Self-Consistent Electronic Structure of a $d_{x^2-y^2}$ and a $d_{x^2-y^2} + id_{xy}$ Vortex

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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 $Bi_2Sr_2CaCu_2O_8$. [S0031-9007(98)06230-9]

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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 [1–3]. While there exists experimental evidence for each of these effects [4–6], 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 [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 μ, and the low-lying eigenvalues are $E_\mu \simeq \mu(\Delta_0^2/E_F)$ with $\mu = 1/2, 3/2, \ldots$, Δ_0 the bulk gap, and E_F the Fermi energy. This prediction has been later confirmed in detail by numerical computations [8] and by experiments on $NbSe_2$ [9]. 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 $\xi \simeq v_F/\pi\Delta_0$ and height Δ_0, a suitable analogy in a d-wave case would involve a potential well whose radius and height depend on the polar angle θ, 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 [6,10–12].

The problem of a vortex in a $d_{x^2-y^2}$ superconductor has been considered theoretically by a number of authors [13–17], but the detailed nature of quasiparticle core states has not been addressed. Very recently Morita, Kohmoto, and Maki [18] studied this problem using an approximate version of the Bogoliubov–de Gennes (BdG) theory. As pointed out in a subsequent Comment [19], this approximation improperly neglects an essential element of the physics of $d_{x^2-y^2}$ superconductors and yields unphysical results.

In this Letter 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 [20]. 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 [6,10] of a large gap, $E_0 \approx \Delta_0/5$, to the lowest core state in $YBa_2Cu_3O_{7-\delta}$. We propose that one can reconcile the theory with experiment by assuming a parity and time reversal symmetry violating $d_{x^2-y^2} + id_{xy}$ state which has recently been invoked to explain the thermal conductivity data on $Bi_2Sr_2CaCu_2O_8$ in finite magnetic fields [21,22]. Such a state is fully gapped, and for a sufficiently large d_{xy} component it can support true bound states in the core of the nature similar to the s-wave case.

The BdG equations for a d-wave vortex have been previously solved numerically on the lattice [13,14]. In this work we adopt a continuum formulation of the problem, which has been used to study conventional s-wave vortices [8]. 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 superconductor can be written as [23]

$$\hat{\mathcal{H}}_e u(\mathbf{R}) + \int d\mathbf{r}\, \Delta(\mathbf{R}-\mathbf{r}/2,\mathbf{r}) v(\mathbf{R}-\mathbf{r}) = Eu(\mathbf{R}),$$
$$-\hat{\mathcal{H}}_e^* v(\mathbf{R}) + \int d\mathbf{r}\, \Delta^*(\mathbf{R}-\mathbf{r}/2,\mathbf{r}) u(\mathbf{R}-\mathbf{r}) = Ev(\mathbf{R}). \tag{1}$$

Here $\hat{\mathcal{H}}_e$ is the single electron Hamiltonian, which we assume to have a simple free particle form

$$\hat{\mathcal{H}}_e = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 - E_F, \tag{2}$$

and $\Delta(\mathbf{R},\mathbf{r}) = V(\mathbf{r})\langle c_\uparrow(\mathbf{R}-\mathbf{r}/2)c_\downarrow(\mathbf{R}+\mathbf{r}/2)\rangle$ is the order parameter which is a function of the center-of-mass and the relative coordinate $\mathbf{R}$ and $\mathbf{r}$. In terms of the quasiparticle amplitudes $[u_n, v_n]$ the order parameter is self-consistently determined from the gap equation

$$\Delta(\mathbf{R},\mathbf{r}) = V(\mathbf{r})\sum_n{}' [u_n(\mathbf{R}-\mathbf{r}/2)v_n^*(\mathbf{R}+\mathbf{r}/2) + u_n(\mathbf{R}+\mathbf{r}/2)v_n^*(\mathbf{R}-\mathbf{r}/2)] \times \tanh(E_n/2T), \tag{3}$$

