Physical Mechanism of the $d \rightarrow d + is$ Transition

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We discuss the basic physical mechanism of the $d \rightarrow d + is$ transition, which is the currently accepted explanation for the results of tunneling experiments into $ab$ planes \cite{7}. Using the first-order perturbation theory, we show that the zero-bias states drive the transition. We present various order-of-magnitude estimates and consistency checks that support this picture.

It has now been firmly established \cite{1} that the order parameter in cuprate superconductors has a $d$-wave symmetry. An inhomogeneity may therefore scatter a quasiparticle between directions that experience opposite signs of the order parameter. This effect is strongest for specular reflection off the 110 surface. Here the sign of the order parameter along every quasiclassical trajectory changes sign upon reflection (see Fig. 1). As a consequence of this and the Atiyah-Patodi-Singer index theorem \cite{2}, the Andreev equation along each trajectory has a normalizable eigenstate of zero energy \cite{3}. These all contribute to the local density of states, and are the source of the zero-bias anomaly observed in tunneling experiments \cite{4,5}.

The tunneling data \cite{7} show that the zero-bias peak splits as the temperature is lowered below 1 or 2 K. This splitting is probably due to an additional symmetry-breaking transition, most likely $d \rightarrow d + is$ transition where a subdominant $s$-wave order parameter appears close to the surface with a $\pi/2$ phase shift compared to the dominant $d$-wave. Such a transition had been anticipated theoretically \cite{8} prior to the experiment. Subsequent calculations of the surface phase diagram \cite{9,10} included the effects of the surface roughness, and gave results that are in good agreement with the experimental data.

These calculations are done within the Eilenberger approach to superconductivity \cite{11}, which uses the quasiclassical approximation of the local Green function. This (so-called Eilenberger) function
then satisfies a transport-like equation. Unfortunately, this approach is very formal, so it hides, rather than explains, the physics behind the calculations, especially when the equations are solved numerically in the imaginary-time domain \[8,12\]. As new experimental results \[13\] call the \(d + is\) interpretation into question, it is even more important to have a direct physical understanding of the transition.

We believe the Andreev quasiclassical picture \[14\], which deals with single-particle states rather than local Green functions, contributes to such understanding by showing how the energy costs and benefits of the \(d \to d + is\) transition are distributed among the degrees of freedom in the system. As we mentioned above, due to the presence of the 110 surface, there are many zero-bias states (ZBSs) in the spectrum. The main purpose of this paper is to show that these states drive the transition.

Our approach was inspired by the study of a weak-coupling BCS superconductor modeled by a Fermi sea with an attractive local four-fermion interaction

\[
V \psi_+^\dagger(r) \psi_-^\dagger(r) \psi_-(r) \psi_+^\dagger(r);
\]

\(V < 0\) is the coupling constant. One decouples this interaction by the Hubbard-Stratonovich (HS) transformation, which introduces the pairing field \(\Delta\). The instability to superconductivity can then be detected by going to \(T = 0\) and looking at the energy change due to the opening of the gap \(|\Delta|\).

The occupied single-particle states lower their energy as \(|\Delta|^2 \ln |\Delta|\) while the system raises its energy by \(|\Delta|^2/(-V)\), which is the extra term in the hamiltonian introduced by the HS transformation.
Since the non-analytic decrease wins over the analytic increase as $|\Delta| \to 0$, an arbitrarily weak attractive $V$ will, at low enough temperature, make the system superconducting. The decrease of the single-particle energies is non-analytic due to contribution from the states initially close to the Fermi surface. We conclude, therefore, that these low-energy states drive the BCS transition.

A similar argument works for the $d \to d + is$ transition. If there is an attractive interaction in the $s$-wave channel with strength $V_s < 0$, we may use the HS transformation to introduce the $s$-wave component of the pairing field $\Delta_s$ on top of the dominant $\Delta_d$, leading to an extra positive term in the Hamiltonian $|\Delta_s|^2/(-V_s)$, just as in the BCS case. When the “$is$” component appears close to the surface, the shape of the order parameter along the trajectory in Fig. 1 changes, as shown in Fig. 2. To study the instability to the transition, we again look at $T = 0$ and $|\Delta_s| \to 0$. The energy of the ZBSs 1 to the lowest, that is first, order in $\Delta_s$ then changes to

$$E_\theta[\Delta_s] = \pm \int_{-\infty}^{+\infty} d\rho 2|f(\theta, \rho)|^2 \text{Im}\Delta_s,$$

(1)

where the upper (lower) sign corresponds to the up- (down-)moving trajectory. Here

$$\begin{pmatrix} f(\theta, \rho) \\ g(\theta, \rho) \end{pmatrix}$$

is a solution of the Andreev equation along the trajectory in the direction $\theta$ at the point $\rho$. For the ZBSs, $g(\theta, \rho) = \mp if(\theta, \rho)$. At $T = 0$, only the down-moving ZBSs will be occupied, and their energy will decrease linearly. It turns out 15 that the energy changes of the remaining states (non-ZBSs) cancel each other out. Thus, upon the appearance of small $|\Delta_s|$, the energy of the occupied (zero-bias) states is lowered linearly, which, for small enough $|\Delta_s|$, wins over the quadratic increase of the HS term for arbitrarily weak $s$-wave attraction $V_s$. It follows that the transition $d \to d + is$ is driven by the ZBSs.

