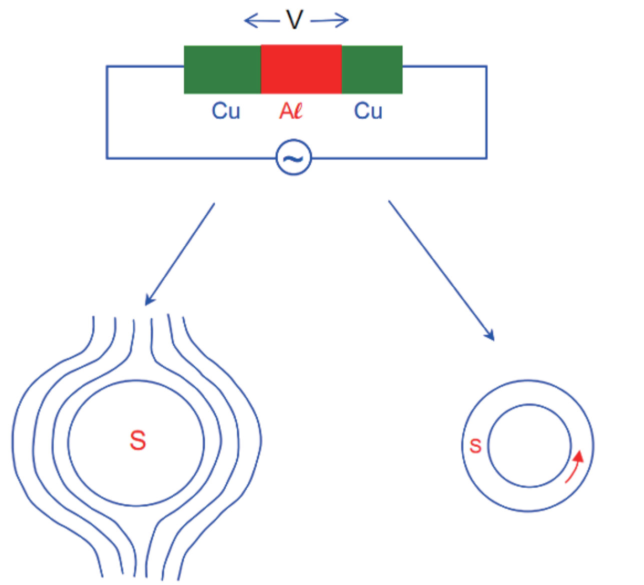
Lecture 8. Exotic Superconductivity : discussion

1) **What do all exotic superconductors have in common?**
2) **Some theoretical approaches**
3) **General considerations on energy saving in "all-electronic" superconductors.**

1) What do all exotic superconductors have in common?

First, (obviously !) superconductivity itself.
What does this mean, and what does it imply?



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" $\Psi(\boldsymbol{r})$ ← Schrödinger-like

$$\Psi(r) = |\Psi(\boldsymbol{r})| \exp(i\phi(\boldsymbol{r})) \leftarrow \text{must be single valued mod. } 2\pi$$

vector potential

$$\text{electric current} \rightarrow \boldsymbol{J}(\boldsymbol{r}) \propto |\Psi(\boldsymbol{r})|^2 (\nabla\phi(\boldsymbol{r}) - e^* \boldsymbol{A}(\boldsymbol{r}))$$

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

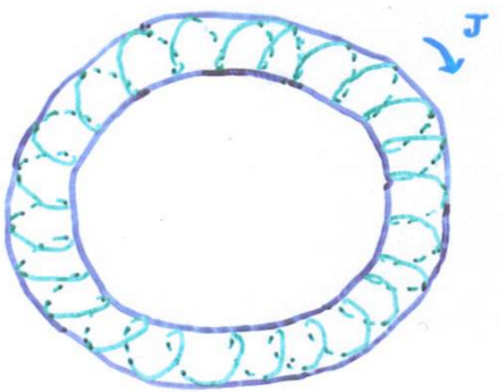
Meissner Effect : exact analog of atomic diamagnetism

$$\int \nabla\phi(\boldsymbol{r}) \cdot d\boldsymbol{l} = 0 \Rightarrow \boldsymbol{J} = -\frac{ne^2}{m}\boldsymbol{A} = -\lambda_L^{-2}\boldsymbol{A}$$

$$\Rightarrow \nabla^2 \boldsymbol{B} = \lambda_L^{-2}\boldsymbol{B} \Rightarrow \boldsymbol{B} = \boldsymbol{B_0} \exp\left(-\frac{z}{\lambda_L}\right) \text{ in atom, supr}$$

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

Persistent current



$n \equiv \frac{1}{2\pi} \int \nabla\phi(\boldsymbol{r}) \cdot d\boldsymbol{l}$

conserved unless $|\Psi(\boldsymbol{r})| \rightarrow 0$ across some X-section

(highly unfavorable energetically)

