Impurity scattering and localization in \textit{d}-wave superconductors

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Strong evidence is presented for the localization of low energy quasiparticle states in disordered \textit{d}-wave superconductors. Within the framework of the Bogoliubov-de Gennes (BdG) theory applied to the extended Hubbard model with a finite concentration of non-magnetic impurities, we carry out a fully self-consistent numerical diagonalization of the BdG equations on finite clusters containing up to 50 \times 50 sites. Localized states are identified by probing their sensitivity to the boundary conditions and by analyzing the finite size dependence of inverse participation ratios.

In conventional \textit{s}-wave superconductors nonmagnetic impurities have little effect on the superfluid density and the transition temperature, which may be understood from Anderson’s theorem \cite{1}. The situation is dramatically different in the high temperature cuprate superconductors where nonmagnetic impurities exhibit a strong pair breaking effect \cite{2}. This is interpreted as a manifestation of unconventional, most likely \textit{d}-wave pairing symmetry. Understanding the role that impurities play in such superconductors is crucial for the interpretation of experimental data. A good example of this is the interpretation of experiments measuring the temperature dependent penetration depth \cite{3,4} in YBa$_2$Cu$_3$O$_{7-x}$. The behavior of various quantities in the presence of disorder also serves as an important test for theoretical models of microscopic pairing interaction.

In the present paper we concentrate on the possibility of localization of the low-energy quasiparticle states in \textit{d}-wave superconductors with line nodes in the gap on the fermi surface. We wish to address the question of whether these low lying states are strongly localized with a relatively short localization length $\xi_L$ or whether they are essentially extended. This is a question of significant importance for many experiments since the transport and thermodynamic properties are largely determined by these low energy excitations.

The problem of localization in \textit{d}-wave superconductors was first considered by Lee \cite{5} who, appealing to arguments from the scaling theory of localization, found that in the limit of unitary \textit{(i.e.} strong) scatterers the quasiparticle states are strongly localized below the mobility gap $\gamma_0$, even if the impurity concentration is sufficiently small that the normal state wavefunctions are essentially extended. For moderate concentrations of strong scatterers, $\gamma_0$ is a reasonable fraction of the maximum gap which allows for the possibility of experimental confirmation. One consequence of such a scenario is the prediction of a universal limit of conductivity $\sigma(\omega \rightarrow 0) \sim (e^2/2\pi\hbar)\xi_0/a$, independent of the scattering rate $\tau^{-1}$ ($\xi_0$ is a coherence length and $a$ is the lattice constant).

Infrared reflectance data on ion-irradiated YBa$_2$Cu$_3$O$_{7-x}$ have been interpreted using this picture \cite{6}.

More recently Balatsky and Salkola \cite{7} presented results that contradict this scenario. Their argument is based on a physical picture of a single impurity wavefunction which, according to an earlier calculation within the self-consistent \textit{T}-matrix approximation \cite{8}, is highly anisotropic with slowly decaying ($\sim 1/r$) tails along the (11) and (11) diagonals. Overlaps between these tails lead to strong interactions between the quasiparticle states on distant impurities, which then form a network of extended impurity states capable of carrying current. This network percolates across the entire system and inhibits the localization by disorder at the lowest energies, creating an “inverse mobility gap” $\gamma_c < \gamma_0$.