where n labels the eigenstates of (1) and the prime means the usual restriction to energies smaller than a cutoff scale Ω_c. $V(\mathbf{r})$ is the pairing interaction which we assume to have the following model form:

$$V(\mathbf{r}) = V_0\delta(\mathbf{r}) + V_1 g(\varphi)\frac{1}{a}\delta(r-a), \tag{4}$$

with $\mathbf{r} = (r,\varphi)$. The potential (4) 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 ϵ 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 [24]. 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 $\hat{\mathcal{H}}_e$ 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 (2), and we furthermore neglect the vector potential $\mathbf{A}$, 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 (4) implies that the order parameter depends on the relative coordinate $\mathbf{r}$ only through its polar angle φ. It is convenient to expand it in terms of the 2D angular momentum eigenstates,

$$\Delta(\mathbf{R},\mathbf{r}) = \Delta(R,\theta;\varphi) = \sum_{p,l} e^{-ip\theta}e^{il\varphi}\Delta_{pl}(R), \tag{6}$$

where $\mathbf{R} = (R,\theta)$. 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: $\Delta(R,\theta;\varphi) = 2e^{-i\theta}\cos(2\varphi)\Delta_{1,\pm 2}(R)$.

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 $\hat{\mathcal{H}}_e$:

$$[u(\mathbf{R}), v(\mathbf{R})] = \sum_{\mu,m} e^{i\mu\theta}\Phi_{\mu m}(R)[u_{\mu m}, v_{\mu m}]. \tag{7}$$

Here $\Phi_{\mu m}(R) = [\sqrt{2}/R_0 J_{\mu+1}(\alpha_{\mu m})]J_\mu(\alpha_{\mu m}R/R_0)$, $J_\mu(z)$ is the Bessel function of order μ, and $\alpha_{\mu m}$ is the mth zero of $J_\mu(z)$. The integrodifferential 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 μ and the resulting radial problem can be solved for each μ separately. The crucial new element in the d-wave case is that, due to the complicated structure of the pairing term (6), the angular momentum channels remain coupled and one has to solve the *full* 2D problem. This essential feature was ignored in [18].

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 $\Delta_{1,\pm 2}(R) = \Delta_0\tanh(R/\xi_0)$, where $\xi_0 = v_F/\pi\Delta_d$ is the coherence length [25]. 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 $\Delta_{pl}(R)$ appear in the self-consistent solution reflecting the spatial anisotropy of the dominant $d_{x^2-y^2}$ component and nucleation of various subdominant order parameters near the core. Figure 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

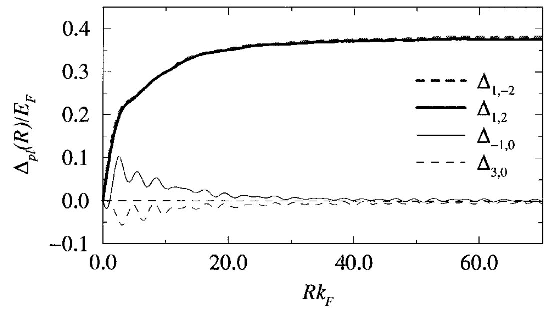

FIG. 1. Dominant order parameter components for system size $R_0 k_F = 120$. In terms of conventional notation we have $|d_{x^2-y^2}| \propto (\Delta_{1,-2} + \Delta_{1,2})$; $|d_{xy}| \propto (\Delta_{1,-2} - \Delta_{1,2})$; and $|s| \propto |e^{i\varphi}\Delta_{-1,0} + e^{-3i\varphi}\Delta_{3,0}|$.

ξ_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 ξ_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 ξ' but is more consistent with algebraic $\sim 1/r^2$ relaxation. Figure 1 also shows sizable components with s-wave 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 $\sim 26 k_F^{-1}$ from the origin.

