Quasiparticles of $d$-wave superconductors in finite magnetic fields

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We study quasiparticles of $d$-wave superconductors in the vortex lattice by self-consistently solving the Bogoliubov-de Gennes equations. It is found for a pure $d_{x^2−y^2}$ state that: (i) low-energy quasiparticle bands in the magnetic Brillouin zone have rather large dispersion even in low magnetic fields, indicating absence of bound states for an isolated vortex; (ii) in finite fields with $k_Fξ_0$ small, the calculated tunneling conductance at the vortex core shows a double-peak structure near zero bias, as qualitatively consistent with the STM experiment by Maggio-Aprile et al. [Phys. Rev. Lett. 75 (1995) 2754]. We also find that mixing of a $d_{xy}$- or an $s$-wave component, if any, develops gradually without transitions as the field is increased, having little effect on the tunneling spectra.

Quasiparticles in superconductors have been a matter of a central theoretical interest in condensed matter physics, underlying almost all phenomena of superconductors. With a growing number of experiments in zero magnetic field which support the $d_{x^2−y^2}$-wave scenario for the high-$T_c$ cuprates [1,2], efforts have also been made to clarify their properties in finite magnetic fields. Experimentally, the scanning tunneling microscope (STM) is one of the most powerful tools to study them. It was Hess et al. [3] who clarified its potential to probe the quasiparticles [4]. Choosing a conventional $s$-wave material NbSe$_2$, they obtained a beautiful vortex-core spectrum with a characteristic zero-bias peak. Its origin was soon attributed, through numerical calculations based on the Bogoliubov-de Gennes (BdG) equations for an isolated vortex [5], to the bound quasiparticles around the vortex core predicted long ago by Caroli et al. [6]. Although a direct observation of the discrete levels is yet to be performed, the experiment confirmed the existence of bound states in the $s$-wave pairing and stimulated further theoretical studies on quasiparticles in the vortex states as well as similar experiments on high-$T_c$ materials.

The first microscopic theoretical study on a $d$-wave pairing was carried out by Wang and MacDonald using a lattice model in finite magnetic fields [7]. With parameters chosen appropriate for the cuprates, the calculated differential tunneling conductance at the vortex core shows a single broad peak near zero bias, whereas that of the corresponding $s$-wave model exhibits a clearly resolved bound-state structure. On the other hand, the measurement on YBa$_2$Cu$_3$O$_{7−δ}$ by Maggio-Aprile et al. [8] reveals a double-peak structure around zero bias, which they attributed by using the $s$-wave result to a couple of bound states split widely due to the large energy gap [9]. This discrepancy between the theory and the experiment raised a couple of questions: (i) whether or not bound states exist for the $d_{x^2−y^2}$-wave pairing where the gap closes along lines; (ii) why the double-peak structure appears. Himeda et al. focused on the strong-correlation effect to answer the second question [10]. Choosing the two-dimensional $t$-$J$ model, using a Gutzwiller wavefunction, and adopting the Gutzwiller approximation, they reported that a double-peak structure may show up in the low-doping region due to the induced $s$-wave component which brings a fully opened gap in the core region. However, the validity of using the Gutzwiller approximation is not well understood here. On the other hand, Franz and Tesanović investigated an isolated vortex of a continuum model through a direct diagonalization of a large matrix [11]. They have shown that: (i) no bound states exist in the $d_{x^2−y^2}$ model; (ii) the pure $d_{x^2−y^2}$ model also yields a single broad peak near zero bias as inconsistent with the experiment; (iii) the observed double-peak structure may be explained by a $d_{x^2−y^2} + id_{xy}$ model where the gap opens for an arbitrary direction so that there exist bound states in the core region. However, the model (iii) suffers from an inconsistency with the experiments that the gap is open everywhere even in zero magnetic field.

With these backgrounds, this letter focuses on a more detailed study on a continuum $d$-wave model. Due to technical difficulties, investigations on this fundamental model started rather recently, and only the special case of an isolated vortex has been considered by now [12,13]. We here consider the whole range $H_{c1} ≤ H ≤ H_{c2}$ in a unified way towards a thorough understanding of the basic $d$-wave model, which will also be useful when treating lattice models with strong correlations or disorders in the vortex lattice. The technique we use may be called “Landau-level expansion method,” developed firstly for the $s$-wave vortex lattice of $κ ≥ 1$ [14,15], and then suitably generalized to include anisotropic pairings and the magnetic-field variation [16]. We thereby clarify those effects caused by the formation of the vortex lattice and seek alternative mechanisms for the double-peak structure. We also consider the possibility of mixing of a $d_{xy}$- and an $s$-wave component into the pure $d_{x^2−y^2}$ state to see how it develops with the field strength and how it affects the physical properties. This topic has attracted much attention recently due to an observation of a plateau in thermal conductivity $κ(H)$ [17], followed by a theoretical proposal that it may imply a phase transition between the $d_{x^2−y^2}$ and the $d_{x^2−y^2} + id_{xy}$ states [18]. The origin of the plateau is still controversial [19], and it will be worth clarifying theoretically whether or not the
transition is really possible.

