

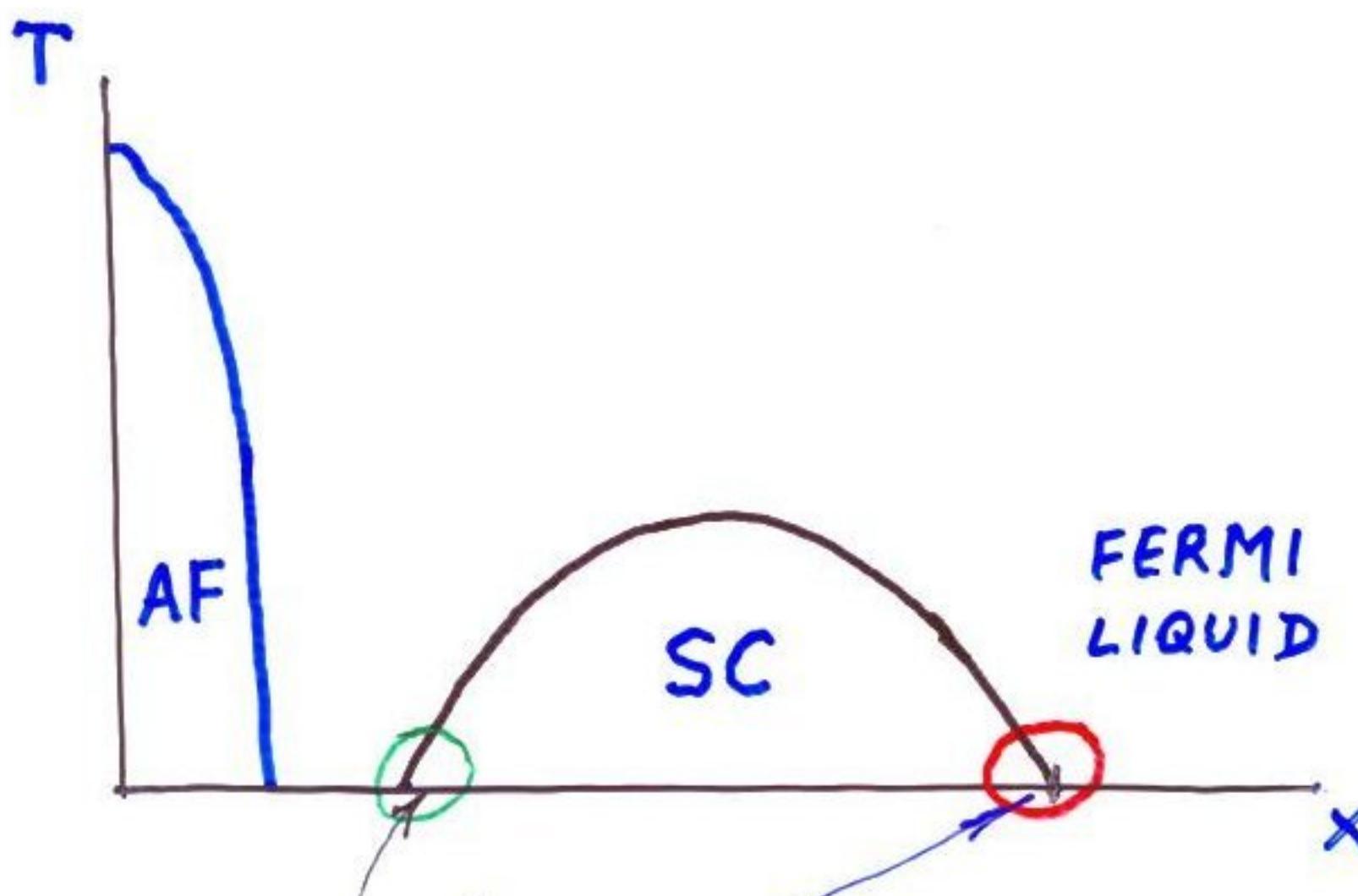
ELECTRON PAIRS FOR HTS

(simple picture of superconductivity in cuprates)

- We demonstrate the existence of a small region in phase diagram of CuO_2 planes (in the vicinity of the maximum hole-doping level compatible with superconductivity) where physical picture of superconductivity is very simple.
- This picture possesses characteristic features that are observed in HTS:
 - high- T_c
 - dx^2-y^2 symmetry of order parameter
 - coexistence of a well-defined one-electron Fermi surface and a pseudogap (which is attributed to the presence of preformed electron pairs)

PHASE DIAGRAM OF HIGH- T_c CUPRATES

For example $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$
where x is the hole doping level.



here T_c is also small but
the normal state is very compli-
cated (strong correlations, locali-
zation etc.)

