Self-consistent electronic structure of a $d_{x^2−y^2}$ and a $d_{x^2−y^2} + id_{xy}$ vortex

M. Franz and Z. Tešanović
Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218
(October 9, 2018)

We investigate quasiparticle states associated with an isolated vortex in a $d$-wave superconductor using a self-consistent Bogoliubov-de Gennes formalism. For a pure $d_{x^2−y^2}$ superconductor we find that there exist no bound states in the core; all the states are extended with continuous energy spectrum. This result is inconsistent with the existing experimental data on cuprates. We propose an explanation for this data in terms of a magnetic-field-induced $d_{x^2−y^2} + id_{xy}$ state recently invoked in connection with the thermal conductivity measurements on Bi$_2$Sr$_2$CaCu$_2$O$_8$.

Behavior of superconductors in a magnetic field has been traditionally at the center of the condensed matter research because of the rich variety of fascinating phenomena in such systems and also because of its considerable technological importance. With the advent of high-$T_c$ cuprates the subject became even more interesting owing to the realization that their order parameter is unconventional, exhibiting most likely a $d_{x^2−y^2}$ symmetry. A number of novel effects associated with the existence of low-lying quasiparticle excitations near the gap nodes have been predicted \cite{6}. While there exists experimental evidence for each of these effects \cite{6,11}, it is by no means conclusive and an active debate continues. Several fundamental issues remain unresolved. Among the most interesting is the electronic structure of magnetic vortices, where a coherent physical picture is still lacking despite the number of theoretical and experimental investigations. Notably the nature of quasiparticle core states in $d$-wave superconductors remains poorly understood. These states are of considerable importance as they impact on various static and dynamic properties of the mixed state such as the structure of the flux lattice, pinning and flux-flow resistance.

It was established more than three decades ago by Caroli, de Gennes and Matricon \cite{7} that discrete quasiparticle states exist localized in vortex cores of conventional $s$-wave superconductors. These states are labeled by the angular momentum quantum number $\mu$, and the low-lying eigenvalues are $E_\mu \simeq \mu(\Delta_0^2/E_F)$ with $\mu = 1/2, 3/2, \ldots, \Delta_0$ the bulk gap and $E_F$ the Fermi energy. This prediction has been later confirmed in detail by numerical computations \cite{9} and by experiments on NbSe$_2$ \cite{10}. In a $d_{x^2−y^2}$ superconductor the situation becomes considerably more complex owing to the nontrivial structure of the gap function which vanishes along the four nodes on the Fermi surface. While the $s$-wave bound states can be intuitively understood by drawing an analogy to a simple quantum-mechanical problem of a particle in the cylindrical well of the radius $\xi \simeq v_F/\sqrt{\pi} \Delta_0$ and height $\Delta_0$, a suitable analogy in a $d$-wave case would involve a potential well whose radius and height depend on the polar angle $\theta$, with $\Delta(\theta)$ vanishing along the four diagonal directions causing $\xi(\theta)$ to diverge. Under such circumstances one would expect low-lying states to be extended along the node directions, rather than localized, unless the mixing of the core levels into the continuum is prevented by some higher symmetry. The existing experimental work, however, appears consistent with localized core states with large energy spacing \cite{4,5}.

The problem of a vortex in a $d_{x^2−y^2}$ superconductor has been considered theoretically by a number of authors \cite{8,7} but the detailed nature of quasiparticle core states has not been addressed. Very recently Morita, Kohmoto and Maki \cite{12} studied this problem using an approximate version of the Bogoliubov-de Gennes (BdG) theory. As pointed out in a subsequent Comment \cite{13}, this approximation improperly neglects an essential element of the physics of $d_{x^2−y^2}$ superconductors and yields unphysical results.

In this article we present, for the first time, a fully self-consistent numerical solution of the continuum BdG theory for a single isolated vortex in a $d$-wave superconductor. In agreement with the above qualitative argument we find that for a pure $d_{x^2−y^2}$ gap there exist no truly localized core states \cite{14}. We find low lying states that are strongly peaked in the core but have tails along the gap node directions which do not appear to decay to zero far from the core. The energy spectrum of these states becomes continuous in the limit of infinite system size. This is consistent with their extended nature, but inconsistent with the experimental finding \cite{14} of a large gap, $E_0 \approx \Delta_0/5$, to the lowest core state in YBa$_2$Cu$_3$O$_{7−\delta}$. We propose that one can reconcile the theory with experiment by assuming a purity and time reversal symmetry violating $d_{x^2−y^2} + id_{xy}$ state which has been recently invoked to explain the thermal conductivity data on Bi$_2$Sr$_2$CaCu$_2$O$_8$ \cite{15,16}.

