Localized States in a d-Wave Superconductor

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Impurity scatterers, particularly in the unitary limit, produce low energy quasiparticles in a two-dimensional d-wave superconductor. We argue that even if the impurity concentration is small so that the wave functions in the normal state are essentially extended, the quasiparticles in the superconducting state become strongly localized for a short coherence length d-wave superconductor. An effective mobility gap then leads to thermally activated behavior for the microwave conductivity and possibly for the London penetration depth. We argue that this observation allows some puzzling data on oxide superconductors to be reconciled with the hypothesis of d-wave pairing.

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A number of recent experiments on the oxide superconductors give strong indications that the pairings state may be of $d_{x^2−y^2}$ symmetry. For example, strong anisotropy is observed in the energy gap in the angular resolved photoemission [1]. Low lying spin excitations remain below $T_c$ in the $(\pi,\pi)$ direction [2]. The unusual dependence of NMR relaxation rate on magnetic field direction is best explained by $d$ pairing [3,4]. In contrast, the temperature dependence of the London penetration depth $\lambda(T)$ was claimed to be thermally activated and consistent with conventional BCS theory [5]. More recently, a $T^2$ dependence was found to be consistent with experiments in YBCO (Y-Ba-Cu-O) thin films [6], and a linear $T$ dependence was reported for single crystals [7]. Nevertheless, at least in some samples, for $T \lesssim 0.2T_c\lambda$ is definitely flatter than a $T^2$ fit would permit [8]. The problem is further complicated by a report of excellent agreement with BCS theory down to low temperatures in an electron doped material [9]. Theoretically, the d wave is often the preferred state for nonphonon mechanisms based on strong correlations [10–12] or exchange of spin fluctuations [13].

According to conventional wisdom, a single experiment showing activated behavior is sufficient to invalidate the d-wave hypothesis, whereas power law behavior can often be explained away as BCS with some extrinsic broadening. Thus, it is important to examine the effect of extrinsic effects such as disorder scattering on the d-wave state. We find that due to special features of two dimensions, conventional wisdom fails and activated behavior can be consistent with d pairing. We shall present our results in terms of a $d_{x^2−y^2}$ state where $\Delta_k = \Delta_0 (\cos k_x a − \cos k_y a)$, even though our conclusions are general for any state where $\Delta_k$ vanishes linearly along a direction parallel to the Fermi surface.

We consider two models of disorder. In model I we assume a correlated random potential $U(r)$ such that $\langle U(r)U(0) \rangle = u_0 \delta^3(r)$. In the normal state, the Born approximation leads to an isotropic scattering rate $\tau^{-1} = 2\pi \rho_0 \mu_0 \delta_0$. In the superconducting state, the wave functions are essentially extended. We argue that this observation allows some puzzling data on oxide superconductors to be reconciled with the hypothesis of d-wave pairing.
wave superconductors, \( g \approx \xi_0/a \) which is of order unity for the oxide superconductors. We can therefore expect localization to play an important role. It is worth remarking that for \( g \) of order unity the scaling to the strong coupling localization fixed point will be stable to small perturbation such as interlayer coupling, so that our conclusions are applicable to weakly coupled layers as well.

While \( \sigma(\omega \to 0) \) is independent of disorder, the amount of disorder controls the energy scale over which this estimate applies. We denote this energy scale by \( \gamma \) and \( \gamma_0 \) for models I and II, respectively. The mean free path which sets the scale of \( \xi_L \) is given by \( l=\nu_F/\gamma \) and \( v_F/\gamma_0 \). We find that for Born scattering (model I), \( \gamma \) is exponentially small in \( \tau \), so that the localization effect is negligible. On the other hand, for model II, \( \gamma_0 \) is given by Eq. (8) and is enhanced compared with \( \tau^{-1} \). The origin of this difference is that for \( d \)-wave superconductors the density of states in the gap is strongly energy dependent so that the effective scattering rate due to static disorder is modified compared with the normal state value. As remarked earlier, the scattering rate has the opposite dependence on the density of states in models I and II. This accounts for the very different behavior of the two models.