KEY POINT:

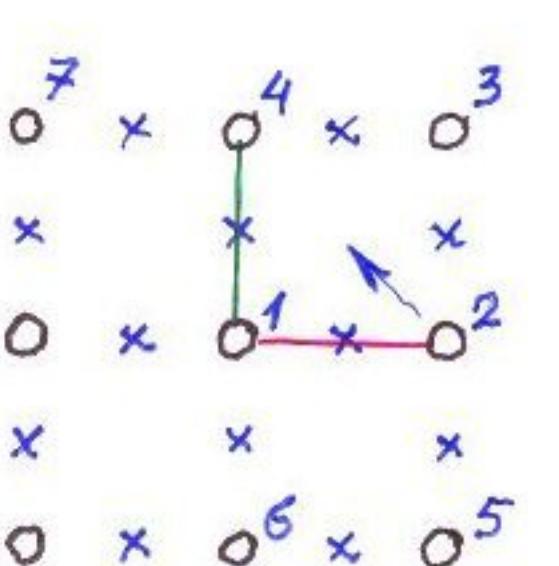
The existence of very mobile pair-quasiparticles in crystals in conditions of the tight-binding:

$$U \gg t$$

where U is electron-electron interaction at distances of the order of atomic spacing, t is the electron tunneling amplitude to neighboring lattice sites. Similar quasiparticles: in helium quantum crystals (A.A., 1982) and as a model of bipolarons in HTS (Alexandrov and Kornilovich, 2002)

SQUARE LATTICE OF CuO_2

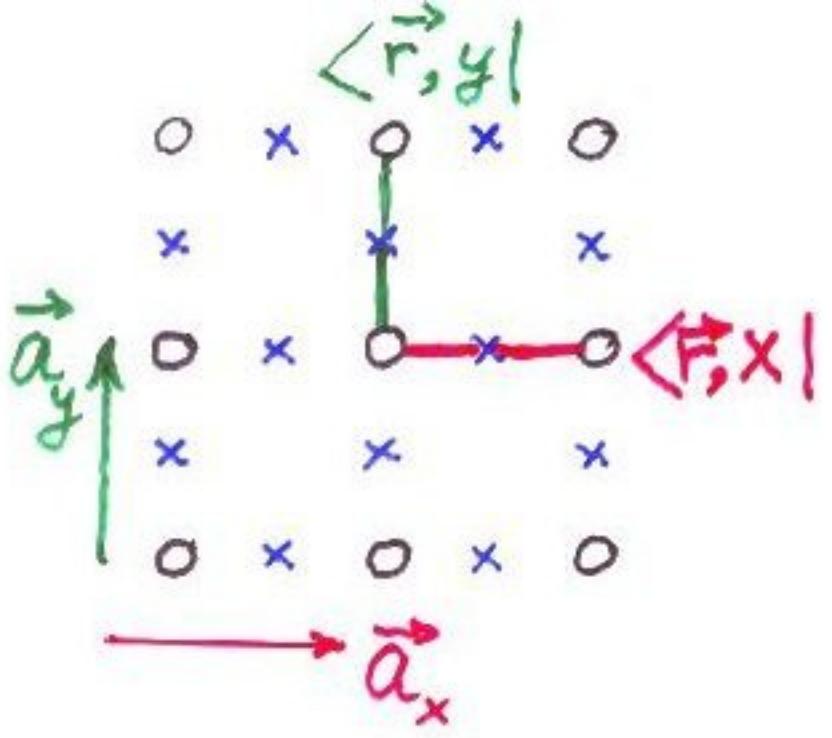
Two electrons localized at nearest-neighboring (1 and 2) copper atoms (more generally, in unit cells containing these atoms).



Tunneling of the single electron
 $2 \rightarrow 4$ (or $2 \rightarrow 6$) does not
change the total energy due
to lattice symmetry.

The pair moves as a whole coherently over the entire plane ($2 \rightarrow 4$ can be followed by $1 \rightarrow 7$ or $1 \rightarrow 3 \dots$).