\footnote{We shall abuse the terminology and call these states ZBSs even after their energy has been shifted away from zero.}
FIG. 2. The pairing potential along the trajectory in Fig. 1a). The corresponding twist of the phase of the order parameter is clockwise.

For YBCO, the experiments give $|\Delta_d| \sim 30$ meV (amplitude) and $|\Delta_s| \sim 1$ meV, so we assume the first-order perturbation formula (1) holds up to the experimental value of $|\Delta_s|$. We can then calculate $|\Delta_s|$ by minimizing the energy of the system. When we sum over all occupied ZBSs, we find that the energy per CuO plane per unit length of the surface is

$$E[s(x)] = \int_0^\infty dx s^2(x)(-V_s) + \int_{-\pi/2}^0 \frac{k_F}{2\pi} d\theta \cos \theta E_\theta[s(x)],$$

(2)

where $s(x) = \text{Im}\Delta_s(x)$. Since $s$ extends into the bulk only as far as the $d$-wave coherence length $\xi \equiv \hbar v_F/|\Delta_d|$, we can estimate

$$E[s] \sim \frac{s^2}{(-V_s)} \xi - k_F s,$$

(3)

which gives

$$s \sim \frac{(-V_s)k_F}{\xi}.$$  

(4)

The experimental values $s \sim 1$ meV, $k_F \sim 1$ Å$^{-1}$, and $\xi \sim 10$ Å give us $|V_s| \sim 10$ meV Å$^2$. (Since the CuO plane is two-dimensional, $V_s$ has dimension $EL^2$ rather than $EL^3$.)

The full variational calculation is presented in [15]. We only remark here that the solution of the variational equation obtained from (2) agrees with the contribution to $\Delta$ from the occupied ZBSs in the gap equation

$$\Delta_{ZBS}(x) = i(-V_s) \int_{-\pi/2}^0 \frac{k_F}{2\pi} d\theta 2|f(\theta, x/\cos \theta)|^2;$$

(5)
that is, \( \Delta_{ZBS}(x) = is(x) \), which shows the internal consistency of the picture. Unlike the BCS gap equation, (5) is an explicit formula for \( \Delta_{ZBS}(x) \); there is no \( \Delta_{ZBS} \) on the right-hand side. The physical reason for this is that within the first-order perturbation theory, it is only the sign of \( s(x) \) (and not its magnitude) that determines which ZBSs are occupied.

Our argument has shown only that \( d + is \) is the favorable state at \( T = 0 \). To see what happens at finite temperatures, we need to minimize the free energy \( F[s(x)] \), which is obtained from (2) when we replace \( E_\theta[s(x)] \) by \( -(T) \ln(1 + \exp( -E_\theta[s(x)]/T)) \), making the lowest order quadratic in \( s(x) \). The order-of-magnitude estimate gives

\[
F[s] \sim \left( \frac{\xi}{(-V_s)} - \frac{k_F}{T} \right) s^2 + O(s^4).
\]

Hence, the system is unstable to the transition to the \( d + is \) state even at finite temperatures. The transition temperature is

\[
T_s \sim \frac{(-V_s)k_F}{\xi},
\]

which is of the same order of magnitude as \( |\Delta_s|_{T=0} \) (see (4)).

Now we shall go back to \( T = 0 \) and observe that the presence of the \( is \) component induces a twist in the phase \( \varphi \) of the order parameter from \(-\pi\) to 0 for an up-moving trajectory and from 0 to \( \pi \) for a down-moving one, see Fig. 2. This twist implies a current flowing down; its density at the point \( \rho \) of a quasiclassical trajectory labeled by \( \theta \) is equal to

\[
j(\theta, \rho) = \frac{e}{2m} n^{(1d)} \partial_\rho \varphi(\theta, \rho),
\]

where \( n^{(1d)} \equiv k_F/\pi \) is the density of the one-dimensional Fermi sea (\( k_F \) is the Fermi wave vector). Current flowing down is also expected from our previous argument that showed that only the down-moving ZBSs are occupied. Each of them contributes

\[
j(\theta, \rho) = ev_F(|f(\theta, \rho)|^2 + |g(\theta, \rho)|^2)
\]

to the current density at a given point; it turns out again [15] that the contributions from the non-ZBSs cancel. In both approaches, we get the total current by summing up contributions from all the quasiclassical trajectories. The result is
I = \frac{ev_Fk_F}{4\pi} \tag{10}

per CuO plane in both calculations. To get an order-of-magnitude estimate, we take $v_F \sim 10^5$ m/s and $k_F \sim 10^{10}$ m$^{-1}$, so $I \sim 10^{-5}$ A. The agreement shows that all the current is carried by the ZBSs.

It is important that not only the magnitude, but also the direction of the current, agrees in both calculations. The reason for this agreement is that the ZBSs moving in the direction of the current are shifted down in energy and thus occupied, whereas those moving against the current are shifted up and unoccupied. We wish to stress that this is exactly opposite to the sign of the Doppler shift: the states moving along the current would be Doppler-shifted up, whereas those moving against the current would be Doppler-shifted down.

In conclusion, the first-order perturbation theory shows that the $d \to d + is$ transition is driven by the ZBSs and that the transition temperature is finite and of the order $|\Delta_s|_{T=0}$. The ZBSs that are being pushed down by the $is$ component carry surface current; they are not Doppler-shifted by this current.

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