Quasi-particle spectra around a single vortex in a d-wave superconductor

Y. Morita$^1$, M. Kohmoto$^1$ and K. Maki$^2$

$^1$Institute for Solid State Physics, University of Tokyo 7-22-1 Roppongi Minato-ku, Tokyo 106, Japan

$^2$Department of Physics and Astronomy, University of Southern California Los Angeles, Cal. 90089-0484, USA

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Abstract

Using the Bogoliubov-de Gennes equation, we study the quasi-particle spectra around a single vortex in a d-wave superconductor, where a magnetic field is parallel to the c-axis. In the temperature region where the Ginzburg-Landau theory is valid, we find that the local density of states preserves a circular symmetry when the symmetry of the superconducting order parameter is pure d-wave. It, however, exhibits a four-fold symmetry when the mixing of a s-wave component occurs. A peak with a large energy gap is found in the local density of states at the center of the vortex, which corresponds to the lowest bound state. Our results are consistent with a recent scanning tunneling microscopy experiment in an YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) monocystal. The breakdown of the Eilenberger theory in YBCO in particular and in the high-$T_c$ superconductors in general is discussed.
It is now well established that most of the properties of the high-$T_c$ superconductors are described in terms of a d-wave superconductor \cite{1,2} with possible exception of the electron-doped Nd$_{2-x}$Ce$_x$CuO$_4$ \cite{3}. Therefore it is of great interest to study vortex states in a d-wave superconductor \cite{4,5,6}. For example, in a magnetic field parallel to the c-axis, it was predicted that a square lattice of vortices tilted by $\pi/4$ from the a-axis is the most stable for $T < 0.8T_c$ \cite{5}, which has been seen recently by a small angle neutron scattering \cite{7} and a scanning tunneling microscopy (STM) experiment \cite{8} in YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) monocrystals at low temperatures ($T < 10K$), although elongated in the b direction. One of the interpretations is that this distortion is due to the orthorhombicity of YBCO, although there are alternative interpretations based on the (d+s) admixture \cite{9,10}.

Here we shall restrict ourselves to a single vortex in a d-wave superconductor, where a magnetic field is parallel to the c-axis. Early analyses of the quasi-particle spectra around a single vortex in a d-wave superconductor within the Eilenberger theory (a semi-classical theory of a superconductor) \cite{11} exhibits a surprising fourfold symmetry in the local density of states \cite{12,13}, which has not been seen experimentally \cite{8}. These analyses rely on the Riccati equation which is obtained in \cite{12} by simplifying the Eilenberger equation \cite{11}. It is to be noted that, in \cite{13}, the low-temperature region, where the Ginzburg-Landau (GL) theory is invalid, is also investigated by solving the Eilenberger equation self-consistently.

We believe that the above Eilenberger theory, which is essentially a semi-classical approximation, is invalid for the high-$T_c$ superconductors \cite{14}. In order to clarify the point, we shall give an analysis of the experimental results.

In YBCO \cite{8}, no peaks are found in zero-bias tunneling conductance at the center of the vortex, in contrast to a s-wave superconductor NbSe$_2$ \cite{15}. Further, at the center of the vortex, there is a peak around $E = 0.25\Delta$ in the tunneling conductance, where $\Delta=280K$ is the superconducting order parameter of YBCO at $T = 0K$. 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 \cite{16}. Since the lowest bound-state energy is given approximately by $E_0 = \Delta/\pi(p_F\xi)^{-1}$ \cite{12,19}, where $p_F$ and $\xi$ are
the Fermi momentum and the coherence length respectively, this implies \( p_F \xi \sim 1 \) in YBCO. 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 \[17, 18\].

Therefore in order to describe the quasi-particle spectra around a single vortex in high-\( T_c \) superconductors, it is crucial to study the Bogoliubov-de Gennes equation which is given by

\[
\left\{ -\frac{1}{2m} (\nabla - ieA(x))^2 - \mu \right\} u_n(x; \hat{k}) + \Delta(x; \hat{k}) v_n(x; \hat{k}) = \epsilon_n(\hat{k}) u_n(x; \hat{k}),
\]

\[
-\left\{ -\frac{1}{2m} (\nabla + ieA(x))^2 - \mu \right\} v_n(x; \hat{k}) + \Delta^*(x; \hat{k}) u_n(x; \hat{k}) = \epsilon_n(\hat{k}) v_n(x; \hat{k}),
\]