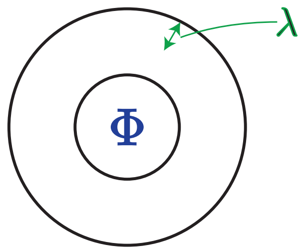
$\Rightarrow J \sim n =$ conserved

For these arguments to work, there must exist a complex order parameter $\Psi(\boldsymbol{r})$ such that
(a) nonzero values of $|\Psi(\boldsymbol{r})|^2$ are (locally) stable
(b) spatial gradients of the phase of $\Psi(r)$ correspond to charge currents.
Overwhelmingly natural guess: $\Psi(\boldsymbol{r})$ represents macroscopically occupied eigenfunction of n-particle density matrix(i.e. system possesses ODLRO). More rigorous arguments (Yang, Kohn + Sherrington) claim to show

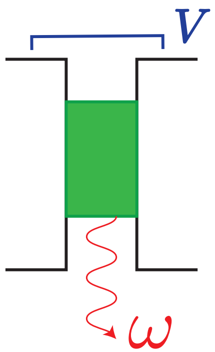
ODLRO is a necessary and sufficient condition for superconductivity.

($\Uparrow$: "anyon superconductivity" not a counterexample)
Even if true, "theorem" says nothing about value of n. Since electrons are fermions, n must be even. But in principle, could be 4,6,.....

How can we tell?
(a) In (thick) ring geometry, Φ (trapped flux) quantized in units of h/ne
(b) In Josephson effect, (principal) frequency $\omega = neV/\hbar$
No evidence for any value of n other than 2 in any (exotic) superconductor



$\Rightarrow$ Superconductivity = Formation of Cooper Pairs



WHAT ELSE (i.e. apart from superconductivity itself) DO THE VARIOUS EXOTIC SUPERCONDUCTORS HAVE IN COMMON?

Apparently, not much! Even if we exclude alkali fullerides,

- not all non-phonon (?) (organics)
- not all quasi-2D (heavy Fermions)
- not all close to AF phase (some heavy Fermions, Sr_2RuO_4)

However, if we restrict ourselves to "high-temperature" superconductors (cuprates, ferropnictides, organics) then,

(a) all strongly 2D

(b) all have AF phase close by

(c) all have charge reservoirs well separated from (super) conducting layers.

SOME THEORETICAL APPROACHES (schematic, mostly cuprates)

1. Generic "BCS-like" approach

   try to identify quantitatively dominant physical effect, write down effective low-energy Hamiltonian encapsulating it. (example: bipolarons, excitons, d-density wave, chiral plaquettes,...)

   Problem: not obvious that only (single-electron) states with $|\varepsilon| \ll k_B T_c$ are relevant! (cf. optical properties of cuprates)

2. Approaches based on Hubbard model:

$$\hat{H}_{\text{eff}} = -t \sum_{\sigma,i,j\in\text{n.n.}} (a_{i\sigma}^\dagger a_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

   Problem: not (known to be) analytically soluble (even in 2D)

   Some possible strategies:

   (a) (Digital) numerical simulations (typically up to $\sim 10 \times 10$)

   (b) Analog simulation (ultracold atoms in optical lattices)

   (c) "Guesses" at analytic solution.

   e.g. $\Psi_{\text{N}} \sim \hat{\mathcal{P}}_{\text{G}} \Psi_{\text{BCS}}$

   $\hat{\mathcal{P}}_{\text{G}}$: Gutzwiller projection, removes all terms corresponding to double occupation of any site.

   Problem: Hubbard model may omit important physical effects (e.g. long-range part of Coulomb interaction)

3. AF spin fluctuations exchange

In all high-T_c superconductors, S phase occurs close to an AF one, Moreover, both NMR and neutron scattering (in cuprates) imply that the spin susceptibility $\chi(q,\omega)$ is (in N phase) featureless as $f(\omega)$ but strongly peaked as $f(q)$ as $Q \equiv (\pi/a, \pi/a)$ (superlattice Bragg vector in AF phase).

