Low-lying excitations around a single vortex in a d-wave superconductor

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A full quantum-mechanical treatment of the Bogoliubov-de Gennes equation for a single vortex in a d-wave superconductor is presented. First, we find low-energy states extended in four diagonal directions, which have no counterpart in a vortex of s-wave superconductors. The four-fold symmetry is due to 'quantum effect', which is enhanced when $p_F\xi$ is small. Second, for $p_F\xi \sim 1$, a peak with a large energy gap $E_0 \sim \Delta$ is found in the density of states, which is due to the formation of the lowest bound states.

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After a few years of controversy, d-wave nature of the high-\(T_c\) superconductors is now well established \[1, 2\], although superconductivity in the electron-doped Nd\(_{2-x}\)Ce\(_x\)CuO\(_4\) appears to be of s-wave \[3\]. Therefore it is important to understand the nature of vortex states in a d-wave superconductor \[2, 4\]. An earlier analysis of the vortex state based on the Gor'kov equation shows that a square lattice of vortices tilted by \(\pi/4\) from the a-axis is the most stable except in the immediate vicinity of \(T = T_c\) or in a weak magnetic field \[5\]. Such a square lattice of vortices, though distorted, has been seen by a small angle neutron scattering \[6\] and a scanning tunneling microscopy (STM) \[7\] in YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) (YBCO) at low temperatures (\(T < 10\)K). We believe that this distortion of the vortex lattice is due to the orthorhombicity of the YBCO, although there are alternative interpretations based on the (d+s) admixture \[8, 9\]. One of the most remarkable results in the STM experiment is that the vortex appears to have a circular symmetry as in an s-wave superconductor. It is in sharp contrast to earlier results obtained within the Eilenberger theory (a semi-classical theory of a superconductor) \[10\], where a clear four-fold symmetry was obtained in the local density of states \[11, 12, 13\]. Further, at the center of the vortex, a peak with a large energy gap \(E_0 \sim \Delta\) was found in the local density of states, where \(\Delta\) is the superconducting order parameter. Then the most natural interpretation is that this corresponds to the lowest bound state for a vortex in a d-wave superconductor analogous to the one predicted by Caroli, de Gennes and Matricon \[14\].

In the previous study \[15\], in order to understand the results from the STM experiment, we have solved the Bogoliubov-de Gennes (B-dG) equation for a d-wave superconductor and obtained quasi-particle spectra around a single vortex. In the temperature region where the Ginzburg-Landau (GL) theory is valid, we found that the local density of states exhibits a circular symmetry and a peak with a large energy gap \(E_0 \sim \Delta\) is found in the local density of states at the center of the vortex, which is consistent with the STM experiment. In ref. \[15\], it is crucial to set \(p_F \xi \sim 1\) for YBCO, where \(p_F\) and \(\xi\) are the Fermi momentum and the coherence length respectively. The value of \(p_F \xi\) is obtained by an approximate formula for the lowest bound state \(E_0 = \Delta/(\pi p_F \xi)\) \[12, 16\]. This is also consistent with the chemical potential of YBCO deduced from the analysis of the spin gap seen in an inelastic neutron scattering experiment from monocrystals of YBCO \[17, 18\]. In the above analysis, however, we neglected the noncommutability between \(\hat{k}\) and \(x\) (’quantum effect’) \[19\], where \(\hat{k}\) and \(x\) are the quasi-particle momentum and coordinate respectively, and the local density of states has a perfect circular symmetry except when the mixing of an s-wave component occurs \[20\]. The correction is \(O(1/p_F \xi)\) and irrelevant at least in the study of systems with a long coherence length \(e.g.\) the superconducting phases of the heavy-ferimon systems \((p_F \xi \sim 10)\) and the \(^3\)He superfluidity \((p_F \xi \sim 100)\), but may have a serious influence in the study of the high-\(T_c\) superconductors, where \(p_F \xi \sim 1\) as is discussed above.

In this paper, a full quantum-mechanical treatment of the B-dG equation for a d-wave superconductor is reported, where the ’quantum effect’ is taken into account. As shown below, the four-fold symmetry appears in the local density of states. Similar four-fold
symmetry was obtained in the previous studies [11, 12, 13]. But it should be noted that the four-fold symmetry discussed here has totally different origin from that obtained in the earlier studies. The B-dG equation for a d-wave superconductor is given by

\[
\left\{ \frac{1}{2m} (\nabla - ieA(x))^2 - \mu \right\} u_n(x) = \epsilon_n u_n(x),
\]

\[
-\left\{ \nabla (\Delta(x) \partial_x) - \partial_y (\Delta(x) \partial_y) \right\} v_n(x) = \epsilon_n v_n(x),
\]

where \( u_n(x) \) and \( v_n(x) \) are the quasi-particle amplitudes, \( \Delta(x) \) is the pair potential, \( A(x) \) is the vector potential which is neglected assuming \( H \ll H_{c2} \), and \( \mu \) is the chemical potential which is identified with the Fermi energy. The parameters are set as \( 2m\xi^2\Delta = 2.82 \) and \( R/\xi = 30 \), where \( \xi \) is the coherence length and \( R \) is radius of the system and the pair potential \( \Delta(x) \) is given by

\[
\Delta(x) = \Delta \tanh(r/\xi) e^{i\phi}, \tag{0.1}
\]

where \( r \) and \( \phi \) are defined by \( x = (r \cos(\phi), r \sin(\phi)) \). This form of pair potential is obtained by the Ginzburg-Landau (GL) theory for a d-wave superconductor [12, 20] and applicable at not too low temperatures (an estimate of the temperature region where the GL theory is valid is \([0.5T_c, T_c]\) for an s-wave superconductor, when one consider the quasi-particle spectra around a single vortex).