We now investigate the nature of quasiparticle core states by computing the generalized inverse participation ratios, defined as [26]

$$a_n = (R_0 k_F)^2 \frac{\langle |u_n|^4 \rangle_s + \langle |v_n|^4 \rangle_s}{(\langle |u_n|^2 \rangle_s + \langle |v_n|^2 \rangle_s)^2}, \qquad (8)$$

where $\langle \cdots \rangle_s = \int \cdots d\mathbf{R}$. 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 $\xi_L \ll R_0$. Figure 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 $E_n < \Delta_0$. Figure 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 of 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 nonmagnetic impurity [28].

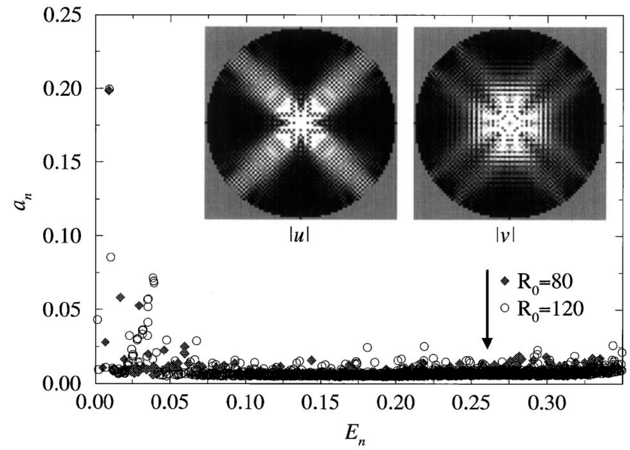

FIG. 2. Inverse participation ratios a_n as a function of energy. The arrow marks the maximum bulk gap Δ_d. Inset: amplitudes $|u_n(\mathbf{R})|$ and $|v_n(\mathbf{R})|$ of the lowest core state.

Although not truly localized these core states should still give rise to enhanced tunneling conductance from the cores. In Fig. 3(a) 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

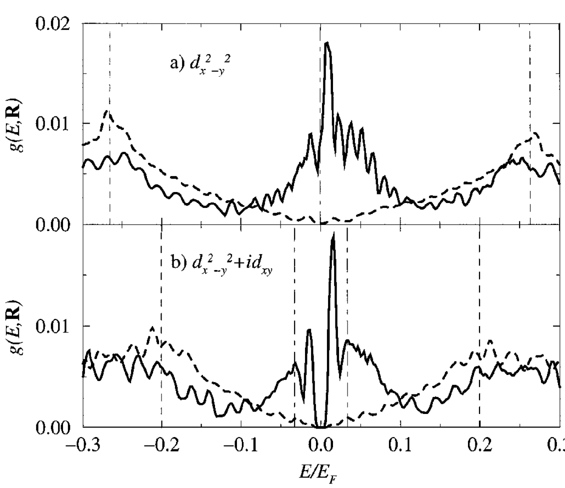

FIG. 3. Tunneling conductance $g(E, \mathbf{R})$ at the center of the vortex (solid line) and far from the vortex (dashed line), both spatially averaged over a circular ring $2k_F^{-1}$ wide. Dashed and dash-dotted vertical lines mark the maximum and minimum bulk gaps, respectively; $R_0 k_F = 120$.

finding of a large $\sim\Delta_d/5$ gap to the lowest core state [6,10]. It is in principle possible that the intragap spectral features found experimentally are, in fact, resonances rather that true bound states. Even so, we find no indication of such resonant behavior in our calculation. Reference [6] also reports that the core states are spatially isotropic, in contradiction to strong anisotropies found by this work and by quasiclassical computations [15,16].

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 cuprates 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 $d_{xy} \simeq 0.17 d_{x^2-y^2}$, roughly consistent with Laughlin's prediction [22] for $T = 0$ and $B = 6$ T. 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. Figure 3(b) 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 experimental result; we find that the agreement becomes better for larger d_{xy} component. Note that within the present model the d_{xy} component is brought about by change in the pairing interaction, rather than magnetic field, and it 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 $\mathbf{A}$ in the kinetic energy (2); 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 [22]. 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 [5,29]. 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.

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