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EXPERIMENTAL WORKSHOP ON
"HIGH TEMPERATURE SUPERCONDUCTORS"
(30 March - 14 April 1989)

PHENOMENOLOGY AND THEORY OF SUPERCONDUCTIVITY
Lecture III :
'MICROSCOPIC BASIS OF SUPERCONDUCTIVITY - PAIRING'

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These are preliminary lecture notes, intended only for distribution to participants.

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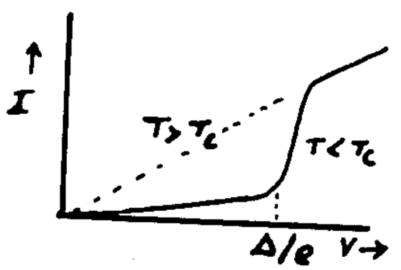
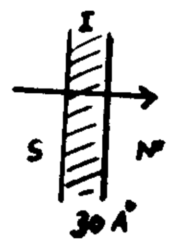
SUPERCONDUCTIVITY - PAIRING

- Identification of Order Parameter Ψ with a MACROSCOPIC EFFECTIVE WAVEFUNCTION for the multi-electron system, provides a useful description for
  1. All macroscopic coherence phenomena - Josephson Junction SC tunneling, SQUID dc & rf
  2. Response to magnetic fields, field penetration, vortex structure, flux quantization
  3. Thermodynamics of type I &, importantly, type II SC, H_{c_1}, H_{c_2}, H_c
  4. parametrization of GL functional from exptl. data
- But the exact Nature of Ψ itself remains obscure.
- Also, there are single-particle (quasiparticle) aspects that lie outside phenomenology
- Example: Quasiparticle tunneling S/N





quasiparticle Injection

Tunneling gap Δ (very different from semicond. type gap)

- Also INFRARED, ULTRA SOUND Absorption gap 2Δ
- other kinetic effects (NMR relaxation $1/T_1$) etc.
- These require microscopic treatment of the many-electron system, and quasiparticle spectrum
- It is at the microscopic level that the New HTSC may turn out to be profoundly different.
- For LTSC, the GL free energy and Ψ are derivable from BCS theory.

• 1. Normal metallic state is a Fermi-Liquid with well defined Fermi surface (FS).
Recall Landau theory of Fermi Liquids: one-to-one correspondence between the Ground- and the excited states of the real interacting electrons with those of ideal non-interacting electron gas.
The strongly interacting bare particles are replaced by weakly interacting dressed "quasiparticles" infinitely long lived at Fermi surface and good for phenomena involving Low Lying excitations. These quasiparticles are spin $\frac{1}{2}$ Fermions carrying electronic charge and well defined momentum $\hbar \underset{\sim}{k}$ and energy $\epsilon_{\underset{\sim}{k}}$ for Uniform system.
These dressed objects are the particles that are to be paired in SC.

• 2. PAIRING Instability of the Normal state for attraction between particles at FS, arbitrarily weak.

• 3. Non-perturbative modification of Normal state, by Coherent Superposition of paired states taking maximum advantage of pairing attraction to lower energy

• 4. Pairs act on other particles/pairs by a meanfield PAIR POTENTIAL to be determined self-consistently — something similar to self-consistent

Field Approximation out the Normal Hartree-Fock replaced by an anomalous (Gor'kov) factorization, i.e.

$$c_1^+ c_2^+ c_3 c_4 \simeq \langle c_1^+ c_2^+ \rangle c_3 c_4 + c_1^+ c_2^+ \overbrace{\langle c_3 c_4 \rangle}^{\text{Anomalous}} \cdots$$

instead of

$$c_1^+ c_2^+ c_3 c_4 \simeq -\langle c_1^+ c_3 \rangle c_2^+ c_4 + \overbrace{\langle c_1^+ c_4 \rangle}^{\text{Normal}} c_2^+ c_3 - c_1^+ c_3 \langle c_2^+ c_4 \rangle + c_1^+ c_4 \langle c_2^+ c_3 \rangle \cdots$$

- Non-vanishing of anomalous averages involving both annihilation (or creation operators), and, therefore, not-diagonal in particle number and requiring grand canonical ensemble formally, is the essence of Superconducting Coherence (OFF-DIAGONAL LONG RANGE ORDER ≡ ODLRO).
- This Anomalous Expectation $\langle cc \rangle$ is the GL order parameter Ψ, a measure of superfluid density or condensate.
- The many-body prollem is complicated by the relative smallness of the effect to be calculated.