(1)

where \( u_n(x; \hat{k}) \) and \( v_n(x; \hat{k}) \) are the quasiparticle amplitudes, \( \Delta(x; \hat{k}) \) is the pair potential, \( A(x) \) is the vector potential which is neglected assuming \( H \ll H_{c2} \) \[16\], and \( \mu \) is the chemical potential which is identified with the Fermi energy. In this paper, we consider two types of the pair potential \( \Delta(x; \hat{k}) \), which are 'pure d-wave' \[12, 20\]

\[
\Delta(x; \hat{k}) = \Delta \tanh(r/\xi) \cos(2\theta(\hat{k})) e^{i\phi},
\]

(2)

where \( r, \phi \) and \( \theta(\hat{k}) \) are defined by \( x = (r \cos(\phi), r \sin(\phi)) \), \( (\hat{k}_x, \hat{k}_y) = (\cos(\theta(\hat{k})), \sin(\theta(\hat{k}))) \), \( \Delta \) is a real constant and \( \xi \) is the coherence length of the superconductor; and 'd+s-wave'

\[
\Delta(x; \hat{k}) = \Delta \tanh(r/\xi) \cos(2\theta(\hat{k})) e^{i\phi} + b_0(r/\xi) e^{-i\phi} + b_1(r/\xi) e^{3i\phi}
\]

for \( 0 < r \leq \xi \),

\[
\Delta(x; \hat{k}) = (\Delta \tanh(r/\xi) + a_0(\xi/r)^2) \cos(2\theta(\hat{k})) e^{i\phi} + (\xi/r)^2 \cdot \cos(2\theta(\hat{k}))(a_1 e^{-3i\phi} + a_1 e^{5i\phi}) + (b_0 e^{-i\phi} + b_1 e^{3i\phi})
\]
The pair potentials are obtained by the GL theory for an anisotropic 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 the s-wave superconductors, when one consider the quasi-particle spectra around a single vortex \[19\]).

In writing (1), we neglected the non-commutability between \(\hat{k}\) and \(x\) \[21\] \[22\]. The correction is \(O(1/p_F\xi)\) and irrelevant at least in the study of systems with a long coherence length e.g. a superconducting phase of a heavy-fermion system \((p_F\xi \sim 10)\) and \(^3\)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. But our results seem to be consistent with experimental results of YBCO as will be discussed below. Here it is to be noted that, in contrast to a usual semi-classical theory of a superconductor (the Eilenberger theory), our method takes into account quantization of the angular momentum. In fact, as we shall see, the quasi-particle spectra is totally different from ones obtained semi-classically \[12,13\].

In order to solve the Bogoliubov-de Gennes equation (1) numerically, it is convenient to expand the quasi-particle amplitudes \(u_n(x; \hat{k})\) and \(v_n(x; \hat{k})\) as

\[
\begin{align*}
  u_n(x; \hat{k}) &= \sum_{l=-\infty}^{\infty} \sum_{j=1}^{\infty} u_{n,l,j}(\hat{k}) \psi_{j,|l|}(r) \exp(il\phi), \\
  v_n(x; \hat{k}) &= \sum_{l=-\infty}^{\infty} \sum_{j=1}^{\infty} v_{n,l,j}(\hat{k}) \psi_{j,|l-1|}(r) \exp(i(l-1)\phi).
\end{align*}
\]

Here \(\psi_{i,\nu}(x) = \frac{1}{\sqrt{2\pi RJ_{\nu+1}(\alpha_{i,\nu})}} J_{\nu}(\alpha_{i,\nu}x/R)\) \((J_{\nu}(x)\) is the Bessel function), \(\alpha_{j,\nu}\) is the \(j\)th positive zero point of \(J_{\nu}(x)\) and \(R\) is the radius of the system. In our numerical calculation, the number of the basis is about 80000 for pure d-wave and about 4800 for (d+s)-wave. It is sufficient to discuss physical properties around a single vortex in a d-wave superconductor.