The BdG equations for a $d$-wave vortex have been previously solved numerically on the lattice \cite{17,18}. In this work we adopt a continuum formulation of the problem, which has been used to study conventional $s$-wave vortices. Such formulation allows us to directly exploit various symmetries of the system and as a result we are able to consider much larger systems with a reasonable spectral resolution. The BdG equations for a $d$-wave su-
per conductor can be written as \[23\]
\[
\hat{H}_e u(R) + \int dr \Delta(R - r/2, r)v(R - r) = Eu(R),
\]
\[
-\hat{H}_e^* v(R) + \int dr \Delta^*(R - r/2, r)u(R - r) = Ev(R). \tag{1}
\]
Here \(\hat{H}_e\) is the single electron Hamiltonian, which we assume to have a simple free particle form
\[
\hat{H}_e = \frac{1}{2m} \left( p - \frac{e}{c} A \right)^2 - E_F, \tag{2}
\]
and \(\Delta(R, r) = V(r) \langle c_{\uparrow}(R - r/2) c_{\downarrow}(R + r/2) \rangle\) is the order parameter which is a function of the center-of-mass and the relative coordinate \(R\) and \(r\). In terms of the quasiparticle amplitudes \([u_n, v_n]\) the order parameter is self-consistently determined from the gap equation
\[
\Delta(R, r) = V(r) \sum_n \left[ u_n(R - r/2) v_n^*(R + r/2) + u_n(R + r/2) v_n^*(R - r/2) \right] \tanh(E_n/2T), \tag{3}
\]
where \(n\) labels the eigenstates of \([1]\) and the prime means the usual restriction to energies smaller than a cutoff scale \(\Omega_c\). \(V(r)\) is the pairing interaction which we assume to have the following model form:
\[
V(r) = V_0 \delta(r) + V_1 g(\varphi) \frac{1}{a} \delta(r - a), \tag{4}
\]
with \(r = (r, \varphi)\). The potential \([1]\) consists of a contact repulsion term \(V_0 > 0\), meant to model the on-site Coulomb repulsion between holes, and a short range attractive part \(V_1 < 0\), necessary to establish superconducting pairing. In order to model the lattice structure of cuprates we allow this attraction to be angle dependent with
\[
g(\varphi) = (1 - \epsilon) \cos^2(2\varphi) + \epsilon \sin^2(2\varphi), \tag{5}
\]
where \(\epsilon\) is a parameter used to tune the relative strength of this model’s analog of nearest and second nearest neighbor attraction. The nature of superconducting instability in this model depends on the dimensionless parameter \(\eta = ak_F\). In the absence of magnetic field the ground state has a d-wave symmetry for \(\eta > 1.9\) and is extended s-wave for \(\eta < 1.9\). This is consistent with the phase diagram of the related lattice model, where d-wave is known to be stable only close to half filling \([2]\). Furthermore, in the d-wave regime, the ground state is a pure \(d_{x^2-y^2}\) for \(\epsilon = 0\), a pure \(d_{xy}\) for \(\epsilon = 1\), and a \(d_{x^2-y^2} + id_{xy}\) admixture for \(0 < \epsilon < 1\). More generally one can also allow for anisotropy in the single particle Hamiltonian \(\hat{H}_e\) to account for the band structure effects in cuprates. We find that such anisotropies do not modify the phase diagram significantly and have only secondary effect on the vortex core structure. In the following we therefore limit ourselves to the simple form \([3]\) and we furthermore neglect the vector potential \(A\), as appropriate for the extreme type-II cuprates \([7]\). The magnitude of the contact repulsion \(V_0\) has little effect on the physics in the d-wave regime \([24]\). For simplicity we therefore take \(V_0 = 0\).