Our starting point towards those purposes is the BdG equations for the eigenfunctions \( u_s \) and \( v_s^* \) labeled by the quantum number \( s \) with a positive eigenvalue \( E_s \):

\[
\int \! dr' \left[ \begin{array}{cc}
\mathcal{H}(r,r') & \Delta(r,r') \\
-\Delta^*(r,r') & -\mathcal{H}(r,r')
\end{array} \right] \left[ \begin{array}{c}
u_s(r') \\
-v_s^*(r')
\end{array} \right] = E_s \left[ \begin{array}{c}
u_s(r) \\
-v_s^*(r)
\end{array} \right].
\]  

(1)

Here \( \Delta \) is the pair potential and \( \mathcal{H} \) denotes the normal-state Hamiltonian giving a quadratic dispersion in zero magnetic field \([22]\); both are \( 2 \times 2 \) matrices to include the spin degrees of freedom. The pair potential is determined self-consistently by

\[
\Delta(r,r') = V(r-r') \Phi(r,r'),
\]

(2)

where \( V \) denotes the interaction and \( \Phi \) is the order parameter defined by

\[
\Phi(r,r') \equiv \sum_s u_s(r)v_s^T(r') - v_s(r)u_s^T(r') \frac{2\tanh E_s}{2k_B T},
\]

(3)

with \( ^T \) denoting the transpose.

To solve these equations efficiently for the vortex-lattice states, we use the Landau-level expansion method mentioned above, which is sketched as follows \([13]\). Consider specifically that the field is along the \( c \) axis of a layered two-dimensional material. We fix the mean flux density \( B \) rather than the external field \( H \), and expand \( u_s \) and \( v_s \) in the eigenfunctions of the magnetic translation group whose unit cell covers the area \( \phi_0/B \) (\( \phi_0 \): the flux quantum). Those eigenfunctions \( \{|\psi_{Nk\alpha}(r)\rangle\} \) are labeled by the Landau-level index \( N \), the magnetic Bloch vector \( k \), and the quantum number \( \alpha = (1,2) \) which signifies two-fold degeneracy of the orbital states. Now, Eq. \([4]\) can be solved separately for each \( (k,\alpha) \) due to the translational symmetry of the vortex lattice; the corresponding eigenstate is labeled explicitly by \( s = (\nu k 2\pi \alpha) \) with \( \nu \) (the band) and \( \sigma \) (the spin) index. On the other hand, Eq. \([2]\) is handled via a double expansion of \( \Delta \) and \( \Phi \) with respect to the center-of-mass and the relative coordinates. Convenient bases to this end are given by \( \{|\psi^{(c)}_{Nk\alpha}(r+r')/2\rangle\} \) and \( \{|\psi^{(c)}_{Nk\alpha}(r-r')\rangle\} \), respectively, with \( q \) another magnetic Bloch vector and \( m \) the angular momentum along the \( c \) axis \((m = -N,-N+1,-N+2,\ldots) \). The overlap between \( \psi^{(c)}_{Nk\alpha}(r+r')/2 \psi^{(c)}_{Nk\alpha'}(r-r') \) and \( \psi_{Nk\alpha}(r)\psi_{Nk\alpha'}(r') \) is calculated rather easily, vanishing unless \( q = k + k' \) and \( \alpha_1 = \alpha_2 \). Also worth noting here is that \([22]\): (i) a single \( q \) suffices to describe the conventional vortex lattice due to its broken translational symmetry; (ii) \( N \)'s for the conventional hexagonal (square) lattice are multiples of 6 (4). Finally \( \langle Nm|V|N'm \rangle \) is estimated most conveniently in the momentum representation. To this end, we expand the pair scattering amplitude in zero field: \( V_{pp'} \equiv (2\pi)^2 \langle p|V|p' \rangle \) as

\[
V_{pp'} = \sum_{mm'} V^{(m,m')}(p,p') \epsilon^{m+m'+1} \phi_p,
\]

where \( \phi_p \) denotes the angle of the wavevector \( p \) with the \( a \) axis. Then the matrix element in finite fields is obtained as \( \langle Nm|V|N'm \rangle = (m-m')(1)^{N-N'}V^{(m,m')}(p,p')/4\pi l_B^2 \) with \( l_B \) the magnetic length and \( p = \sqrt{N}/l_B \). Once \( V_{pp'} \) is given explicitly, we can thereby calculate the properties of the vortex-lattice state over \( H_{c1} \leq H \leq H_{c2} \).