Both theories described above resort to approximations when treating the scattering from impurities and they ignore the gap relaxation near the impurity sites resulting from their pair breaking property. Since the arguments for and against localization are quite subtle it may well be that the above mentioned details are important, in which case perhaps the best way to address the problem is through numerical calculations. Hatsugai and Lee \cite{9} studied localization numerically in a simpler but related model of Dirac fermions on the lattice, whose excitation spectrum is similar to that of a \textit{d}-wave superconductor. By examining the sensitivity of the wavefunction to boundary conditions they concluded that the low energy states are indeed strongly localized. This would seem to be in qualitative agreement with the theory of Lee \cite{5}, however since the system possessed no off-diagonal long range order, the quantitative predictions of this theory could not be verified. While this work was strongly suggestive, without treating a system with superconducting order one cannot establish the existence of localization in a \textit{d}-wave superconductor. A convenient framework for studying the effect of impurities within a simple lattice model of \textit{d}-wave superconductivity was outlined by Xiang and Wheatley \cite{10}. The same model was later used to study localization induced by \textit{weak} disorder, modeled by a white noise random component added to the chemical potential \cite{11}. This corresponds to the scattering in the Born limit where the localization effect had been predicted to be negligible \cite{8}. The numerical work indeed confirmed that the localization length in the superconducting state remains comparable to its normal-state value \textit{(i.e., very large)} down to the lowest energies.
In the present work we address the case of a dilute density of strong (nearly unitary) scatterers. It is this limit that has precipitated controversy \[3\], and that is most relevant experimentally (e.g., for Zn doped \( \text{YBa}_2\text{Cu}_3\text{O}_{6-\delta} \)). In order to confront the question of localization in such systems we solve a simple tight binding model with an on-site repulsion and nearest neighbor attraction which give rise to superconductivity in the \( d \)-wave channel, on finite clusters using the selfconsistent Bogoliubov-de Gennes (BdG) technique. The main advantage of such an approach is that the impurity scattering is treated \textit{exactly} and that it is \textit{directly} relevant to \( d \)-wave superconductors. Our principal result is that quasiparticle states are strongly localized at low energies below a mobility gap \( \gamma_0 \). The value of \( \gamma_0 \), as well as the localization length \( \xi_L \), are in a good agreement with the theory of Lee \[4\].

The Hamiltonian we consider has been used previously to study the vortex structure \[12\] and impurities \[10,11\] in a \( d \)-wave superconductor:

\[
H = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_i n_{i\sigma} + \sum_i V_{i}^{\text{imp}} n_{i\sigma} + V_0 \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{V_1}{2} \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}
\]

Here \( \langle ij \rangle \) stands for nearest neighbor pairs, and the notation is otherwise standard. The last term models strongly repulsive impurities: \( V_{i}^{\text{imp}} = V_{i}^{\text{imp}} > 0 \) at randomly chosen sites with density \( n_{i\text{imp}} \) and \( V_{i}^{\text{imp}} = 0 \) on all other sites. If one takes \( V_0 > 0 \) and \( V_1 < 0 \) this model gives rise to pairing in the \( d \)-wave channel. In mean field theory \[4\] can be solved by defining the pairing amplitudes

\[
\Delta_0(r_i) = V_0(c_{i\uparrow}^\dagger c_{i\downarrow}), \quad \Delta_\delta(r_i) = V_1(c_{i\uparrow} + \delta c_{i\downarrow}^\dagger c_{i\downarrow}), \tag{2}
\]

where \( \delta = \pm x, \pm y \) are nearest neighbor vectors for a square lattice. The resulting mean field Hamiltonian is then diagonalized using the Bogoliubov transformation \[14\]

\[
c_{i\uparrow} = \sum_n [\gamma_n \uparrow u_n(r_i) - \gamma_n \downarrow^\dagger v_n(r_i)], \quad c_{i\downarrow} = \sum_n [\gamma_n \downarrow u_n(r_i) + \gamma_n \uparrow^\dagger v_n(r_i)].
\]

to the quasiparticle operators \( \gamma_n \sigma \). Within mean field theory the Hamiltonian \[4\] is diagonalized when \( u_n \) and \( v_n \) satisfy the BdG equations \[14,12\]

\[
\begin{pmatrix}
\hat{\xi} \\
\hat{\Delta} \\
\end{pmatrix}
\begin{pmatrix}
u_n \\
v_n \\
\end{pmatrix}
= E_n
\begin{pmatrix}
u_n \\
v_n \\
\end{pmatrix}, \tag{3}
\]

where

\[
\hat{\xi} u_n(r_i) = -t \sum_{\delta} u_n(r_i + \delta) + (V_{i}^{\text{imp}} - \mu) u_n(r_i),
\]