Energy scales:

- Fermi energy ~ 5~10 eV
- coulomb correlation ~ 1 eV/electron
- phonon (Debye) energy ~ 10^{-2} - 5×10^{-2} eV
- Supercond. gap 2Δ ($\sim k_B T_c$) ~ 0 - 10^{-3} eV
- supercond. Condensation energy ~ 0 - 10^{-8} eV/electron
- Too small to be obtained by calculating the larg. Normal and SC state energies. MUST directly consider and isolate the PAIRING effects.

* NORMAL GROUND STATE (Fermi sea)

- $|FS\rangle = \prod_{k<k_F} c^+_{k\sigma}|0\rangle$, all states up to E_F filled.

<u>SC</u> GROUND STATE with $+k\uparrow, -k\downarrow$ <u>paired occupation</u>

- $|BCS\rangle = \prod_k (u_k + v_k c^+_{+k\uparrow} c^+_{-k\downarrow})|0\rangle$

  $(u_k^2 + v_k^2 = 1)$

  $|v_k|^2$ = prob. $(k\uparrow - k\downarrow)$ state occupied

  $|u_k|^2$ = " $(k\uparrow - k\downarrow)$ " unocc.

- <u>Recall</u> $1 + a c^+_{k\uparrow} c^+_{-k\downarrow} \equiv e^{a c^+_{k\uparrow} c^+_{-k\downarrow}}$

  ($\because$ Fermions : $c^2 = 0 = (c^+)^2$)

$\therefore |BCS\rangle \propto e^{\sum_k \frac{v_k}{u_k} c^+_{k\uparrow} c^+_{-k\downarrow}} |0\rangle$

$\equiv e^{\sum_k \phi_k b^+_k}|0\rangle \equiv e^{b^+}|0\rangle$

(b^+_k creates pair, $\equiv c^+_{k\uparrow} c^+_{-k\downarrow}$)

- ϕ_k is just Fourier transform of singlet "Cooper" pair state :

  $\langle r | \sum_k \phi_k b^+_k |0\rangle \equiv \Phi(r)$; $r = r_1 - r_2$

- $|BCS\rangle = \left(1 + b^+ + \frac{(b^+)^2}{2!} + \cdots\right)|0\rangle$

  no pair, one pair, 2 pairs ...

  <u>Coherent</u> <u>superposition</u> of states with different no. of pairs

- Let $b^+ \to e^{i2\theta} b^+$; θ a phase.

  $|\theta\rangle_{BCS} = \left(1 + e^{i2\theta} b^+ + e^{i4\theta}\frac{(b^+)^2}{2!} + \cdots \frac{e^{iN(2\theta)}}{N!}(b^+)^N \cdots\right)|0\rangle$

  state with fixed phase θ (<u>same</u> for each pair)

- $|N\rangle = \frac{1}{2\pi}\int_0^{2\pi} e^{-i2N\theta}|\theta\rangle_{BCS}\, d\theta$ state with fixed N.

  (θ, N) are <u>conjugate</u>.

- This state incorporates the pairing correlation. Treat u_k and v_k as variational parameter and minimise energy (or free energy at $T \neq 0\,K$) for fixed average particle number (Grand canonical ensemble).

- The pairs so far are in zero-momentum state: $(k\uparrow, -k\downarrow)$

$$\langle r_1 r_2 | \sum_k \phi_k C_{k\uparrow}^{+} C_{-k\downarrow} |0\rangle \equiv \tilde{\Phi}(r_1 - r_2)$$

- With non-zero-current carrying state, the pair acquires net momentum:

$$\tilde{\Phi}(r_1 - r_2) \rightarrow \tilde{\Phi}(r_1 - r_2)\, e^{iq\cdot\frac{(r_1 + r_2)}{2}}$$

- Spatial spread of the internal pair wave function $\tilde{\Phi}(r_1 - r_2)$ is the coherence length ξ_0.

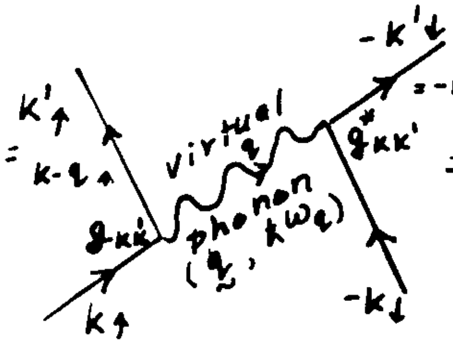
- Thus SC state is not just collection of pairs, but phased (coherent) superposition of states with different no. of pairs: Mean number $\langle N\rangle$ but spread $\langle \delta N^2\rangle^{1/2} \sim \langle N\rangle^{1/2} \ll \langle N\rangle$ as $\langle N\rangle \rightarrow \infty$.