Possible ansatz for $\chi(q,\omega)$ ($\equiv \chi_{\mathrm{NAFL}}(q,\omega)$) (Pines et al):

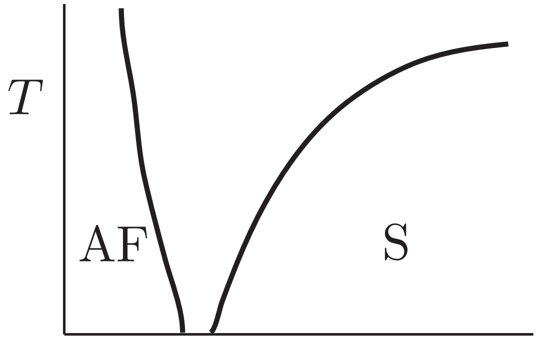
far from pseudo-Bragg vector $Q \equiv (\pm\pi/a, \pm\pi/a)$, $\chi_{\mathrm{NAFL}}(q,\omega)$ has Fermi liquid-like form:

$$\chi_{\mathrm{NAFL}}(q,\omega) \cong \frac{\chi_{\boldsymbol{q}}}{1 - i\omega/\Gamma_{\boldsymbol{q}}} \cong \frac{\chi_0}{1 - i\omega/\Gamma_0}$$

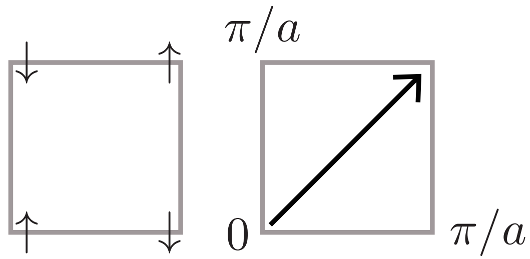
However, near a pseudo-Bragg vector,

$$\chi_{\mathrm{NAFL}}(q,\omega) \cong \frac{\chi_{\boldsymbol{Q}_i}\ (\gg \chi_{\boldsymbol{q}})}{1 + (\boldsymbol{Q}_i - \boldsymbol{q})^2 \xi^2(T) - i\omega/\omega_{\mathrm{SF}}}$$

where $\omega_{\mathrm{SF}} \ll \Gamma_0$ is AF fluctuation frequency, and $\xi(T)$ is AF correlation length.



(cuprates)



real space k-space

Ansatz (not directly testable in experiment):

Electrons couples strongly to AF spin fluctuations, whose exchange then generates an effective electron-electron attraction (cf ^{3}He)

Striking prediction of spin-fluctuation theories (rather generic):

(a) points on Fermi surface most nearly connected by $\boldsymbol{Q}_i$ are at $(\pi, 0)$, $(0, \pi)$ (etc.) $\Rightarrow$ expect gap max. there.

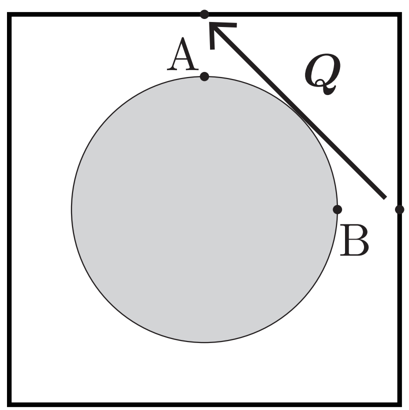
(b) sign of pair wave function $F(\boldsymbol{k})$: scattering processes should as far as possible leave F invariant.

But emission of virtual spin fluctuation flips spin, changes momentum by $\boldsymbol{Q}$. If state is singlet, spin flips $\Rightarrow \times(-1)$. Hence to preserve F, momentum change A $\to$ B must also $\times(-1)$.

Hence, from (a) F must be large at $(\pi, 0)$ (b) F must change sign under $\hat{R}_{\pi/2}$. Of 4 even-parity irreps of C_{4v}, only $d_{x^2-y^2}$ works. Thus,

Spin Fluctuation theories unambiguously predict $d_{x^2-y^2}$ symmetry.

Problem: many fitted parameters



WHICH ENERGY IS SAVED IN THE SUPERCONDUCTING (or any other) PHASE TRANSITION?)