\[
\hat{\Delta} v_n(r_i) = \Delta_0(r_i) + \sum_{\delta} \Delta_\delta(r_i) v_n(r_i + \delta), \tag{4}
\]

subject to the constraints of self-consistency

\[
\Delta_0(r) = V_0 \sum_n u_n(r) v_n^* (r) \tanh(E_n/2k_BT),
\]

\[
\Delta_\delta(r) = \frac{V_1}{2} \sum_n [u_n(r + \delta) v_n^* (r) + u_n(r) v_n^* (r + \delta)] \times \tanh(E_n/2k_BT), \tag{5}
\]

where the summation is over positive eigenvalues \( E_n \) only.

For a system of linear size \( L \), solving the system of equations \[4\] with periodic boundary conditions requires diagonalizing a \( 2L^2 \times 2L^2 \) matrix. For a suitably chosen initial order parameter distribution we solve the system \[4\] using the standard LAPACK diagonalization routine. We then compute new gap functions from Eqs. \[4\] and iterate until the desired convergence is achieved. Typically 7-8 iterations are necessary to establish five-digit
convergence in the free energy and the average gap. Periodically we perform longer runs of 25-30 iterations to confirm the accuracy of the solutions. No significant deviations are found between short and longer runs.

We have solved the BdG equations (3) at $T = 0$ for the following set of model parameters: $\mu = -t$, corresponding to the band filling factor $n \approx 0.68$ ($n = 1$ is a half-filled band); $V_0 = 3t$, and $V_1 = -4.5t$. In the absence of disorder Eqs. (3) are easily solved analytically by appealing to translational invariance. One obtains the usual BCS type excitation spectrum $E_k = (\epsilon_k^2 + |\Delta_k|^2)^{1/2}$ with $\epsilon_k = -2t(\cos k_x + \cos k_y) - \mu$ and $\Delta_k = 2\Delta_d(\cos k_x - \cos k_y)$. For the above parameters we obtain $\Delta_d = 0.67t$. With respect to real materials this value is exaggerated; however, our choice of parameters was motivated by the desire to have the large mobility gap $\gamma_0$ (which according to Lee [3] scales with $\Delta_0^{1/2}$), necessary to study localization numerically in a finite system.

In Fig. 1 we display the amplitudes of $d$- and extended s-wave order parameters defined as [12]

$$d(r) = \frac{1}{|\Delta_x(r) + \Delta_y(r) - \Delta_y(r) - \Delta_y(r)|}$$
$$s(r) = \frac{1}{4}(\Delta_x(r) + \Delta_y(r) + \Delta_y(r) + \Delta_y(r))$$

in the vicinity of a single impurity with $V^{\text{imp}} = 100t$. The $d$-wave order parameter is suppressed at the impurity site and recovers its bulk value over 2-3 lattice spacings, just as one would expect for a pair-breaking impurity. The s-wave, which vanishes in the bulk, is nucleated near the impurity site and displays an interesting real space structure with a “d-wave” symmetry: it vanishes along the $|x| = |y|$ diagonals and changes sign upon 90° rotation. This behavior can be easily understood from the corresponding Ginzburg-Landau theory [15]. We note that being of the form $d \pm s$ this state does not break time reversal symmetry.

For a finite density of impurities we probe for localization in two different ways. First, for a given system size and disorder configuration we evaluate a generalized inverse participation ratio [16],

$$a_n = \frac{\langle |u_n|^4 \rangle + \langle |v_n|^4 \rangle}{\langle (|u_n|^2 + |v_n|^2)^2 \rangle^2},$$

where $\langle \ldots \rangle$ stands for the sum over all sites. As a function of increasing system size $L$ this quantity decreases as $\sim 1/L^2$ for extended states and approaches a constant value $\sim (a/\xi_L)^2$ for a state localized within the characteristic length $\xi_L$. Second, we study the sensitivity of states to boundary conditions by applying a uniform phase twist $\chi$ across the length of the system. We consider wavefunctions with the “twisted” boundary condition along the $x$-direction, $\Psi(x + L, y) = e^{i\chi} \Psi(x, y)$, and periodic along $y$, and we compute the stiffness of the $n$-th eigenvalue

$$\kappa_n = \frac{1}{2} \left( \frac{\partial^2 E_n}{\partial \chi^2} \right)_{\chi=0}.$$

Extended states will be sensitive to twist, and thus $\kappa_n$ is expected to be large. Localized states with $\xi_L \ll L$ will be insensitive to twist and $\kappa_n$ is expected to be small.