- All pairs in zero-momentum state ~ Bose condensation as in ^4He. But large ξ_0 means overlapping pairs unlike ^4He. This strong overlap $\rightarrow$ gap in spectrum in SC.

ORIGIN OF EFFECTIVE ATTRACTIVE INTERACTION : EXCHANGE OF VIRTUAL PHONONS, or other Bosonic EXCITATIONS e.g. electronic polarization etc

- BASIC IDEA: Polarization CREATED by one electron attracts the other electron (Water-bed effect) $\Rightarrow +k\uparrow, -k\downarrow$ singlet pairs

- FORMALLY: 2^{nd} order in electron-phonon coupling $g_{kk'} \rightarrow$



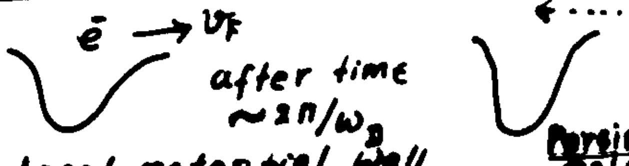
$$\Rightarrow \sum_{k,q} \underbrace{\frac{|g_{kk'}|^2 \hbar\omega_q}{(\varepsilon_{k-q} - \varepsilon_k)^2 - (\hbar\omega_q)^2}}_{-ve \text{ (attractive) for}} C^\dagger_{-k+q\downarrow} C^\dagger_{k-q\uparrow} C_{k\uparrow} C_{-k\downarrow}$$

$|\varepsilon_{k-q} - \varepsilon_k| < \hbar\omega_q \sim$ Debye cut-off $\hbar\omega_D$

- This attractive interaction $V_{kk'}$ ($\equiv V_P$) due to phonons averaged over FS gives $\langle V_{kk'} \rangle_{FS} = -V$ for $|\varepsilon_k - E_F|, |\varepsilon_{k'} - E_F| < \hbar\omega_D$
  $= 0$ otherwise assumed.

- But what about the relatively stronger repulsive Coulomb potential between the Landau quasiparticles:
  Screened Coulomb potential $\sim \frac{e^2}{r} e^{-k_s r}$ (real space)
  (Here $k_s^2 = \frac{6\pi n e^2}{E_F}$ Thomas-Fermi screening) $\sim \frac{4\pi e^2}{q^2 + k_s^2}$ (Reciprocal space)
  Averaged over FS : $\left\langle \frac{4\pi e^2}{q^2 + k_s^2} \right\rangle_{FS} \equiv V_c >> V_p$

- Still, phonon mediated attraction weak but retarded dominates stronger Coulomb repulsion which is Instantaneous:



Local potential well due to lattice polarization that persists for time $\sim \frac{2\pi}{\omega_D}$

this condition gives $E_F >> \hbar\omega_D$ Holds for good metals.

- Now, if $v_F \cdot \frac{2\pi}{\omega_D} > \frac{2\pi}{k_s} \sim n^{1/3}$ (screening length) the other electron will see the attractive well (retarded) but not the instantaneous screened repulsion.

• Intuitively, this means that the retarded phonon attraction and the Instantaneous Coulomb repulsion are effective at different space-time points.

• $\Rightarrow$ replaces V_c by a pseudo potential

$$V_c^* = \frac{V_c}{1 + N(0)V_c \ln\underbrace{(E_F/\hbar\omega_D)}} \ll V_c,$$ acting in the same Debye-cutoff shell.

retardation ratio effect ~ 10^2; $N(0)$ = density of states at FS.

• Dimensionless phonon attraction

$$\lambda \equiv N(0)V$$

• Dimensionless Coulomb repulsion

$$\mu^* = N(0)V_c^*$$

• $\lambda - \mu^* < 0$ is the effective Pairing interaction that enters the BCS theory (in the weak-coupling limit ($\lambda \ll 1$)). Strong coupling $\lambda \gg 1$ limit requires proper treatment of damping, retardation.

• Same λ enters phonon induced normal state resistivity at high temp, $\rho \propto T$.