We therefore reach the conclusion that for short coherence length \( d \)-wave superconductors with a dilute concentration of strong scatterers, the low energy quasiparticles with \( E < \gamma_0 \) are strongly localized. What are the experimental consequences? To answer this, we introduce yet another energy scale \( \Delta w \) given in Eq. (10), which is the typical energy level spacing between states within a localization length of each other. For \( T < \Delta w \), the localized states begin to decouple and the conductivity becomes activated. For \( \Delta w < T < \gamma_0 \) we expect the dc or microwave conductivity to be \( \sigma = (e^2/2\pi h) \xi_0/a \). For \( T > \gamma_0 \), the quasiparticles are well defined and a Boltzmann description applies, so that \( \sigma = T^2 \) where one factor of \( T \) comes from the density of states and a second factor comes from a lifetime which is proportional to the density of states. In contrast, in model I, we find that \( \sigma \) is essentially the normal state conductivity for \( T > \gamma_0 \). This is because \( \tau \) is now inversely proportional to the density of states and the temperature dependence cancels. There is a rapid crossover to \( \sigma = (e^2/2\pi h) \xi_0/a \) for \( \gamma < T < \gamma_0 \). Activated behavior will set in only below \( \Delta w \) which is very small in this case. We note that experimentally the microwave conductivity appears to be linear in \( T \) below 40 K for clean samples [6]. While this disagrees with both models I and II, we emphasize that if the density of states is energy dependent, an interpretation assuming a constant scattering rate should be viewed with some caution. For the clean samples, the dimensionless conductance is of order 400 at about 40 K and the low temperature behavior is sensitive to a background subtraction due to extraneous surface absorption [6] so that the localization effects discussed here cannot be tested. Samples with more disorder are more promising candidates to test the effects discussed here.

The London penetration depth has been calculated ignoring localization effect. While the results have been mainly numerical [19], it is easy to show that \( \lambda^{-2}(T) \sim \lambda^{-2}(0) \) is linear in \( T \) for \( T > \gamma_0 \) and \( T^2 \) for \( T < \gamma_0 \). We expect the effect of localization to be manifest for \( T < \Delta w \). However, since \( \lambda^{-2}(T) \) measures the spectral weight of the conductivity, the effect of localization is more subtle. For example, it is not at all clear that it should be activated at low temperatures the way the absorptive part \( \sigma(\omega) \) is. Nevertheless, for \( T < \Delta w \), it is reasonable to expect a flattening of the temperature dependence of \( \lambda(T) \). Because of the difficulties in dealing with localized wave functions, we are only able to provide some suggestive formal argument below.

We now supply some of the technical details. We begin with model I. The self-consistent Green functions are \( G = -(i\tilde{\omega} + \xi_k)/D \) and \( F = \Delta_k/D \) where \( D = \omega_0^2 + \xi_k^2 + \Delta_k^2 + k^2 - 2m - \mu \). Here \( \omega_0 = \omega_n + i\Sigma(\omega_n) \) and

\[
\Sigma(\omega_n) = \nu \sum_k G(k, \omega_n) \tag{1}
\]

The \( F \) function does not appear in Eq. (1) because its contribution vanishes upon angular average over \( k \). We shall expand around the point \( \mathbf{k}_0 \) on the Fermi surface in the \((1,1)\) direction. It is convenient to introduce a coordinate system parallel \( (\mathbf{k}_1) \) and perpendicular \( (\mathbf{k}_2) \) to the Fermi surface at \( \mathbf{k}_0 \). Then \( \xi_k = \nu F_{k_2} \Delta_k = \nu v k_1 k_2 \) where \( k_1 = (k_x - k_y)/\sqrt{2}, \ k_2 = (k_x + k_y)/\sqrt{2} - |\mathbf{k}_0|, \) and \( v = \sqrt{\Delta} \Delta_d \sin(k_0 a) \). The Green function near each zero of \( \Delta_k \) is given by

\[
G(k, \omega_n) = -(i\omega_n + \nu F_{k_2})/(\omega_0^2 + \nu^2 k_1^2 + \nu^2 k_2^2) \tag{2}
\]

and Eq. (1) becomes \( \Sigma(\omega_n) = \nu M \sum_k G(k, \omega_n) \) where \( M = 4 \) is the number of gap zeros. Upon analytic continuation and taking \( \omega \) to zero, it is clear that the integral is logarithmically divergent and is cut off by \( \gamma = \lim_{\omega \to 0} \Sigma(\omega) \). This explains why it is necessary to treat the self-energy self-consistently. The solution for \( \Delta_0 \) is

\[
\gamma = \Delta_0 \exp(-2\pi^2 \rho_0 v_F \tau) \tag{3}
\]

The quantity in the exponent is of order \( \Delta_0 \). The broadening of the quasiparticle state in momentum representation by \( \gamma \) in turn leads to a finite density of states \( \rho \) at \( \omega = 0 \) given by Eq. (1) as \( \rho = \rho_0 \tau \).