The quantity of interest for comparison to STM experiments is a local density of states in a superconductor

\[
N(E, x) = \sum_{\hat{k}, n} [ |u_n(x, \hat{k})|^2 \delta(E - \epsilon_n(\hat{k})) \\
+ |v_n(x, \hat{k})|^2 \delta(E + \epsilon_n(\hat{k}))].
\]
The local densities of states \( N(E, \mathbf{x}) \) for pure d-wave are shown in Figs. 1-4 for \( r/\xi = 0.0, 1.0, 2.0 \) and \( 10.0 \), respectively. The parameters are chosen as \( p_F\xi = 1.41 \) and \( 2m\xi^2\Delta = 2.82 \), from the experimental condition [8]. We also set \( R/\xi = 40 \). One can see peaks in the local densities of states corresponding to bound states around a single vortex, which are localized near the vortex center.

For \( r/\xi = 0.0 \) and \( 1.0 \) (Figs. 1 and 2), a peak with a large energy gap, which corresponds to the lowest bound state, appears in the local density of states. The peak has a width due to the internal degree of freedom in the \( \hat{k} \) space. The result is consistent with a recent STM experiment [8]. For \( r/\xi = 10.0 \) (Fig. 4), \( N(E, \mathbf{x}) \)’s around a vortex and without a vortex are almost identical. This indicates that the bound state is localized within this distance. We believe that the large energy gap is closely related to the quantization of the angular momentum. We note that there is a clear asymmetry in the local density of states at \( E \) and \(-E\) due to the formation of the bound states [23].

The integrated local densities of states near the zero energy \( \int_{0}^{0.17\Delta} dE \, N(E, \mathbf{x}) \) are shown in Figs. 5 and 6 for pure d-wave and (d+s)-wave respectively. The parameters are chosen as \( p_F\xi = 1.33, R/\xi = 30, 2m\xi^2\Delta = 2.82, 2m\xi^2a_m = 0.05 (m = -1, 0, 1) \) and \( 2m\xi^2b_m = 0.05 (m = 0, 1) \). The choice of high energy cutoff does not change the results quantitatively. Note that the local density of states preserves a circular symmetry for pure d-wave. On the other hand, it exhibits a clear four-fold symmetry when the mixing of a s-wave component occurs (see Fig. 6).

In conclusion, we have investigated the quasi-particle spectra around a single vortex in a d-wave superconductor by solving the Bogoliubov-de Gennes equation numerically. The local densities of states are consistent with a recent STM experiment [8]. The result shows a peak with a large energy gap in the local density of states at the center of the vortex, which corresponds to the lowest bound state. We find that the local density of states preserves a circular symmetry when the symmetry of the superconducting order parameter is pure d-wave. It, however, exhibits a four-fold symmetry when the mixing of a s-wave component occurs. However it is possible that a four-fold symmetry of a local density of states without
a mixing of a s-wave component \[12,13\] appears due to the noncommutability between \( \hat{k} \) and \( \mathbf{x} \). A fully quantum-mechanical treatment of the Bogoliubov-de Gennes equation is left as a future problem. Also a self-consistent treatment is needed in low temperatures, where the GL theory is invalid. Moreover, a treatment of a vortex lattice is essential when one investigates the thermodynamic quantities.

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Fig. 1 The local density of states $N(E, x)$ around a vortex ($\diamond$) and that without a vortex (+), where $r/\xi = 0.0$. The rescaled energy is defined by $E/\Delta$.

Fig. 2 The local density of states $N(E, x)$ around a vortex ($\diamond$) and that without a vortex (+), where $r/\xi = 1.0$. The rescaled energy is defined by $E/\Delta$.

Fig. 3 The local density of states $N(E, x)$ around a vortex ($\diamond$) and that without a vortex (+), where $r/\xi = 2.0$. The rescaled energy is defined by $E/\Delta$.

Fig. 4 The local density of states $N(E, x)$ around a vortex ($\diamond$) and that without a vortex (+), where $r/\xi = 10.0$. The rescaled energy is defined by $E/\Delta$. Weak anisotropy appears due to boundary effect.

Fig. 5 The integrated local density of states $\int_{0}^{0.17\Delta} dE N(E, x)$ for pure d-wave (left) and that for (d+s)-wave (right), where $\phi = 3\pi/8$. The lines are guide for eyes.

Fig. 6 The integrated local density of states $\int_{0}^{0.17\Delta} dE N(E, x)$ for pure d-wave ($\diamond$) and that for (d+s)-wave (+), where $r/\xi = 3.0$. The lines are guide for eyes.