A. Dirac Hamiltonian(non-relativistic limit):

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

$$\hat{K} = \sum_i \frac{\hat{p}_i^2}{2m} + \sum_\alpha \frac{\hat{P}_\alpha^2}{2M}$$

$$\hat{V} = \frac{1}{8\pi\varepsilon_0}\left\{\sum_{i,j}\frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} + \sum_{\alpha,\beta}\frac{(Ze)^2}{|\boldsymbol{R}_\alpha - \boldsymbol{R}_\beta|} - 2\sum_{i,\alpha}\frac{Ze^2}{|\boldsymbol{r}_i - \boldsymbol{R}_\alpha|}\right\}$$

Consider competition between “best” normal and superconducting ground state:
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 $E_{\mathrm{cond}} = \langle\hat{H}\rangle_{\mathrm{N}} - \langle\hat{H}\rangle_{\mathrm{S}} > 0$,

$$\langle\hat{V}\rangle_{\mathrm{S}} < \langle\hat{V}\rangle_{\mathrm{N}}$$

i.e. total Coulomb energy (e-e, e-n, n-n) must be saved in superconducting transition.

B. Intermediate-level description:

partition electrons into "core"+"conduction", ignore phonons. Then, effective Hamiltonian for conduction electrons is

$$\hat{H} = \hat{K}_{\text{eff}} + \hat{V}_{\text{eff}}$$
$$\hat{K}_{\text{eff}} = \sum_i \frac{\hat{p}_i^2}{2m} + \hat{U}(\boldsymbol{r}_i)$$
$$\hat{V}_{\text{eff}} = \frac{1}{8\pi\varepsilon_0} \sum_{i,j} \frac{e^2}{\varepsilon |\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

with $U(\boldsymbol{r}_i)$ independent of ε (?), where ε is high-frequency dielectric constant(from ionic cores).

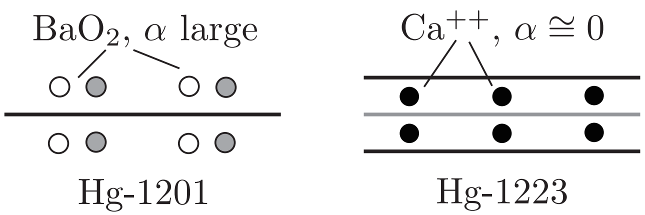
If this is right, can compare 2 systems with same form of $U(\boldsymbol{r})$ and carrier density but different ε.

Hellman-Feynman:

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

Hence provided $\langle \hat{V} \rangle$ decreases in N $\to$ S transition, (assumption!) $\dfrac{\partial E_{\text{cond}}}{\partial \varepsilon} < 0$, i.e. "other things" $(U(\boldsymbol{r}), n)$ being equal, advantageous to have as strong a Coulomb repulsion as possible ("more to save"!)

e.g.: Hg-1201 vs (central plane of) Hg-1223



ENERGY CONSIDERATION IN "ALL-ELECTRONIC" SUPERCONDUCTORS

(neglect phonons, inter-cell tunneling)

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

$\hat{T}_{(\parallel)}$: in-plane e^- KE

$\hat{U}$: potential energy of condensation electrons in field of static lattice

$\hat{V}_c$: inter-conduction e^- Coulomb energy (intraplane and inter plane)

AND THAT'S ALL

(DO NOT add spin fluctuations, excitons, anyons...)

At least one of $\langle\hat{T}\rangle$, $\langle\hat{U}\rangle$, $\langle\hat{V}_c\rangle$ must be decreased by formation of Cooper pairs. Default option: $\langle\hat{V}_c\rangle$

Rigorous sum rule:

$$\langle\hat{V}_c\rangle \sim -\int d^3\boldsymbol{q}\int d\omega\,\mathrm{Im}\left\{\frac{1}{1+V_{\boldsymbol{q}}\chi_0(\boldsymbol{q},\omega)}\right\}$$

$$[3D \equiv \int d^3\boldsymbol{q}\int d\omega\,(-\mathrm{Im}\,\varepsilon(\boldsymbol{q},\omega)^{-1})]$$

where $V_{\boldsymbol{q}}$ is Coulomb interaction (repulsive) and $\chi_0(\boldsymbol{q},\omega)$ is bare density response function.

Where in the space of $(\boldsymbol{q},\omega)$ is the Coulomb energy saved (or not)?