The electron pair behaves as a Bose quasiparticle with band width of the order of t .



Stationary states with
a given quasimomentum

$$\sum_{\vec{r}} \psi^{(n)} e^{i \vec{k} \vec{r}} | \vec{r}, n \rangle$$

where $n = x, y$ determines
the orientation of the two-
electron "dumb-bell".

$$(*) \quad \{\mathcal{E}(\vec{k}) - \varepsilon_0\} \psi^{(x)} = t \psi(y) (1 \pm e^{-i k_x}) (1 \pm e^{i k_y})$$

$$\{\mathcal{E}(\vec{k}) - \varepsilon_0\} \psi^{(y)} = t \psi(x) (1 \pm e^{i k_x}) (1 \pm e^{-i k_y})$$

where $\hbar_{x,y} = \vec{k} \cdot \vec{a}_{x,y}$, ε_0 is the energy of the initial localized state of the pair,
the upper or lower sign is for spin-singlet or spin-triplet state, respectively. t is known to be positive.

$$\min \mathcal{E}(\vec{k}) = \varepsilon_0 - 4t \text{ for } \begin{cases} \hbar_x = \hbar_y = 0 \\ (\text{singlet}) \\ \hbar_x = \hbar_y = \pi \\ (\text{triplet}) \end{cases}$$

This degeneracy is removed by the electron exchange (antiferromagnetic!) in the initial localized pair: energy minimum for singlet.

From (*) for $\hbar_x = \hbar_y = 0$ we have $\psi^{(x)} = -\psi^{(y)}$

The ground-state wave function $\Psi \equiv \psi^{(x)}$ change sign upon rotation by $\pi/2$ and upon reflection in the diagonal plane.

Ψ transforms in accordance with

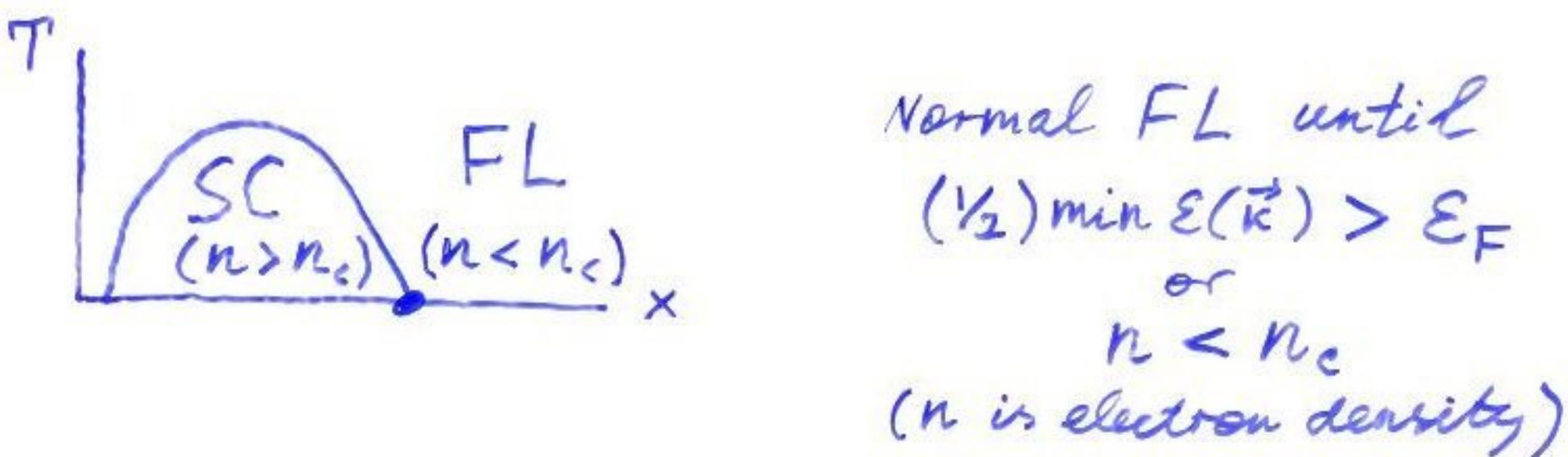
$d_{x^2-y^2}$ representation!

SUPERCONDUCTIVITY

assume that all other two-, three-, etc. electron configurations are energetically disadvantageous as compared to above pairs.