• Density of state (effective mass) enhancement in sp. heat: $(1+\lambda)$ factor in linear electronic sp. heat.

• Good SC are bad metals (large electron-phonon scattering.

• Typically $\lambda \sim 0.2 - $ [illegible]
$\mu^* \sim$ [illegible] $- 0.25$

• Higher λ often causes metastability and $\rightarrow$ less symmetric phase with lower λ.

** A formal way of deriving the effective electron-electron interaction uses the Dielectric function: $V_{eff} = \frac{4\pi e^2}{q^2 \varepsilon(q,\omega)}$

* BCS Hamiltonian (pairing terms)

$$H_{\underline{Red}} = \underbrace{\sum_{k,\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma}}_{\text{Free electron}} + \underbrace{\sum_{k,k'} V_{kk'} C^+_{k'\uparrow} C^+_{-k'\downarrow} C_{-k\downarrow} C_{k\uparrow}}_{\text{Attractive interaction (assumed weak)}}$$

Important: The interaction term contributes infinetesimally to normal state (in the H-F factorization). It is only in the SC state with anticipated anomalous (Gor'kov) factorization, that it becomes effective. Thus, we have already isolated the crucial term.

Also, this term conserves pairing condition → pairs scattered to pairs; this motivates ⇒

- Orderparameter (anomalous expectation) Gor'kov

$$\Delta_k = -\sum_{k'} V_{kk'} \langle C_{-k\downarrow} C_{k\uparrow} \rangle ;$$ off-diagonal in occupation numbers.

$$\Downarrow$$

- $$H_{Gor'kov} = \sum_{k,\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} - \sum_k (\Delta_k c^+_{k\uparrow} c^+_{-k\downarrow} + h.c) + \text{constants}$$

Thus Δ_k acts as a 1-body potential, of a strange kind though.

This is a bilinear form and can be readily diagonalized.

Andreev Reflection:

electron scattered to electron

$U_{kk'}$ ordinary 1-body potential: $\sum_{kk'} U_{kk'} c^+_{k'\uparrow} c_{k\uparrow}$

electron $(k\uparrow)$ → hole $(-k\downarrow)$

$\sum_k \Delta^*_k C_{-k\downarrow} C_{k\uparrow}$

$(k\uparrow)$ pairs up with $(-k\downarrow)$ and condenses, leaving a hole in $(-k\downarrow)$ backscattered.

* SPECTRUM (QUASI-PARTICLE)

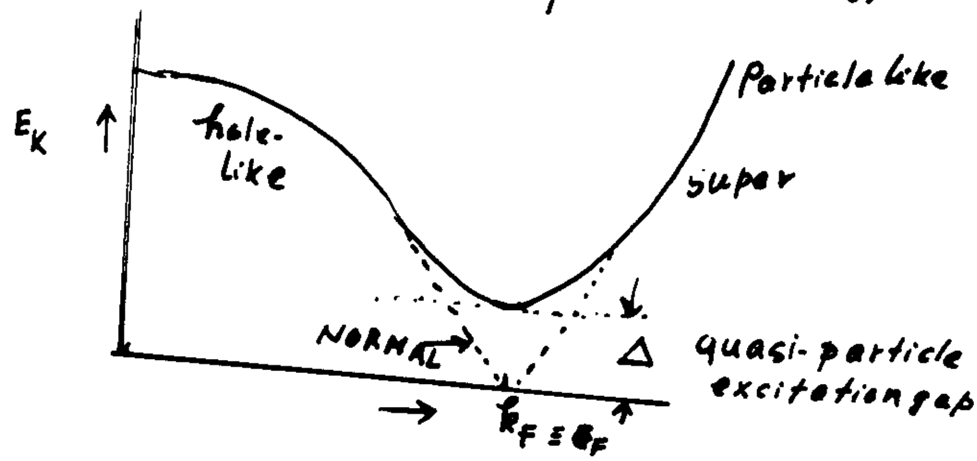
Introduce canonical transformation to diagonalise:

$$c_{k\uparrow} = u_k^* \alpha_k + v_k \beta_k^+ \qquad u_k^2 + v_k^2 = 1$$

$$c_{-k\downarrow}^+ = -v_k \alpha_k + u_k \beta_k^+ \qquad u_k^2 = \frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right)$$

Here α_k, β_k new fermions $\qquad v_k^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right)$

- $\xi_k = \epsilon_k - E_F$, $E_k = \sqrt{\Delta_k^2 + \xi_k^2}$
  Quasi-particle energy