The pairing interaction we use is given by

\[
N_0 V_{pp'} = -2 \left( \frac{p}{k_B T} \right)^2 \left( \frac{p'}{k_B T} \right)^2 \left( g_{xy} - g_{yz} \right) \cos 2\phi_p \cos 2\phi_p' \left( g_{xy} \sin 2\phi_p \sin 2\phi_p' + g_s \Theta(p) \Theta(p') \right),
\]

(4)

where \( N_0 \) is the density of states for both spin in zero field, \( g \)'s are the coupling constants, \( k_B \) is the Fermi wavenumber, and \( \Theta(p) \) denotes a smooth cut-off \([7]\): \( \Theta(p) = e^{-|p^2-k_F^2|/p_c^2} \) with \( p_c \) a cut-off wavenumber. We then utilize the quantity \( T_{c0}^{(1)} = T_{c1}^{(1)}(g_{xy},p_c) \) \((j = x^2-y^2, xy, s)\), defined as the transition temperature in zero field for the state \( j \) in the absence of other two channels, as parameters to measure the strength of the pairing interaction for the channel \( j \). This procedure may be justified for the weak-coupling model. Indeed, we find little difference in the calculated results among several choices of \( (g_{xy},p_c) \). Another important parameter in the model is the coherence length \( \xi_0 = v_F/\Delta_0 \), where \( v_F \) is the Fermi velocity and \( \Delta_0 \) denotes the maximum of the energy gap at \( H = T = 0 \). We will clarify below the \( kp_\xi \) dependence of the differential tunneling conductance which is proportional to

\[
N(E,r) = -\sum_s \left[ |u_s(r)|^2 f'(E-E_s) + |v_s(r)|^2 f'(E+E_s) \right],
\]

(5)

with \( f(E) = (e^{E/k_B T} + 1)^{-1} \). Although they can be included easily, we here neglect: (a) the spatial variation of the magnetic field since \( \kappa \) is quite large for the high- \( T_c \) materials; (b) the Pauli paramagnetism for simplicity. The square vortex lattice is assumed throughout \([22]\), and the expansion over \( N_c \) (the center-of-mass Landau-level index) is cut at some \( N_c^{max} \), typically \( N_c^{max} = 8 \sim 16 \), with the convergence checked by changing \( N_c^{max} \).

We now present the results on the pure \( d_{x^2-y^2} \) model \( (g_{xy} = 0) \). Figure 1(a) shows the quasiparticle spectrum in the magnetic Brillouin zone with \( k_F \xi_0 = 5 \) for a low-temperature and low-field state: \( T/T_c = B/H_{c2} = 0.1 \). For comparison, the corresponding one of the \( s \)-wave model (hexagonal lattice) is presented in Fig. 1(b). We can clearly observe the following difference between the two. In Fig. 1(b) (\( s \)-wave), a qualitative change in the dispersion curves is seen around \( E_s \sim \Delta_0 \): the curves for \( E_s \sim \Delta_0 \) are closely spaced with a little dispersion, whereas the lower-energy bands are flat and occur in pairs with the level spacing of the order of \( \Delta_0^2/\varepsilon_F \) (\( \varepsilon_F \) : Fermi energy). As already pointed out by Norman et al. \([7]\), these correspond to the bound core states of an isolated vortex with little tunneling probability between adjacent
cores; one can check that the number of states for the lowest pair of bands is exactly the same as the number of vortices. In contrast, the low-energy d-wave bands in Fig. 1(a) are densely packed with large dispersion, indicating extended nature of the corresponding wavefunctions (this feature also shows up in the case of the hexagonal lattice).