Assume that $(\frac{1}{2}) \min \epsilon(\vec{k}) = (\frac{1}{2})(\epsilon_0 - 4t)$ is within the one-electron energy band.

Upon an increase in the electron number at $T=0$ (decrease in the hole-doping level) :



With further decrease in the hole-doping all additional $n - n_c$ electrons ($n - n_c$ is small enough!) pass into BE-condensate of pair-quasiparticles:

superconductor (boson-fermion models)

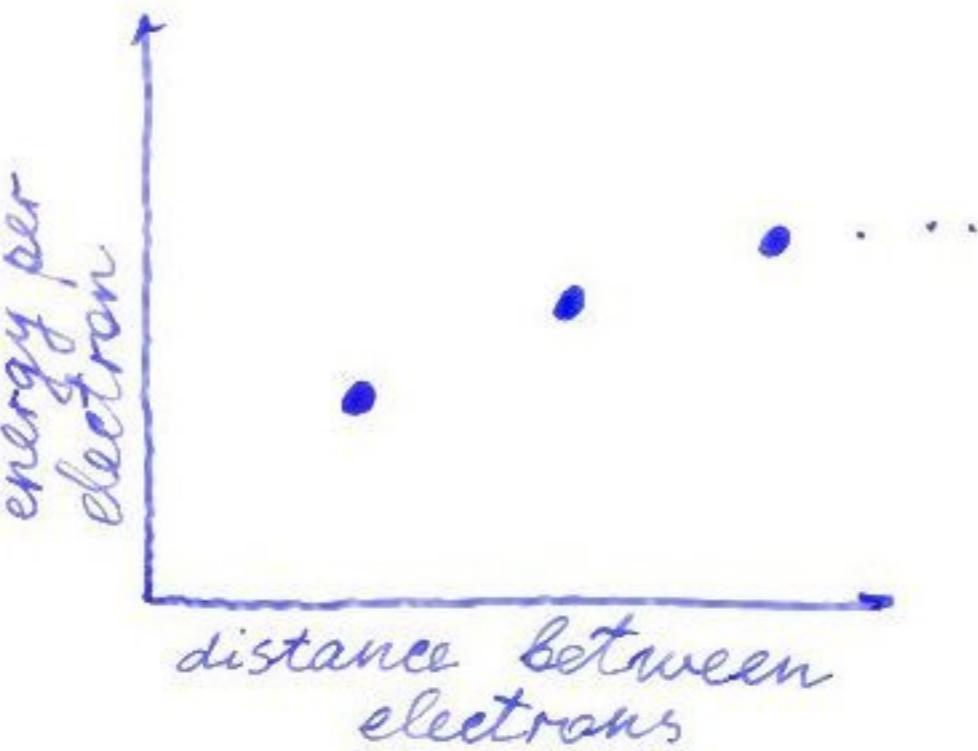
Superconducting order parameter

$$\psi \equiv \psi^{(x)} = -\psi^{(y)}$$

transforms in accordance with the $d_{x^2-y^2}$ representation of the CuO_2 plane symmetry.

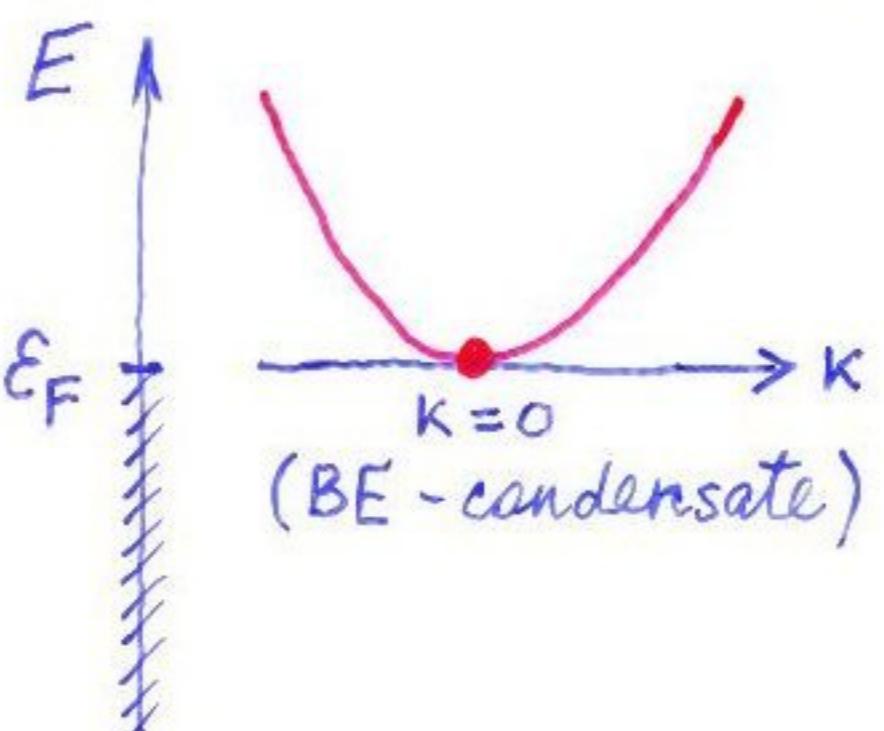
Important points:

1. Decay of pairs into single electrons is negligible:



To decay a pair
has to overcome
a great energy
barrier!

2. Similar to that in Landau Fermi-liquid theory:



Pairs with low excitation energy ε :

$$\varepsilon = \frac{k^2}{2m} \text{ where } m = \frac{\hbar^2}{t a^2}, \\ a = |\vec{a}_x| = |\vec{a}_y|.$$

Uncertainty δE in the energy E of a pair arising from collisions with one-electron Landau quasiparticles is small compared to E ($\delta E \propto E^2$) because of the limitations posed by the energy conservation and Pauli principle even when the single-electron concentration N is not small.

Thus, the proposed picture of superconductivity in the vicinity of maximal doping level (the concentration $\frac{1}{2}(n-n_c)$ of electron pairs is small enough) remains valid even when n is not small and the pair-single electrons interaction is important.

Generally, $\epsilon(\vec{k})$ and $\min \epsilon(\vec{k})$ are functionals of the single-electron distribution function.

So, our pairs \rightarrow collective property of the whole electron system.

Fermi quasiparticles

Usual electron-electron interaction

$$\sum U c^+ c^+ c \underline{c}$$

(c^+ , c are electron operators)

creates (due to $\langle \psi \psi \rangle \propto \psi$) an effective potential $\Delta_{\vec{k}}$ acting on fermions as in traditional superconductors:

$$H_{\text{int}} = \sum_{\vec{k}} (\Delta_{\vec{k}} c_{\vec{k}\uparrow}^+ c_{-\vec{k}\downarrow}^+ + h.c.)$$

in view of the symmetry of ψ , we have

$$\Delta_{\vec{k}} = V(\hat{k}_x^2 - \hat{k}_y^2) \psi$$

where $\hat{k} = \vec{k}/|\vec{k}|$ and V is an invariant interaction.

Owing to this interaction Fermi-quasiparticles in our superconducting state acquire features typical for ordinary superconductors with $d_{x^2-y^2}$ symmetry.

Critical Temperature

The density N' of uncondensed pairs at finite T is

$$N' = \int \frac{2\pi K dK}{(2\pi k)^2} \frac{1}{e^{\epsilon/kT} - 1} = \frac{mT}{2\pi k^2} \log \frac{T}{\tau}$$

The integral diverges at small $\epsilon = \kappa^2/2m$, so it is cut off at $2\sim\tau$ where τ is a small tunneling amplitude for electrons in direction perpendicular to Cu_2 plane.

We have $n - n_c = 2N' + 2N_0$

where N_0 is the pair number in the condensate.

T_c is defined by $N_0(T_c) = 0$ or

$$n - n_c = \frac{m T_c}{\pi k^2} \log \frac{T_c}{\tau}.$$

This T_c is quite high:

for $n - n_c \sim \bar{a}^{-2}$ it differs from t only by a logarithm term.

Normal State Thermodynamics — Pseudogap

Pair spectrum: $E = E_m(\mu) + \varepsilon$ where $\varepsilon = \kappa^2/2m$.

Pair density at $T > T_c$:

$$N = \int_0^\infty \frac{2\pi\kappa dk}{(2\pi\hbar)^2} \frac{1}{e^{\frac{\varepsilon+\varepsilon}{T}-1}} = \frac{mT}{2\pi\hbar^2} \log \frac{1}{1-e^{-\frac{\varepsilon}{T}}} \quad (\xi \gg z)$$

where $\xi = \frac{\partial \varepsilon_m}{\partial \mu} \delta\mu - 2\delta\mu$, $\mu = \mu(n_c) + \delta\mu$, $2\mu(n_c) = \varepsilon_m(n_c)$

Electron number conservation with changing T :

$$n - n_c = 2N + \frac{\partial n}{\partial \mu} \delta\mu.$$

From this we find $\xi = \xi(T)$ and then all other quantities.