- Self-consistent equation for Δ_k :

$$\Delta_k = -\sum_{k'} V_{kk'} \Delta_{k'} \left(1 - 2 f(E_{k'})\right) / 2E_{k'}$$

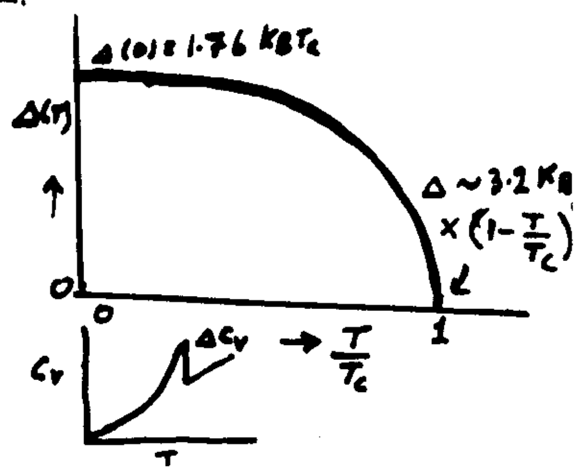
fermi-function

For the simple model : $\boxed{V_{kk'} = -V, \ \xi_k, \xi_{k'} < \hbar\omega_D \\ = 0 \ \text{otherwise}}$

⇓ GAP EQUATION

- $$\boxed{1 = \frac{V}{2}\sum_k \frac{\tanh \frac{E_k}{2k_B T}}{E_k}}$$ ⇒ gives Δ as function of T.

Δ non-zero for $T < T_c$



- $k_B T_c = 1.14\, \hbar \omega_D \exp\left(-\frac{1}{N(0)V}\right)$
- $\frac{2\Delta(T=0)}{k_B T_c} = 3.5$ GAP RATIO
- $\because \omega_D \propto M^{-1/2} \Rightarrow$ isotope effect.
- Sp. heat discontinuity $\frac{\Delta C_v}{\gamma V T_c} \approx 1.43$
- NMR Acoustic attenuation (a)

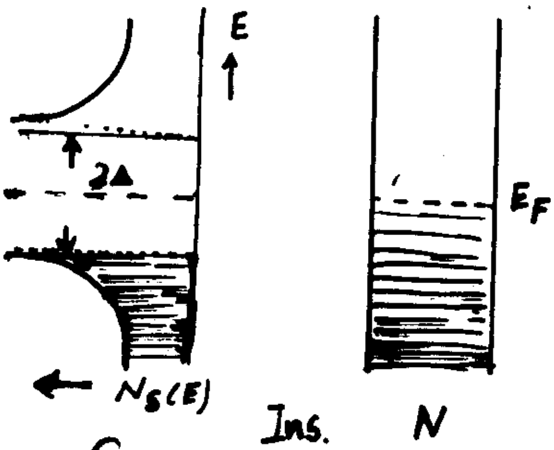
• From the excitation spectrum

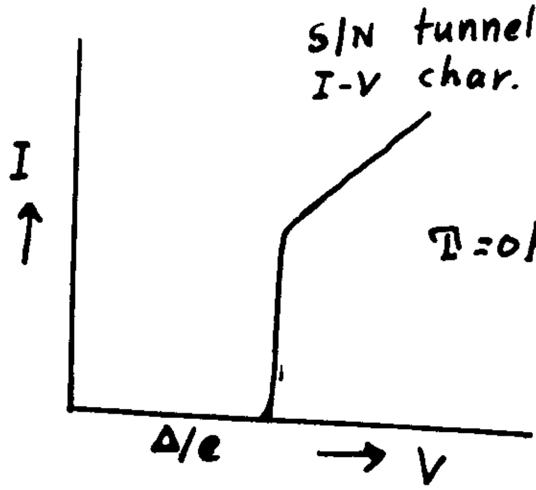
$$E_K = \sqrt{\Delta^2 + (\epsilon_K - E_F)^2}$$

we infer the <u>density</u> of states $N_s(E)$ of Quasiparticles

$$\frac{N_s(E)}{N(0)} = \frac{E}{(E^2 - \Delta^2)^{1/2}}, \quad E > 0 \qquad \text{E measured from } E_F.$$