From this comparison, we may conclude that no bound states exist for the d-wave model even in the zero-field limit of an isolated vortex, in agreement with the result of Franz and Tešanović [12]. A remark is necessary at the limit of an isolated vortex, in agreement with the result of Franz and Tešanović [12]. A remark is necessary at the limit of an isolated vortex, in agreement with the result of Franz and Tešanović [12].

where Tr implies integration and summation over the space and the spin coordinates, respectively. The second term on the right-hand side is expected not to depend strongly on the details of the quasiparticle spectrum. The first term, on the other hand, is quite sensitive to the structure of the local density of states. In particular, high density of states at $\omega = 0$ is energetically unfavorable so that the system tends to reduce it by using any perturbation available. We identify this perturbation with the hopping probability of the low-energy quasiparticles, whose magnitude may be measured by the dimensionless distance between adjacent vortices, $k_F l_B \sim k_F \xi_0 / \sqrt{B/H_{c2}}$. Hence the identification tells us that the double-peak structure becomes clearer as $k_F \xi_0$ $(B/H_{c2})$ decreases (increases), which is consistent with our numerical results. Our calculations performed for other values of $k_F \xi_0$ reveal that the peak splitting shows up at intermediate fields for $k_F \xi_0 \lesssim 5$. Since $k_F \xi_0$ is of the order of unity for the high-$T_c$ materials, the above mechanism may well explain the tunneling spectrum observed at $H = 6T$ [10]. A detailed experiment on the field dependence may be worth carrying out.

We finally consider the mixing of a $d_{xy}$-wave or an s-wave component into the dominant $d_{x^2-y^2}$ wave to study how it affects physical properties in finite magnetic fields. Such a state has been suggested to be realized in finite fields at low temperatures accompanying a phase transition [19,20]. Franz and Tešanović treated this problem in the zero-field limit of an isolated vortex, where parameters were chosen in such a way that $d_{x^2-y^2} + id_{xy}$ state is already formed in zero magnetic field. Clearly this is not consistent with various experiments which indicate a $d_{x^2-y^2}$ pairing in zero field. We hence choose the parameter $g_{xy}$ or $g_s$ in Eq. (5) in such a way that a pure $d_{x^2-y^2}$ state is stabilized in zero field. More specifically, $T_{c0}(xy)/T_c (T_{c0}^{(s)}) / T_c$ is put 0.31 (0.36) in the following $d_{xy}$-wave (s-wave) study, whereas the critical value is 0.33 (0.38) above which $d_{x^2-y^2} + id_{xy}$ $(d_{x^2-y^2} + is)$ state is formed in zero field below a certain critical temperature $T_c^{(xy)} (T_c^{(s)})$ lower than $T_{c0}^{(xy)} (T_{c0}^{(s)})$. Notice incidentally that $T_c = T_{c0}^{(s^2-y^2)}$. Figure 3 shows the field dependence.
of the maximum-gap ratios $|\Delta_{xy}|/|\Delta_{x^2-y^2}|$ and $|\Delta_4|/|\Delta_{x^2-y^2}|$ at the midpoint of the next-nearest-neighbor vortices of the square lattice. One can see clearly that the component $|\Delta_{xy}|$ develops gradually without any transitions with the field strength. This fact can also be realized on a purely group-theoretical ground as follows. There are four mirror reflections in zero field which distinguish the $d_{xy}$ state from the $d_{x^2-y^2}$ state. Those symmetry operations, however, no longer exist at finite fields due to the supercurrent flowing in the system. It hence follows that the mixing starts immediately above $H_{c1}$. The same is true for the $s$-wave mixing as already pointed out [25-26]. The result implies that the reason for the observed plateau in thermal conductivity [19,21], and $k_F \xi_0 = 5$. A similar result has been found for the case of the $s$-wave component. These results suggest that the mixing without a transition brings only small changes for the physical properties in finite magnetic fields.

In summary, we have carried out fully self-consistent calculations of the BdG equations for a basic $d$-wave model with continuously varying the field strength. We have thereby presented several new results connected closely with the detailed nature of the $d$-wave quasiparticles in the vortex lattice. The method used here will be helpful for the microscopic understanding of other anisotropic superconductors in finite magnetic fields as well as rotating Fermi superfluids.

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Fig. 3. Field dependence of the ratio $|\Delta_{xy}|/|\Delta_{x^2-y^2}|$ and $|\Delta_4|/|\Delta_{x^2-y^2}|$ at the center of the vortex-core square with $T/T_c = 0.1$, $k_F \xi_0 = 5$, and $T_{c0}/T_c = 0.31$ ($T_{c0}/T_c = 0.36$).

Fig. 4. The tunneling conductance at the core center for the $d_{x^2-y^2} + id_{xy}$ state (solid line) compared with that of the pure $d_{x^2-y^2}$ state (dashed line). Parameters are $B/H_{c2} = 0.3$, $T/T_c = 0.1$, $k_F \xi_0 = 5$, and $T_{c0}/T_c = 0.31$.