We next compute the quasiparticle contribution to the conductivity \( \sigma(\omega) \) in the limit \( \omega \to 0 \). For isotropic scattering, it is sufficient to keep only the bubble diagram with the self-consistent Green functions derived above. Expanding the standard expression in a spectral representation, we obtain (including spin)

\[
\sigma(\omega \to 0) = \frac{e^2}{h} \frac{4n^2}{\pi} \sum_{k, k'} |G''(\omega = 0, k)|^2 + |F''(\omega = 0, k)|^2 \tag{4}
\]

The imaginary part is obtained from Eq. (2) as \( G''(\omega = 0, \text{~}) \),

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$k) = \gamma/(\gamma^2 + (v_F k_1)^2 + (v_F k_2)^2)$ and $F'(\omega = 0, k) = 0$. The integral over $k_1, k_2$ are easily done, giving

$$\Gamma(\omega = 0) = (e^2/2\pi \hbar)(2/\pi)v_F/v_L.$$  

Next we consider model II. Instead of Eq. (1) the self-energy is given by [20-22]

$$\Sigma(\omega_n) = i\gamma_0(\omega_n)/|e^2 - g^2(\omega_n)|,$$

where $\Gamma = n_0/\pi \rho_0$, $c = \cot \delta_0$, and $\gamma_0(\omega_n) = (\pi \rho_0)^{-1} M \times \sum G(k, \omega_n)$ with $G$ given by Eq. (2). The Born scattering limit [Eq. (1)] is recovered if $c^2$ dominate the denominator in Eq. (6). For simplicity we specialize to the unitary case $\delta_0 = \pi/2$ or $c = 0$. The solution of Eq. (6) in the limit $\omega \to 0$ yields an estimate for $\gamma_0 = \Sigma(\omega = 0)$ to be

$$\gamma_0 = (\Gamma \pi k_F v_L/2)^{1/2} \approx \Delta(\Delta_0 \tau)^{-1/2},$$

where we have ignored a small logarithmic correction of order $\ln(\Delta_0/\Gamma)$. As pointed out before [20-22], the essential point is that for unitary scatterers $\gamma_0$ is enhanced relative to the normal scattering rate $\Gamma$ whereas for Born scatterers $\gamma$ is suppressed relative to $\tau^{-1}$. Indeed, for unitary scatterers, the scattering rate $\gamma(\omega)$ of a quasiparticle with energy $\omega$ is estimated to be $\gamma(\omega) \approx \Gamma \Delta_0/\omega$ for $\gamma_0 < \omega < \Delta_0$.

Now we can estimate the localization length for unitary scatterers. The conclusion that the dimensionless conductance $g = v_F/v_L \approx \gamma_0/\omega = \epsilon_F/\Delta_0$ is not changed. The mean free path, i.e., the distance scale at which diffusion begins, is now given by $v_F/\gamma_0$ and we estimate the localization length to be

$$\xi \approx (v_F/\Delta_0)^{1/2} \exp(\epsilon_F/\Delta_0),$$

which is reasonably short for a short coherence length superconductor even in the clean limit $\Delta_0 \tau \approx 100$.

To ascertain the physical significance of the localization length we estimate the typical energy level spacing between states within a localization length, i.e., $\Delta w = (\gamma^2)^{-1}$. Using Eq. (8) we find

$$\Delta w \approx \gamma_0(\Delta_0/\epsilon_F) \exp(-2\epsilon_F/\Delta_0).$$

For the oxide superconductors, $\Delta_0/\epsilon_F \approx 1$ and we find that $\Delta w$ is a reasonable fraction of $\gamma_0$. The significance of $\Delta w$ is that for $T < \Delta w$ the localized states begin to decouple and conductivity becomes activated. In contrast, in the Born approximation, we find $\Delta w = \gamma(\epsilon_F \tau)^{-1} \exp(-2\epsilon_F/\Delta_0)$ which is very small for $\epsilon_F \tau \gg 1$.