$$= 0 \qquad , E < 0$$



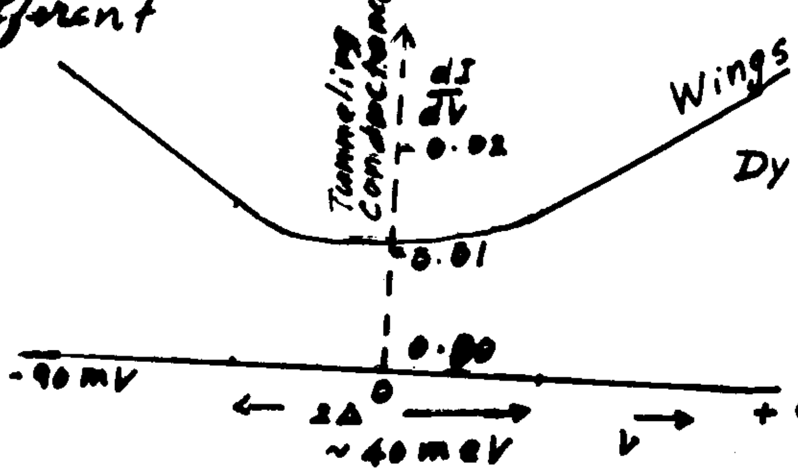


$\left(\frac{dI}{dV}\right)_s \propto N_s(E)\big|_{E=eV}$

(At finite temp. non-zero I for V < Δ/e).

• Actually, there is <u>E- dependence in Δ</u> too (<u>strong coupling effect</u>) ⇒ phonon peaks in dJ/dV (derivative plot). Extremely important probe for electron- phonon coupling and phonon spectral density: <u>$\alpha^2(\omega) F(\omega)$</u>, and Gap measurement.

• HTSC tunneling char. are remarkably different



$DyBa_2Cu_3O_7/Al_2O_3/Al$

$\frac{2\Delta}{K_B T_c} \sim 5$

Connection with GL Order-Parameter Ψ.

- The pair potential $\Delta_k \equiv -\sum_{k'} V_{kk'} \langle c_{k'\uparrow} c_{k'\downarrow} \rangle$ of BCS is the <u>Order</u> <u>Parameter</u> $\Psi(x)$ of GL.

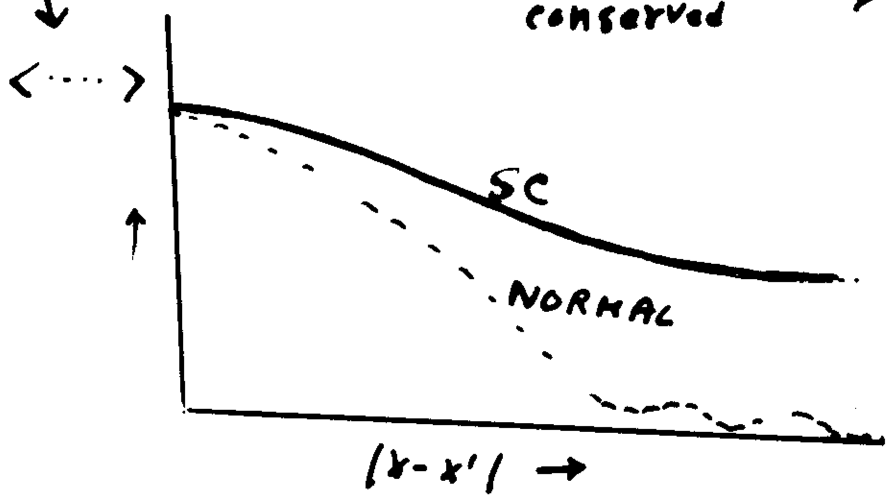
- In real space

$$\Psi(x) = \langle \underbrace{\tilde{C}_\uparrow(x)\, \tilde{C}_\downarrow(x)}_{\text{off-diagonal in particle number! Must think of subsystem.}} \rangle \neq 0, \text{ against naive bias.}$$

- SC is characterized by OFF-DIAGONAL LONG RANGE ORDER (ODLRO):

$$\langle \tilde{C}^{+}_\uparrow(x)\, \underbrace{\tilde{C}^{+}_\downarrow(x)\, \tilde{C}_\downarrow(x')\, \tilde{C}_\uparrow(x')}_{\text{No. of particles conserved}} \rangle \neq 0$$

Limit $|x-x'| \to \infty$ $\to \Psi^{+}(x)\, \Psi(x')$ (factorises)



- $\langle$ODLRO$\rangle$ implies also infinite conductivity.

- " " phase synchronization distant pairs ($\equiv$ quantum coherence on macroscopic scale).