The form of the pairing interaction \([1]\) implies that the order parameter depends on the relative coordinate \(r\) only through its polar angle \(\varphi\). It is convenient to expand it in terms of the 2D angular momentum eigenstates,
\[
\Delta(R, r) = \Delta(R, \theta; \varphi) = \sum_{p, \ell} e^{-i p \theta} e^{i \ell \varphi} \Delta_{p\ell}(R), \tag{6}
\]
where \(R = (R, \theta)\). In such a representation the integer \(p\) characterizes winding of the superconducting phase around the vortex and \(l\) specifies the orbital state of the Cooper pair. Thus, for instance, the dominant order parameter near a singly quantized \(d_{x^2-y^2}\) vortex consists of an equal superposition of \(p = 1, l = \pm 2\) components:
\[
\Delta(R, \theta; \varphi) = 2e^{-i \varphi} \cos(2\varphi) \Delta_{1, \pm 2}(R).
\]

We solve the BdG equations \([1]\) numerically on a disk of the radius \(R_0\) with a suitably chosen initial order parameter and we then iterate Eqs. \((1)\) and \((3)\) until self-consistency is achieved. Following Gygi and Schluter \([8]\) we expand the quasiparticle amplitudes in the basis spanned by the eigenfunctions of \(\hat{H}_e\):
\[
[u(R), v(R)] = \sum_{\mu, m} e^{i \mu \theta} \Phi_{\mu m}(R)[u_{\mu m}, v_{\mu m}]. \tag{7}
\]
Here \(\Phi_{\mu m}(R) = [\sqrt{2/R_0}]_{\mu+1}(\alpha_{\mu m})J_{\mu}(\alpha_{\mu m} R/R_0), J_{\mu}(z)\) is the Bessel function of order \(\mu\) and \(\alpha_{\mu m}\) is the \(m\)-th zero of \(J_{\mu}(z)\). The integro-differential equation \([1]\) thus becomes an eigenvalue problem with an infinite matrix which we truncate at large values of \(|\mu|\) and \(m\), and diagonalize using a standard LAPACK subroutine. In the s-wave case this matrix is block diagonal in the angular momentum \(\mu\) and the resulting radial problem can be solved for each \(\mu\) separately. The crucial new element in the d-wave case is that, due to the complicated structure of the pairing term \([1]\), the angular momentum channels remain coupled and one has to solve the full 2D problem. This essential feature was ignored in \([4]\).

To model a pure \(d_{x^2-y^2}\) case we choose \(\eta = 2, \epsilon = 0, \Omega_c/E_F = 0.3, V_1/E_F = 1.6\) and \(T = 0\). We assume the initial order parameter of the form \(\Delta_{1, \pm 2}(R) = \Delta_0 \text{tan}(R/\xi_0)\), where \(\xi_0 = v_F / \Delta_0\) is the coherence length \([24]\). The above parameters imply \(\Delta_d = 0.26E_F\) and \(\xi_0 = 2.5k_F^{-1}\). In the process of iterating Eqs. \((1)\) and \((3)\), various other components \(\Delta_{p\ell}(R)\) appear in the self consistent solution reflecting the spatial anisotropy of the dominant \(d_{x^2-y^2}\) component and nucleation of various sub-dominant order parameters near the core. Fig. \([1]\), shows the leading components of the self-consistent order parameter. The \(d_{x^2-y^2}\) order parameter relaxes to its bulk value over a distance \(\sim 20k_F^{-1}\), which is much larger than \(\xi_0\). In fact, by varying the coupling strength \(V_1\) in a wide range, we find that for coherence lengths \(\xi_0 k_F \lesssim 10\) the order parameter profile (rescaled to its bulk value) no longer depends on \(\xi_0\) and retains the universal shape showed in Fig. \([1]\). We also find that this profile is not
very well fitted by the usual \( \tanh(R/\xi) \) function for any \( \xi' \) but is more consistent with algebraic \( \sim 1/r^2 \) relaxation. Fig. 1 also shows sizable components with symmetry of the form predicted by the Ginzburg-Landau theory \( [3] \). We have explicitly verified that, in agreement with \( [3] \), they will form four satellite vortices at a distance \( \sim 26k_F^{-1} \) form the origin.

We now investigate the nature of quasiparticle core states by computing the generalized inverse participation ratios, defined as \( [20] \)

\[
a_n = (R_0 k_F)^2 \frac{\langle |u_n|^4 \rangle_s + \langle |v_n|^4 \rangle_s}{\langle |u_n|^2 \rangle_s + \langle |v_n|^2 \rangle_s^2},
\]