From now on we assume that the low lying quasiparticles are localized. For a given realization of the random potential, the effective Hamiltonian is diagonalized by $\gamma_1 = \psi(\tau), \psi^*(\tau) + v_F(\tau)$ and $\gamma_2 = \psi(\tau), \psi^*(\tau)$, where the Fourier transform of the quasiparticle wave functions $u$ and $v$ satisfy the Bogoliubov equations [23]:

$$\xi_k(\epsilon_k) + \sum_{\epsilon_q} U(\epsilon_q)u(\epsilon_k + \epsilon_q) + \Delta_k u(\epsilon_k) = E_\epsilon u(\epsilon_k),$$

$$\xi_k v(\epsilon_k) - \sum_{\epsilon_q} U(\epsilon_q)\epsilon_q v(\epsilon_k + \epsilon_q) + \Delta_k v(\epsilon_k) = E_\epsilon v(\epsilon_k).$$

We now use the discussion of Millis [24] and define the superfluid tensor $\rho^{\alpha\beta} = n_0 u^\alpha v^\beta - \rho_0^{\alpha\beta}$. The normal fluid tensor $\rho^{\alpha\beta}$ is computed by considering the response of the quasiparticles to an electromagnetic field. The response of the order parameter itself is not included in this calculation; this contribution is accounted for by a backflow term in the London kernel which enforces charge conservation [24]. We find

$$\rho^{\alpha\beta} = \sum_{\epsilon_q} \epsilon_q u^\alpha v^\beta \left[ 1 - f(E_\epsilon) - f(E_\epsilon + \epsilon_q) \right],$$

$$\rho^{\alpha\beta} = \sum_{\epsilon_q} \epsilon_q u^\alpha v^\beta \left[ f(E_\epsilon) - f(E_\epsilon + \epsilon_q) \right],$$

where

$$l_{\epsilon_q} = \langle u_\epsilon | -i \partial_{\epsilon_q} / m | u_\epsilon \rangle + \langle v_\epsilon | -i \partial_{\epsilon_q} / m | v_\epsilon \rangle,$$

$$p^{\epsilon_q} = \langle u_\epsilon | -i \partial_{\epsilon_q} / m | v_\epsilon \rangle - \langle v_\epsilon | -i \partial_{\epsilon_q} / m | u_\epsilon \rangle,$$

are the velocity matrix elements of the Bogoliubov wave functions. We note that in the presence of disorder, the first term in Eq. (12) gives a finite contribution even at $T = 0$, and the terms proportional to $f$ constitute finite temperature corrections. For nodeless states these terms lead immediately to thermally activated corrections. In the present case, the states $\alpha, \beta$ may denote localized or essentially extended states, separated by an effective mobility gap $E_g$. If $\alpha$ and $\beta$ are both extended, their contributions are clearly activated. To discuss the case when $\alpha$ and/or $\beta$ are localized, we first consider the conductivity tensor:

$$\sigma_{\mu\nu}(\omega) = e^2/2\pi \hbar \sum_{\epsilon_q} p^{\epsilon_q}_{\mu\alpha} p^{\epsilon_q}_{\nu\beta} \delta(\omega - E_\epsilon - E_{\epsilon_q}) \left[ 1 - f(E_\epsilon) - f(E_{\epsilon_q}) \right] - l_{\epsilon_q}^{\alpha\beta} l_{\epsilon_q}^{\beta\alpha} \delta(\omega - E_\epsilon - E_{\epsilon_q}) \left[ f(E_\epsilon) - f(E_{\epsilon_q}) \right].$$

and note that $e^2/2\pi \hbar \sigma_{\mu\nu}(\omega) = \int_0^\infty d\omega \sigma_{\mu\nu}(\omega)$. The first term in Eqs. (13) and (12) corresponds to the creation of a pair of quasiparticle excitations from the ground state while the second term corresponds to the scattering of a thermally excited quasiparticle. If both $\alpha, \beta$ are localized and $|E_\epsilon - E_{\epsilon_q}| < \Delta w$, the matrix element between them are typically exponentially small and negligible. If both $\alpha$ and $\beta$ are extended, the $T = 0$ conductivity has a threshold at $2E_g$ and the finite temperature corrections are activated at all $\omega$. Finally, if $\alpha$ is extended and $\beta$ localized, it is possible to find a power law in $T$ correction to $\sigma(\omega)$, but only for $\omega > E_g$. Thus, we conclude that $\sigma(\omega)$ as measured in the dissipative part of a microwave experiment [8,9] must be thermally activated.