We have studied systems with $n_l = 0.015$ and $n_i = 0.06$ of strong repulsive impurities with $V^{\text{imp}} = 100t$. In Fig. 2 we display typical results for the inverse participation ratio $a_n$ and stiffness $\kappa_n$ as a function of energy for $n_l = 0.06$. There is a pronounced qualitative difference in $a_n$ between the low energy states below $E/t \approx 1$ and the high energy states. This is strongly suggestive of a mobility gap with a magnitude close to that predicted by Lee; $\gamma_0 \approx 0.84t$ for the parameterized system. While not so pronounced, this mobility gap can also be observed in the behavior of $\kappa_n$. For lower density of impurities, $n_l = 0.015$, we obtain similar results with the apparent mobility gap reduced by roughly a factor of two. This is in agreement with Lee’s prediction that $\gamma_0 \sim n_l^{1/2}$.

Even stronger evidence for the existence of the mobility gap can be obtained by analyzing the system size dependence of $a_n$. To this end we have carried out calculations for $L = 20, 24, 28, 32, 36, 40, 50$ and six independent impurity configurations for each size. The inset of Fig. 2 shows two quantities, $a^c \equiv \langle \langle a_n \rangle \rangle_{E<\gamma_0}$ and $a^g \equiv \langle \langle a_n \rangle \rangle_{E>\gamma_0}$, defined as averages of the inverse participation ratios $a_n$ taken over the indicated range of energy, as a function of $1/L^2$. Data points for $a^g$ lie on a straight line which extrapolates to zero for $L \to \infty$, just as one would expect for the extended states. Values of $a^c$ appear to extrapolate to a finite value of $a^c_{\infty} \approx 0.003$, which implies that these states are localized with $\xi_L/a \approx 20$. We note that this value of $\xi_L$ is in

![FIG. 2. Inverse participation ratio $a_n$ and stiffness $\kappa_n$ plotted as a function of energy for $L = 40$ and $n_l = 0.06$. Dashed line marks the mobility gap $\gamma_0 = 0.84t$ estimated from the theory of Lee [3]. Inset: Finite size scaling of the inverse participation ratio averaged over the energies below ($a^c$) and above ($a^g$) the mobility gap $\gamma_0$. The error bars reflect the scatter of the data from 6 different impurity configurations. Solid and dashed lines are guides to the eye only.](image)
a reasonable agreement with the rough estimate given in Ref. [4], which gives \( \xi_L/a \approx 38 \).

We have inspected visually the amplitudes of wavefunctions \( u_n(r) \) and \( v_n(r) \) for signs of localization. We have found that, in agreement with the above analysis, these states are spatially localized below the mobility gap with the characteristic length scale of about 20–30a, and appear to be extended at higher energies.

The question naturally arises why we do not observe delocalization effects below the inverse mobility gap \( \gamma_c \) predicted in Ref. [7]. In order to clarify this issue we have studied quasiparticle states associated with a single impurity. For the model parameters described above (i.e., strong coupling) we found no evidence for the anisotropic cross-shaped states predicted in Ref. [8]. Thus, it is not surprising that for a finite density of impurities the delocalization mechanism based on long-ranged overlaps is inoperative and all we find is a sharp mobility edge below which all the states are strongly localized. Furthermore we found that in this regime it is very important to treat the order parameter self-consistently; a separate calculation with spatially uniform (i.e., not relaxed) order parameter yielded wavefunctions with different spatial distributions and energy eigenvalues.