Pair density $N(T)$:

1. $n > n_c$ ($T_c > 0$), $T \ll T_c \log \frac{T_c}{T}$:

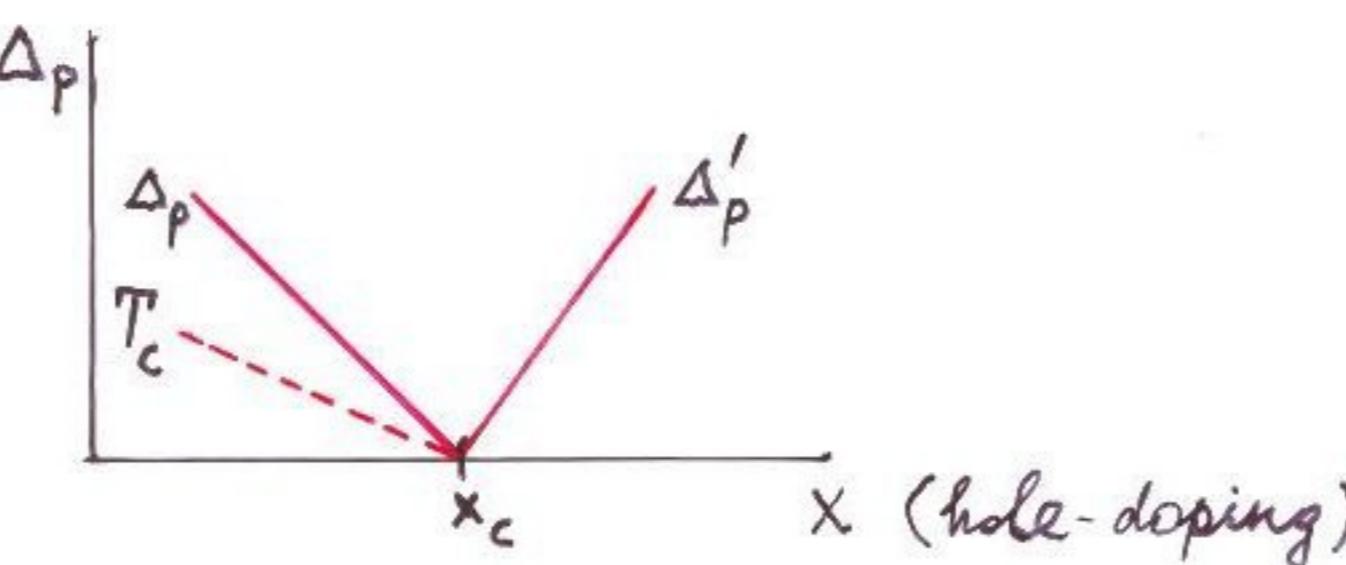
$$\frac{N(T) - N(T_c)}{N(T_c)} = \frac{\partial n / \partial \mu}{2(2 - \partial \varepsilon_m / \partial \mu)} T e^{-\frac{\Delta_p}{T}}$$

where $N(T_c) = (n - n_c)/2$ and

$\Delta_p = T_c \log \frac{T_c}{T} = \frac{\pi \hbar^2}{m} (n - n_c)$ is pseudogap for $n > n_c$.

2. $n < n_c$ ($T_c = 0$): $N(T) = \frac{mT}{2\pi\hbar^2} e^{-\frac{\Delta'_p}{T}}$ ($T \ll \Delta'_p$)

where $\Delta'_p = \frac{\partial \mu}{\partial n} (2 - \partial \varepsilon_m / \partial \mu) (n_c - n)$ is pseudogap for $n < n_c$.



Entropy $S(T)$:

1. $n > n_c$ ($T_c > 0$), $T \ll \Delta_p$

$S(T)$ is almost linear in T with exponential deviations:

$$\frac{S(T)}{T} - \left(\frac{S}{T}\right)_{T=T_c} = -\frac{m}{2\pi\hbar^2} \frac{\Delta_p}{T} e^{-\frac{\Delta_p}{T}}$$

where $\left(\frac{S}{T}\right)_{T=T_c} = \frac{\pi^2}{12} \frac{m}{\hbar^2}$.