In order to solve the B-dG equation numerically, it is convenient to expand the quasi-particle amplitudes \( u_n(x) \) and \( v_n(x) \) as

\[
u_n(x) = \sum_{\nu} \sum_{j} \psi_{n,\nu,j}(r) \exp(i \nu \phi),
\]

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\]

Here \( \psi_{i,\nu}(x) = \frac{1}{\sqrt{2\pi R J_{\nu+1}(\alpha_{i,\nu})}} J_{\nu}(\alpha_{i,\nu}x/R) \) \( J_{\nu}(x) \) is the Bessel function, \( \alpha_{i,\nu} \) is the \( j \)-th positive zero point of \( J_{\nu}(x) \) and \( R \) is the radius of the system. In the previous study [13], in which the 'quantum effect' is neglected, the B-dG equation decouples for \( u_{n,l,j} \)'s and \( v_{n,l,j} \)'s with different \( l \). On the other hand, when the 'quantum effect' is taken into account, \( u_{n,l,j} \)'s and \( v_{n,l,j} \)'s with different \( l \) couple, which plays an important role when \( p_F\xi \) is small. Because of the coupling, the number of basis we can use for numerical diagonalization is small compared to the previous study [13]. However, it is sufficient for the understanding of the qualitative aspects.

At first, consider the density of states \( \sum_i \delta(E - E_i) \) as a function of \( E/\Delta \), where \( p_F\xi = 1.33 \). As is seen in Fig. 1, there is a peak with a large energy gap \( E_0 \sim \Delta \). This
corresponds to the lowest bound state. The peak has a width due to the internal degree of freedom in the \( k \) space. These are consistent with the previous results \[15\] qualitatively, where the 'quantum effect' is neglected.

Next consider a local density of states in a superconductor, which is the quantity of interest for comparison to STM experiments and given by,

\[
N(E, \mathbf{x}) = \sum_n \left[ |u_n(\mathbf{x})|^2 \delta(E - \epsilon_n) 
+ |v_n(\mathbf{x})|^2 \delta(E + \epsilon_n) \right].
\]

In Fig. 2 and 3, \( \int_0^{0.35\Delta} dE N(E, r, \phi) \) is plotted and they show a clear four-fold symmetry in the local density of states. When \( p_F \xi \) is changed from 1.33 to 2.00, the four-fold symmetry is suppressed (see Fig. 3) and the local density of states becomes circular. This supports the idea that the four-fold symmetry is due to the 'quantum effect'. We stress that these low-energy states extended in four diagonal directions are particular to d-wave superconductivity. Therefore 1) these states should give rise to the zero-energy density of states proportional to \( \sqrt{B} \) as discussed by Volovik and others \[21, 4\], 2) they are the most likely the origin of the large flux flow resistivity in YBCO observed recently by Doettinger et al. \[22\] and, 3) when a square lattice of vortices tilted by \( \pi/4 \) from the a-axis is formed, the quasi-particle can move from one vortex to the other through these low-energy states extended in four diagonal directions, which should give rise to a cohesive energy guaranteeing the stability of the square lattice. The clarification of the quasi-particle spectrum in a vortex lattice and, in particular, the tilted square lattice is of immediate interest.

In conclusion, we have investigated the Bogoliubov-de Gennes equation for a d-wave superconductor, where the noncommutability between \( \hat{k} \) and \( \mathbf{x} \) ('quantum effect') is taken into account. We found a peak with a large energy gap \( E_0 \sim \Delta \) in the density of states, which is consistent with the previous results. We found low-energy states extended in four diagonal directions, which is due to the 'quantum effect'. The low-energy states have no counterpart in a vortex of s-wave superconductors. It is natural to consider that these low-energy states cause directional attractive forces between vortices. It is possible that, due to the directional attractive force, a square lattice of vortices becomes stable in some parameter region. Another scenario for a square lattice of vortices is proposed in ref. \[5\], where the higher-order correction in the Ginzburg-Landau theory \[23\] plays an essential role. In this paper, we do not consider the effect of the higher-order correction. The higher-order correction causes the four-fold symmetry in the pair potential. We consider that, in low temperatures, it is needed to take into account both the 'quantum effect' and the higher-order correction in the GL theory self-consistently, and more detailed study is left as a future problem.

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Figure Captions

Fig. 1: $\sum_i \delta(E - E_i)$ as a function of $E/\Delta$, where $k_F\xi = 1.33$.

Fig. 2: $\int_0^{0.35\Delta} dE \ N(E, r, \phi)$, where $k_F\xi = 1.33$ for a) $r/\xi = 3.0$, b) $r/\xi = 9.0$, c) $r/\xi = 15.0$ and d) $r/\xi = 27.0$.

Fig. 3: $\int_0^{0.35\Delta} dE \ N(E, r, \phi)$, where a) $k_F\xi = 1.33$ and $r/\xi = 9.0$ and b) $k_F\xi = 2.0$ and $r/\xi = 9.0$. 
Fig. 1
Fig. 2
Fig. 3 a)
Fig. 3 b)