For the sake of completeness the above analysis was repeated for a different set of model parameters which may be closer to the realistic values for cuprates [13]: \( V_0 = 1.05t, V_1 = -1.05t, \mu = -0.36t \), which imply smaller magnitude of the bulk gap, \( \Delta_d \approx 0.066t \). In this case we have indeed found the predicted highly anisotropic quasiparticle state, however only the electron part of the wavefunction, \( v_n(r) \), exhibited the predicted tails along the diagonal directions. The amplitude of the hole part, \( u_n(r) \), was found to vanish along these diagonals with two tails running parallel to it. Such a structure was recently also obtained from the \( T \)-matrix approximation [17] and it is not clear how it affects the analysis of the localization problem in a system with finite impurity concentration. Within our numerical method we were unable to address this question since for the above parameters the estimated localization length \( \xi_L \) would be much larger than the maximum system size we can handle. Since in this case virtually identical results were obtained with a spatially uniform order parameter, the method employed previously by Xiang [11] may be suitable to address this problem.

Thus, the evidence presently available allows for two distinct scenarios with regards to the existence of the inverse mobility edge. Either (i) there is a crossover from the strong coupling regime which has (as we have explicitly demonstrated) \( \gamma_c = 0 \) to the weak coupling regime with \( \gamma_c > 0 \), or, (ii) it may be that \( \gamma_c = 0 \) for all coupling strengths which could be explained as a consequence of the complicated structure of the quasiparticle states discussed above that was not included in the original analysis of the many impurity problem [8].

To conclude, we have presented clear evidence for strong localization by impurities in \( d \)-wave superconductors at low energies. Compared to earlier analytical work [9], our approach treats impurity scattering exactly within BdG theory and accounts for order parameter relaxation near the impurity sites in a fully self-consistent way. The present model can easily be extended to finite temperatures and frequencies, thus opening possibilities for the analysis of the temperature dependent penetration depth, infrared conductivity, critical temperature, and other physically interesting quantities in the presence of disorder.

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[1] P. W. Anderson, Phys. Rev. Lett. 3, 325 (1959).
[2] K. Ueda and T. M. Rice, in Theory of Heavy Fermions and Valence fluctuations, Ed. T. Kasuya and T. Saso, (Springer, Berlin, 1985) p. 267.
[3] A. T. Fiory et al., Phys. Rev. Lett. 61, 1419 (1988); J. F. Annett, N. D. Goldenfeld and S. R. Renn, Phys. Rev. B 43, 2778 (1991); W. N. Hardy et al., Phys. Rev. Lett. 70, 3939 (1993).
[4] P. J. Hirschfeld and N. D. Goldenfeld, Phys. Rev. B 48, 4219 (1993).
[5] P. A. Lee, Phys. Rev. Lett. 71, 1887 (1993).
[6] D. N. Basov et al., Phys. Rev. B 49, 12165 (1994).
[7] A. V. Balatsky and M. I. Salkola, Phys. Rev. Lett. 76, 2386 (1996).
[8] A. V. Balatsky, M. I. Salkola and A. Rosengren, Phys. Rev. B 51, 15547 (1995).
[9] Y. Hatsugai and P. A. Lee, Phys. Rev. B 48, 4204 (1993).
[10] T. Xiang and J. M. Wheatley, Phys. Rev. B 51, 11721 (1995).
[11] T. Xiang, Phys. Rev. B 52, 6204 (1995).
[12] P. I. Soininen, C. Kallin and A. J. Berlinsky, Phys. Rev. B 50, 13883 (1994).
[13] Y. Wang and A. H. MacDonald, Phys. Rev. B 52, R3876 (1995).
[14] P. G. de Gennes, Superconductivity of Metals and Alloys, (Addison-Wesley, Readings, MA, 1989).
[15] A. J. Berlinsky et al., Phys. Rev. Lett. 75, 2200 (1995); M. Franz, (unpublished).
[16] D. J. Thouless, Phys. Rep. 13, 93 (1974).
[17] M. I. Salkola, A. V. Balatsky and D. J. Scalapino (unpublished).