Bound states and extended states around a single vortex in the $d$-wave superconductors

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Making use of the Bogoliubov-de Gennes equation for the $d$-wave superconductors, we investigate the quasi-particle spectrum around a single vortex. Taking $p_F\xi = 10$, we found that there are bound states which are localized around the vortex core, and extended states which are rather uniform, for $|E| < \Delta$ where $E$ is the quasi-particle energy and $\Delta$ is the asymptotic value of the order parameter for away from the vortex.

Much attention has been paid to the quasi-particle spectrum around a single vortex in $d$-wave superconductors, since the discovery of the high-$T_c$ cuprate superconductors [1, 2]. As is well known, $d$-wave superconductivity in both the hole-doped and the electron doped high-$T_c$ cuprates has been established [4–8]. As is well known, $d$-wave superconductivity in both the hole-doped and the electron doped high-$T_c$ cuprates has been established [4–8].

Contrary to the theoretical expectation [1–3], a) they have not seen any clear fourfold symmetry around a single vortex in [9–11]. Contrary to the theoretical expectation [1–3], a) they observed a bound state with energy $\Delta$, and b) they have not seen any clear fourfold symmetry.

Motivated by these experiments, Morita et al. [12] have abandoned the quasi-classical approximation used in earlier analysis [2] and proposed to study the bound states in terms of Bogoliubov-de Gennes equation [13]. Indeed, this approach appeared to give the correct description of the observation. However, later Franz and Tešanović claimed that there should be no bound states [14]. Further this claim was confirmed by Yasui and Kita [15] and by Takigawa et al. [16] later. In a vortex in $s$-wave superconductors, Caroli et al. [13] have shown there are a series of bound states. Further a detailed structure of the bound state wave function is explored later by Gygi and Schlüter [17]. As we have shown later, there are many bound states in $d$-wave superconductors as in $s$-wave superconductors [17]. We don’t know for sure the origin of this disagreement. But the possible source of their errors in previous studies [14–16] is easy to locate. They neglected in their analysis the conservation of the angular momentum around the vortex. Of course the strict conservation of the angular momentum is broken due to the fourfold symmetry of $\Delta(k)$. On the other hand the angular momentum is still conserved by modulo 4, and this is adequate to guarantee the presence of bound states. Therefore the structure of the bound states in the vicinity of the vortex core of $d$-wave superconductor appears to be very similar to the one in $s$-wave superconductor.

Then the only clear difference is the presence of extended states first discovered in [12]. Also these extended states give rise to the Volovik effect [19], which has been observed as the $\sqrt{H}$-term in the specific heat [20] and more recently as the $H$ linear term in the thermal conductivity [21, 22].

Earlier we have considered extreme quantum limit, i.e. $p_F\xi \approx 1$ [17], but recent experiment shows $p_F\xi \approx 20$, 30 for Bi2212 and YBCO, respectively [22]. Therefore, in this letter, we take $p_F\xi = 10$. We consider quasi-two dimensional $d_{x^2-y^2}$-wave superconductors in a disk with radius R. We put a single vortex at the center of the disk. When $R$ is large enough, the magnetic field is weak and the vector potential is small, so we ignore the vector potential. The Bogoliubov-de Gennes equations are given as,

$$\left[ -\frac{1}{2m_e} \nabla^2 - \mu \right] u_n (r) - \frac{1}{p_F} \left[ \partial_x \Delta (r) \partial_x - \partial_y \Delta (r) \partial_y \right] v_n (r) = E_n u_n (r),$$

$$- \frac{1}{p_F} \left[ \partial_x \Delta (r) \partial_x - \partial_y \Delta (r) \partial_y \right] u_n (r) = E_n v_n (r).$$

The order parameter is given as,

$$\Delta (r) = \sum_n \frac{1}{p_F} \left( 1 - 2f(E_n) \right)$$

$$\times \left[ (\partial_x u_n (r)) (\partial_x v_n^* (r)) - (\partial_y u_n (r)) (\partial_y v_n^* (r)) \right].$$

In the following we assume that the vector potential takes following form,

$$\Delta (r) = |\Delta (r)| e^{-i\theta}.$$
where $\phi_{mj}$ is Fourier-Bessel basis given as,

$$
\phi_{mj} (r) = \frac{\sqrt{2}}{R J_{m+1} (\alpha_{mj})} J_m \left( \frac{\alpha_{mj} R}{R} \right),
$$

Here $\alpha_{mj}$ is the $j$-th zero of the Bessel function of the $m$-th order. Then the Bogoliubov-de Gennes equation becomes as,

$$
\left[ \frac{1}{2m_e} \left( \frac{\alpha_{mj}}{R} \right)^2 - \mu \right] u_{nmj} - \frac{1}{2} \sum_{j} \left( \Delta_{m-1}^{ij} v_{nm-1j'} + \Delta_{m+3}^{ij} v_{nm+3j'} \right) = E_n u_{nmj},
$$

$$
\left[ \frac{1}{2m_e} \left( \frac{\alpha_{mj}}{R} \right)^2 - \mu \right] v_{nmj} - \frac{1}{2} \sum_{j} \left( \Delta_{m+1}^{ij} u_{nm+1j'} + \Delta_{m+3}^{ij} u_{nm+3j'} \right) = E_n v_{nmj}.
$$