This question can be answered by experiment! (EELS, Optics, X-rays)

HOW CAN PAIRING SAVE COULOMB ENERGY?

$$\langle \hat{V}_c \rangle \sim -\int d^3\boldsymbol{q} \int d\omega \, \mathrm{Im} \left\{ \frac{1}{1 + V_{\boldsymbol{q}} \chi_0(\boldsymbol{q}, \omega)} \right\} \quad \text{[exact]}$$

A. $V_{\boldsymbol{q}} \chi_0(\boldsymbol{q}, \omega) \ll 1$ (typical for $q \gg q_{\mathrm{TF}}^{(\mathrm{eff})} \sim \min(k_{\mathrm{F}}, k_{\mathrm{TF}}) \sim 1\text{Å}^{-1}$)

$$\langle \hat{V}_c \rangle_{\boldsymbol{q}} \cong +V_{\boldsymbol{q}} \int d\omega \, \mathrm{Im} \, \chi_0(q, \omega) = V_{\boldsymbol{q}} \langle \rho_{\boldsymbol{q}} \rho_{-\boldsymbol{q}} \rangle_0$$

$\Rightarrow$ to decrease $\langle \hat{V}_c \rangle_{\boldsymbol{q}}$, must decrease $\langle \rho_{\boldsymbol{q}} \rho_{-\boldsymbol{q}} \rangle_0$
but $\delta \langle \rho_{\boldsymbol{q}} \rho_{-\boldsymbol{q}} \rangle_{\mathrm{pairing}} \sim \sum_{\boldsymbol{p}} \Delta_{\boldsymbol{p}+\boldsymbol{q}/2} \Delta^*_{\boldsymbol{p}-\boldsymbol{q}/2}$
$\Rightarrow$ gap should change sign (d-wave?)

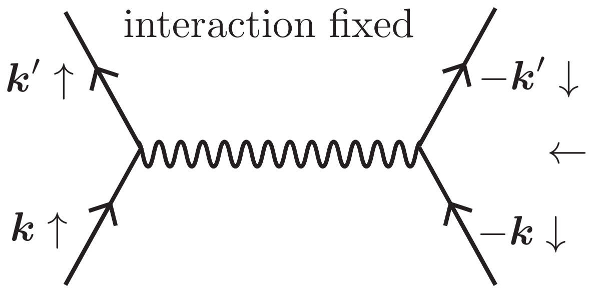
B. $V_{\boldsymbol{q}} \chi_0(\boldsymbol{q}, \omega) \gg 1$ (typical for $q \gg q_{\mathrm{TF}}^{(\mathrm{eff})}$)

$$\langle \hat{V}_c \rangle_{\boldsymbol{q}} \cong \frac{1}{V_{\boldsymbol{q}}} \left(-\mathrm{Im} \chi_0(\boldsymbol{q}, \omega)^{-1} \right) \quad \leftarrow \text{note inversely proportional to } V_{\boldsymbol{q}}$$

$\Rightarrow$ to decrease $\langle \hat{V}_c \rangle_{\boldsymbol{q}}$, (may) increase $\mathrm{Im}\chi_0(\boldsymbol{q}, \omega)$ and thus (possibly) $\langle \rho_{\boldsymbol{q}} \rho_{-\boldsymbol{q}} \rangle_0$

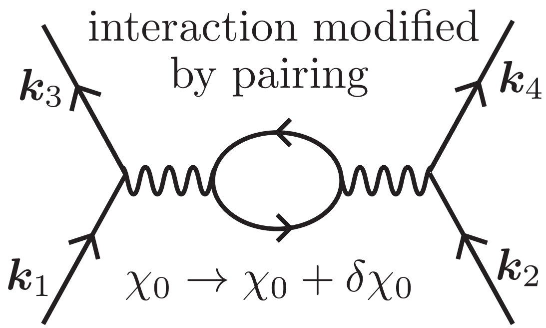
increased correlations $\Rightarrow$ increased screening $\Rightarrow$ decrease of Coulomb energy!