where \( \langle \ldots \rangle_s = \int \ldots dR \). As a function of increasing system size \( R_0 \) this quantity approaches a finite constant for an extended state and grows as \( R_0^2 \) for a state localized within the characteristic length \( \xi_s \ll R_0 \). Fig. 2 shows \( a_n \) as a function of energy for system sizes \( R_0 k_F = 80, 120 \). Over the entire energy range the data for two different sizes behave in a similar way. If there existed localized states in the core their corresponding \( a_n \) would have increased by more than a factor of 2 between sizes \( R_0 k_F = 80 \) and 120. No such increase is observed. We carried out similar analysis for an s-wave case (same parameters with \( \eta = 1 \)), where it is known that only localized states exist at low energies. Indeed, in this case a clear \( a_n \sim R_0^2 \) scaling was observed \( [27] \) for \( E_n < \Delta_0 \). Fig. 2 further shows that, unlike in the s-wave case \( [8] \), there is no discernible pattern in the core energy levels and their spacing decreases with increasing system size. Visual inspection of the amplitudes of these states (inset Fig. 2) reveals that they are highly anisotropic with peaks near the core and tails running along the gap node directions which appear to saturate to a finite amplitude far from the core. Similar states are known to exist near a strongly scattering non-magnetic impurity \( [29] \).

Although not truly localized these core states should still give rise to enhanced tunneling conductance from the cores. In Fig. 3a we display this quantity computed from the present model. The closely spaced core states give rise to a broad peak centered near the zero energy. The peaks corresponding to individual states can still be resolved, but by studying the size dependence of such spectra we conclude that in the limit of infinite size these will form a continuum, similar to that reported by Wang and MacDonald in their lattice calculation \( [14] \). While the fine details of the spectrum depend on parameters of the model as well as on the system size, its gross qualitative features, and in particular the vanishingly small gap to the lowest state, remain remarkably robust for a wide range of parameters considered. These spectra are, unfortunately, in disagreement with the experimental finding of a large \( \sim \Delta_0/5 \) gap to the lowest core state \( [3] \). It is in principle possible that the intragap spectral features found experimentally are in fact resonances rather than true bound states. Even so, we find no indication of such resonant behavior in our calculation. Ref. 1 also reports that the core states are spatially isotropic, in contradiction to strong anisotropies found by this work and by quasiclassical computations \( [13,16] \).

It would thus appear that a model based on a pure \( d_{x^2-y^2} \) order parameter is in all aspects inconsistent with the published experimental data. We therefore propose an explanation in terms of a mixed \( d_{x^2-y^2} + id_{xy} \) state, which may be formed in upturns in finite fields at low temperatures \( [21,22] \). Such a state is fully gapped and we therefore expect the quasiparticle core states to recover some of their localized s-wave character. Within the present model we study such a scenario by taking \( \epsilon = 0.25 \) (with other parameters unchanged). This results in a \( d_{x^2-y^2} + id_{xy} \) state with \( d_{xy} \simeq 0.17d_{x^2-y^2}, \) roughly consistent with Laughlin’s prediction \( [23] \) for \( T = 0 \) and \( B = 6T \). The order parameter distribution near the core remains qualitatively similar to that reported in Fig. 1, but now with unequal magnitudes of \( \Delta_{1,2} \) and \( \Delta_{1,-2} \). Carrying out the analysis of participation ratios we find...
that the core states below the minimum gap $d_{xy}$ are truly localized and nearly isotropic, in agreement with experiment. Fig. 3 shows the corresponding tunneling conductance, which is now qualitatively consistent with experiment in that there exists a finite gap to the lowest core state which is independent of the system size. This gap is however still too small to account for the experiment in that there exists a finite gap to the lowest core state which is independent of the system size. This gap would therefore be present even at zero field. Although we expect that the qualitative features of the core states are insensitive to the origin of $d_{xy}$, a more satisfactory model would correctly describe the transition to the time reversal breaking state as a function of field. This would require explicitly including the vector potential term $A$ in the kinetic energy \(\mathcal{H}\); the work on this is in progress.

Our results firmly establish the absence of localized vortex core states in superconductors with a pure $d_{x^2-y^2}$ gap. We speculate that a sizable admixture of a subdominant order parameter is needed to reconcile theory with experiment. A magnetic-field-induced $d_{xy}$ component appears to be the most acceptable choice at present. This is by no means free of problems. A sufficiently large $d_{xy}$ component could be difficult to justify since on general grounds one would expect $d_{xy}/d_{x^2-y^2}$ to scale as the ratio of the corresponding critical temperatures. Furthermore, a transition to the fully gapped $d_{x^2-y^2} + id_{xy}$ state would be observable in the specific heat or muon-spin-rotation measurements of the penetration depth, but no such effect has been reported. In the present context of the vortex core states, however, our proposition can be easily tested by measuring the core spectra at lower fields (or higher temperatures). If the present spectra are indeed characteristic of a $d_{x^2-y^2} + id_{xy}$ state a dramatic change should be observable at the transition to the pure $d_{x^2-y^2}$ state.