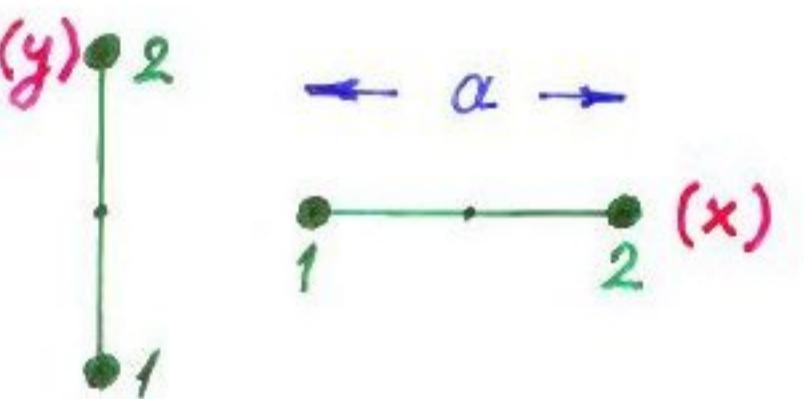
2. $n < n_c$ ($T_c = 0$).

$$\frac{S(T)}{T} = \frac{m}{2\pi\hbar^2} e^{-\frac{\Delta_p'}{T}} \quad (T \ll \Delta_p')$$

3. $T \gg \Delta_p', \Delta_p$.

$$\frac{S(T)}{T} = \frac{m}{\hbar^2} \sigma \quad \text{where } \sigma \text{ is a numerical factor.}$$

New prediction :
Orbital paramagnetism of electron pairs.



For $\vec{K} = 0$ the Hamiltonian of a pair is

$$H = 4t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = 4t \tilde{\sigma}_z,$$

with $\Psi = \Psi^{(x)} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \Psi^{(y)} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

Coordinates of electrons in $\Psi^{(x)}$ -state (with respect to the center of gravity of the pair) are

$$x_1 = -x_2 = -a/2, \quad y_1 = y_2 = 0$$

In $\Psi^{(y)}$ -state we have $x_1 = x_2 = 0, y_1 = -y_2 = -a/2$.

Generally, $x_1 = -\frac{a}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad x_2 = \frac{a}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$
 $y_1 = -\frac{a}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad y_2 = \frac{a}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

The velocities are

$$\dot{\vec{r}}_{1,2} = \frac{i}{\hbar} [H, \vec{r}_{1,2}],$$

or

$$\dot{x}_1 = -\dot{x}_2 = -\dot{y}_1 = \dot{y}_2 = -\frac{2at}{\hbar} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -\frac{2at}{\hbar} \tilde{\sigma}_2.$$

The operator of the pair magnetic moment, which is directed along z -axis, is

$$\mu \equiv \mu_z = \frac{e}{2c} \sum_{1,2} (x\dot{y} - y\dot{x}) = -\frac{2ta^2}{\hbar} \tilde{\sigma}_2.$$

The Hamiltonian of the pair in presence of magnetic field B is

$$H = 4t \tilde{\sigma}_z - \hat{\mu} B. \quad (B \equiv B_z)$$

Weak field :

$$\epsilon_{\min} = -4t - t \frac{e^2 a^4}{8 \hbar^2 c^2} B^2.$$

Magnetic moment of the pair is

$$\langle \mu \rangle = - \frac{\partial \epsilon_{\min}}{\partial B} = \alpha B$$

where magnetic polarizability is

$$\alpha = \frac{e^2 a^4}{4 \hbar^2 c^2} t = \frac{e^2 a^2}{4 m c^2}. \quad (t = \frac{\hbar^2}{m \alpha^2})$$

Magnetic susceptibility of the superconductor (above T_c) is

$$\chi = \frac{e^2 a^2}{4 m c^2} N^0$$

where $N^0 = N(T)/L$ is the volume density of pairs and L is the distance between CuO_2 planes.

Type of magnetism	Anisotropy	Sensitivity to inhomogeneities
Orbital paramagnetism of pairs	strong	no ($\vec{R} = \vec{v} = 0$)
Pauli spin-paramagnetism of singles	no	no
Landau diamagnetism of singles and pairs	strong	strong

can be separated!