For the normal fluid density, it is still true that terms with $\alpha$ and $\beta$ both localized make no contribution because of small overlap. However, if $\alpha$ is extended and $\beta$ is lo-
ized, we find that a small $T^2$ correction may exist. In this case, we argue that for localized states $\nu_\alpha(r)$ and $\nu_\beta(r)$ are strongly admixed so that each exhibits the same kind of random fluctuations, and the matrix elements $\rho_{\alpha\beta}$ and $\rho_{\beta\alpha}$ are statistically indistinguishable. With this approximation we find a near cancellation between the two terms in Eq. (13) resulting in

$$\rho^n(T) - \rho^n(0) = 2m\sum_{\alpha\beta} |\rho_{\alpha\beta}|^2 f(E_\beta) 2E_\beta/(E_\beta^2 - E^2) , \quad (14)$$

which is proportional to $T^2$. Since the state $\beta$ is localized, it is instructive to introduce $T_{\beta\beta}$ and $\rho_{\beta\beta}'$ as matrix elements of $r_\mu$ instead of $-i\delta_\mu/m$. Then we have $T_{\beta\beta}' = \rho_{\beta\beta}' (E_a - E_\beta)$ and $\rho_{\beta\beta}' = \rho_{\beta\beta}' (E_a + E_\beta)$. If we now make what appears to be an equally reasonable assumption that $\rho_{\alpha\beta} = T_{\beta\beta}$, we will obtain a $T^2$ contribution similar to Eq. (14) but with a negative coefficient. Thus it is quite uncertain what this $T^2$ contribution should be, except that the prefactor is proportional to $\rho_{\alpha\beta}'$, i.e., the square of the size of the localized states, which becomes smaller for stronger disorder. Therefore, it is possible that in an intermediate temperature regime, the $T$ dependent correction is dominated by the activated contribution from the extended states.

An immediate consequence of our picture is that if the oxide superconductor is d wave or has a zero gap, the activation gap in the microwave conductivity and possibly in $\lambda$ should be correlated with the amount of disorder in the sample. For the oxide superconductors, it is reasonable that disorder due to defects off the copper-oxygen plane may be treated in the Born approximation and that defects in the plane may be in the unitary limit. For the best materials, $\Delta_0$ or $\rho$ may exceed 100. If these are treated as unitary scatterers, we expect the localization effect to be important at an energy scale below $\gamma_0 = \Delta_0(\Delta_0\tau)^{-1/2}$, which may be of order $0.1T_c$. On the other hand, the electron doped materials are typically strongly disordered. Indeed, $\Delta_0\tau \approx 1$ and $T_c$ may be suppressed due to pair breaking effects. Thus, we expect a large mobility gap in these samples, which may account for the activated behavior found experimentally [9]. To test this idea, it will also be interesting to correlate the activation gap with the linear term in the specific heat which may arise from the finite density of states in the gap. We note that due to repulsion, the localized states may be singly occupied, with a spin which acts like a local moment. The existence of localized states will also call for a reexamination of the Knight shift data at low temperatures [4]. Finally, tunneling into the localized state is potentially a very interesting phenomenon, particular in point-contact tunneling where only states localized near the tip of the electrode may couple, leading to occasional discrete levels in the gap [25].

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Note added.—After the submission of the initial version of this paper, we carried out numerical studies which confirm the localization of quasiparticles near the gap nodes [27].

[1] Z. X. Shen et al. (to be published).
[19] P. Arberg, M. Mansor, and J. P. Carbotte (to be published).
[26] Matthew Fisher (private communication) has suggested that a related disordered Dirac fermion model may describe the transition between quantum Hall plateaus.