The authors are indebted to A. V. Balatsky, A. J. Berlinsky and A. J. Millis for helpful discussions. This research was supported by NSF grant DMR-9415549.

\begin{thebibliography}{99}
\bibitem{1} S. K. Yip and J. A. Sauls, Phys. Rev. Lett. \textbf{69}, 2264 (1992).
\bibitem{2} G. E. Volovik, Sov. Phys. JETP \textbf{58}, 469 (1993).
\bibitem{3} A. J. Berlinsky, \textit{et al.}, Phys. Rev. Lett. \textbf{75}, 2200 (1995).
\bibitem{4} A. Maeda, \textit{et al.}, Phys. Rev. Lett. \textbf{74}, 1202 (1995).
\bibitem{5} K. A. Moler, \textit{et al.}, Phys. Rev. Lett. \textbf{73}, 2744 (1994).
\bibitem{6} I. Maggio-Aprile, \textit{et al.}, Phys. Rev. Lett. \textbf{75}, 2754 (1995).
\bibitem{7} C. Caroli, P. G. de Gennes, J. Matricon, Phys. Rev. Lett. \textbf{9}, 307 (1964).
\bibitem{8} F. Gygi and M. Schluter, Phys. Rev. B \textbf{43}, 7609 (1991).
\bibitem{9} H. Hess, R. B. Robinson, and J. V. Wasczak, Phys. Rev. Lett. \textbf{64}, 2711 (1990).
\bibitem{10} K. Karrai, \textit{et al.}, Phys. Rev. Lett. \textbf{69}, 355 (1992).
\bibitem{11} X. Jiang, \textit{et al.}, Physica C\textbf{254}, 175 (1995).
\bibitem{12} Recent tunneling data on Bi$_2$Sr$_2$CaCu$_2$O$_{8}$ [Ch. Renner, \textit{et al.}, (unpublished)] show no bound states. Instead they indicate a peculiar "pseudogap" behavior in vortex cores.
\bibitem{13} P.I. Soininen, C. Kallin, and A.J. Berlinsky, Phys. Rev. B \textbf{50}, 13883 (1994).
\bibitem{14} Y. Wang and A. H. MacDonald, Phys. Rev. B \textbf{52}, R3876 (1995); preprint [cond-mat/9607094]
\bibitem{15} N. Schoenholtz and K. Maki, Phys. Rev. B \textbf{52}, 490 (1995).
\bibitem{16} M. Ichikawa, \textit{et al.}, Phys. Rev. B \textbf{53}, 15316 (1996).
\bibitem{17} N. B. Kopnin and G. E. Volovik, Phys. Rev. Lett. \textbf{79}, 1377 (1997).
\bibitem{18} Y. Morita, M. Kohmoto and K. Maki, Phys. Rev. Lett. \textbf{78}, 4841 (1997).
\bibitem{19} M. Franz and M. Ichioka, Phys. Rev. Lett. \textbf{79}, 4513 (1997).
\bibitem{20} We note that this result has been anticipated by Ichikawa \textit{et al.} \textbf{[16]} who pointed out that quasi-classical trajectories of these states are open and therefore presumably cannot be quantized. See also Ref. \textbf{[13]}.
\bibitem{21} K. Krishana, \textit{et al.}, Science \textbf{277}, 83 (1997).
\bibitem{22} R. B. Laughlin, preprint [cond-mat/9709004]
\bibitem{23} P. G. de Gennes, \textit{Superconductivity of Metals and Alloys}, (Addison-Wesley, New York, 1992).
\bibitem{24} D. L. Feder and C. Kallin, Phys. Rev. B \textbf{55}, 559 (1997).
\bibitem{25} Here $\Delta_d$ is defined as a maximum gap on the Fermi surface which is related to the real space bulk order parameter $\Delta_0$ by $\Delta_d = 2\Delta_0(\eta)\Delta_0 \approx 0.7\Delta_0$ for $\eta = 2$.
\bibitem{26} M. Franz, C. Kallin, and A. J. Berlinsky, Phys. Rev. B \textbf{54}, R6897 (1996).
\bibitem{27} M. Franz and Z. Tešanović, (unpublished).
\bibitem{28} M. I. Salkola, A. V. Balatsky, and D. J. Scalapino, Phys. Rev. Lett. \textbf{77}, 1841 (1996), and references therein.
\bibitem{29} J. E. Sonier, \textit{et al.}, Phys. Rev. B \textbf{55}, 11789 (1997).
\end{thebibliography}