ELIASHBERG vs. OVERSCREENING



← Eliashberg

REQUIRES ATTRACTION IN NORMAL PHASE



← overscreening

NO ATTRACTION REQUIRED IN NORMAL PHASE

The Role of 2-Dimensionality

As above,

$$\langle V\rangle = -\frac{1}{2}\sum_q \int \frac{d\omega}{2\pi}\mathrm{Im}\Big\{\frac{1}{1+V_q\chi_0(q,\omega)}\Big\}$$
$$= -\frac{1}{2}\frac{1}{(2\pi)^{d+1}}\int_0^\infty d^d q\,\mathrm{Im}\Big\{\frac{1}{1+V_q\chi_0(q,\omega)}\Big\}$$

In 3D, $V_q \sim q^{-2}$,$1+V_q\chi_0(q,\omega)\equiv\varepsilon_{||}(q,\omega)$, so

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

so "small" q strongly suppressed in integrals.

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

$$V_q\chi_0(q,\omega) \sim q\frac{d}{2}(\varepsilon_{3D}(q,\omega)-1)$$

(interplane spacing $\rightarrow d$)

$$\Rightarrow \langle V\rangle \sim \int q\,dq\Big\{-\mathrm{Im}\frac{1}{1+q\frac{d}{2}(\varepsilon_{3D}(q,\omega)-1)}\Big\}$$
$$\sim \frac{1}{d}\int dq\Big\{-\mathrm{Im}\frac{1}{\varepsilon_{3D}(q,\omega)}\Big\}$$

small q as important as large q.

Hence, \$64,000 question :

In 2D-like high-T_c superocnductors (cuprates, ferropnictides, organics...)

is saving of Coulomb energy ,mainly at small q?

Constraints on saving of Coulomb energy at small q

$$\langle V\rangle = V_q\langle\rho_q\rho_{-q}\rangle = V_q\frac{1}{2\pi}\int_0^\infty \mathrm{Im}\chi(q,\omega)d\omega$$

Sum rules for "full" density response $\chi(q,\omega)^*$ (any d)

$$J_{-1} \equiv \frac{2}{\pi}\int_0^\infty \frac{d\omega}{\omega}\mathrm{Im}\chi(q,\omega) = \chi(q,0) \qquad \text{KK-relation}$$

$$J_1 \equiv \frac{2}{\pi}\int_0^\infty \omega d\omega \mathrm{Im}\chi(q,\omega) = \frac{nq^2}{m} \qquad \text{f-sum}$$

$$J_3 \equiv \frac{2}{\pi}\int_0^\infty \omega^3 d\omega \mathrm{Im}\chi(q,\omega) = \frac{q^2}{m^2}\langle A\rangle + q^4\frac{n^2}{m^2}V_q + o(q^4) \qquad \text{(generalized Mihara-Puff)}$$

where:

$$\langle A\rangle \equiv -\frac{1}{\pi}\sum_k (\boldsymbol{k}\cdot\hat{\boldsymbol{q}})^2 U_{-k}\rho_k > 0 \qquad (?)$$

Note in 2D, term in $\langle A\rangle$ is dominant at small q. General Cauchy-Schwartz inequalities (any d):

$$\frac{1}{2}\sqrt{V_q^2 J_{-1}J_1} \geq \langle V\rangle_q \geq \frac{1}{2}\sqrt{V_q^2 J_1^3/J_3}$$

or

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

$\Rightarrow$ for $\langle A\rangle = 0$ ("jellium" model) no saving of Coulomb energy for $q \to 0$. Lattice is crucial!

$*$ M. Turlakov and AJL. Phys. Rev. B **67**, 044517 (2003)

$$\langle V_c\rangle_S - \langle V_c\rangle_N \sim \int d^2q \int d\omega V_q \mathrm{Im}\Big\{\frac{\delta\chi(q,\omega)}{1+V_q\chi_0(q,\omega)}\Big\}$$

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

$*$ WHY 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)

$$T_c^{(n)} - T_c^{(1)} \sim \mathrm{cont}\Big(1 - \frac{1}{n}\Big) \quad \text{(controversial)}$$

Possible explanation:

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 tunneling model
2. Kosterlitz-Thouless
3. Inter-plane Coulomb interactions ← We know they're there !

in-plane wave vector

$$V_{\mathrm{int}}(q) \sim q^{-1}\exp(-qd)$$

← intra-multilayer spacing ($\sim 3.5\mathring{A}$)

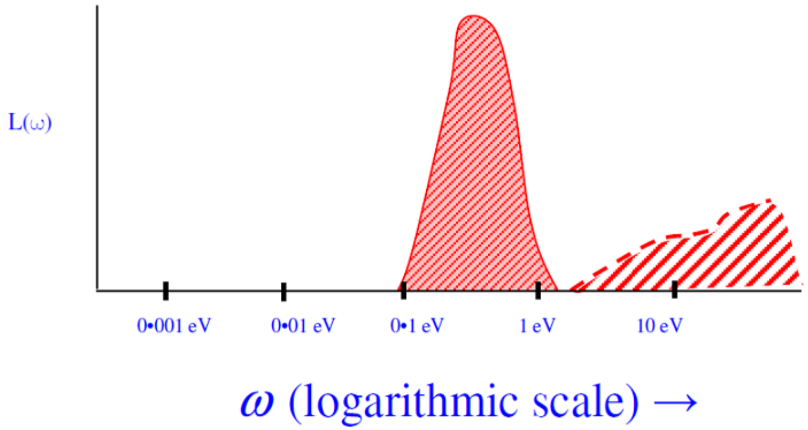
If (3) is right, then even in single plane materials, dominant region of q is $q < d^{-1}$!!

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

N state

MIR (Mid-Infrared) Optical + EELS Spectra of the Cuprates

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



B. EELS

Confirms $q \to 0$ shape of the loss function, and verifies that (roughly) same shape persists for finite q. (at least up to $\sim 0.3\mathring{A}$)

So that's where the money is !

Digression:

This strong peaking of the loss function in the MIR (mid-infrared) appears to be a necessary condition for high-T_c superconductors. Is it also 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 !

ferropnictides?

If saving of Coulomb energy is mainly in Low-q MIR regime...

N→S must decrease-Imε^{-1} in this regime.
i.e. $\text{Im}\frac{\delta\varepsilon}{\varepsilon_n^2} > 0$
but, in MIR regime, in N phase*

$$\varepsilon_n(\omega) \cong \frac{\omega_p^2}{\omega^2} - 1 + i \Rightarrow \varepsilon_n^{-2} \sim \frac{\omega^4}{2\omega_p^4} i$$

⇒ need Re$\delta\varepsilon > 0$ in MIR. By KK-relation, this ⇒

$$\int_0^\infty \omega'^4 \left\{ \frac{1}{2} \log \left| \frac{\omega_e + \omega'}{\omega_e - \omega'} \right| - \frac{\omega_e}{\omega'} \right\} \text{Im}\delta\chi(q, \omega') d\omega' < 0 \quad (\omega_e \sim \omega_p)$$

↑ positive for $\omega' > \overline{\omega}_e \sim \omega_e \sim \omega_p$

negative for $\omega' < \overline{\omega}_e$
⇒ expect spectral weight transfer from $\omega > \omega_p$ to $\omega < \omega_p$ (MIR).

↑ : optics measres $q \ll \xi^{-1}$, whereas saving of Coulomb energy should be mainly from $\xi^{-1} < q \lesssim q_{TF}$.
⇒NEED EELS EXPERIMENT !
(P. Abbamonte, J. Zuo (UIUC))

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* El-Azrak et. al., Phys. Rev. B **49**, 9846 (1994)

If this is right, what are good "ingredients" for enhancing T_c?

1. 2-dimensionality (weak tunneling contact between layers, but strong Coulomb contact)
2. Strongest possible Coulomb interaction (intra-plane and inter-plane)
3. Strong Umklapp $\overset{(?)}{\Rightarrow}$ effects wide and strong MIR peak (may come from strong AF-type fluctuations?)

My bet on robust room temperature superconductivity :
in my lifetime : $\sim 10\%$
in (some of) yours : $> 50\%$