$\Delta_{m-1}^{ij}$'s are matrix elements and given as,

$$
\Delta_{m-1}^{ij} = \int_0^R rdr \Delta (r) \phi_{mj}^d (r) \phi_{m-1j'}^i (r),
$$

$$
\Delta_{m+3}^{ij} = \int_0^R rdr \Delta (r) \phi_{mj}^d (r) \phi_{m+3j'}^i (r),
$$

where $\phi_{mj}^d (r) = \frac{\sqrt{2}}{R J_{m+1} (\alpha_{mj})} J_{m-1} \left( \frac{\alpha_{mj} R}{R} \right)$ and $\phi_{mj}^i (r) = \frac{\sqrt{2}}{R J_{m+1} (\alpha_{mj})} J_{m+1} \left( \frac{\alpha_{mj} R}{R} \right)$. The order parameter is now given by,

$$
\Delta (r) = \frac{\sqrt{2}}{4 \pi} \sum_n \left[ 1 - 2 f (E_n) \right] \sum_{j_1 j_2} \sum_m \left[ \phi_{mj_1}^d (r) \phi_{m+3j_2}^d (r) u_{nmj_1} v_{nm+3j_2} + \phi_{mj_1}^d (r) \phi_{m-1j_2}^d (r) u_{nmj_1} v_{nm-1j_2} \right].
$$

In order to fix the particle density, we determine the chemical potential by the condition,

$$
N_e = 2 \sum_{nmj} \left[ f (E_n) \right] |u_{nmj}|^2 + \left[ 1 - f (E_n) \right] |v_{nmj}|^2,
$$

where $N_e$ is total particle number.

From Eqs. ($6$) and ($7$), there are coupled sequences of $u_m$ and $v_m$ and there are four sectors of them.

0th \; \cdot \cdot \cdot, u_{n-4j}, v_{n-1j}, u_{n0j}, v_{n3j}, \cdot \cdot \cdot

1st \; \cdot \cdot \cdot, v_{n-4j}, u_{n-3j}, v_{n0j}, u_{n1j}, \cdot \cdot \cdot

2nd \; \cdot \cdot \cdot, v_{n-3j}, u_{n-2j}, v_{n1j}, u_{n2j}, \cdot \cdot \cdot

3rd \; \cdot \cdot \cdot, v_{n-2j}, u_{n-1j}, v_{n2j}, u_{n3j}, \cdot \cdot \cdot

(14)

There is a following symmetry between these sectors,

$$
\{ u_{nm}, v_{nm}, E_n \}_1 \leftrightarrow \{ -v_{n-m}, v_{n-m}, -E_n \}_0,
\{ u_{nm}, v_{nm}, E_n \}_2 \leftrightarrow \{ -v_{n-m}, v_{n-m}, -E_n \}_3.
$$

(15)

Therefore we solve Eqs. ($6$) and ($7$) for the 1st and the 2nd sectors and using the symmetry we determine $\Delta (r)$.

For the numerical calculation, we take $R = 15\xi$, $\Delta_0 / E_c = 0.4$ and $p_F \xi = 10$.

First, we show the temperature dependence of the order parameter in Fig. (1).

![Fig. 1](image1.png)

FIG. 1. Temperature dependence of the order parameter. (a) $T / T_c = 0.1$, (b) $T / T_c = 0.2$, (c) $T / T_c = 0.3$, (d) $T / T_c = 0.5$, (e) $T / T_c = 0.7$, and (f) $T / T_c = 0.9$.

There is an oscillation of the order parameter away from the vortex core. This comes from the geometrical resonance of the system and the boundary condition. Comparing with the s-wave superconductors [13, 23], there is no structure inside of the core.

![Fig. 2](image2.png)

FIG. 2. Local density of states as a function of $E$ and $r$ at $T / T_c = 0.1$. It is normalized by density of states of normal state $N_0$.  


FIG. 3. Weight of bound states and extended states for $E/\Delta = 0.05 \pm 0.02$.

FIG. 4. Wave functions of a bound state, (a) $|u(r)|^2$ and (b) $|v(r)|^2$. Its energy eigenvalue is $E/\Delta = 0.0481$.

FIG. 5. Wave functions of an extended state, (a) $|u(r)|^2$ and (b) $|v(r)|^2$. Its energy eigenvalue is $E/\Delta = 0.0331$.

Strictly speaking, we find other set of solutions, which cannot be characterized as the bound state or the extended state. But we believe that they are due to the finite size of our disk which we have studied.

In Summary, making use of the Bogoliubov-de Gennes equation for $d$-wave superconductors [13], we have studied the quasi-particle spectrum around a single vortex with a weak-coupling model and for $p_F\xi = 10$. First, we find many bound states centered around the vortex core as shown in Fig. 2. This picture is very similar to the one found for $s$-wave superconductors [18]. Second, there are extended states with almost uniform amplitude near the vortex core (see Fig. 5). Third, there appear to be a small group of the mixture of the bound state and the extended state. However, we believe this mixing is the finite size effect. In order to clarify this question, we need a pararell study of the quasi-particle spectrum in disks with different size. There remains one mystery. Why STM in YBCO [9] and Bi2212 [11] picked up only a single bound state? Perhaps some of bound states are localized near the vortex core, while the extended states are rather flat. So this should give a quasi-uniform density of states at $E = 0$. These are shown is Fig. 2 and Fig. 5 respectively.
more readily accessible to STM?

FIG. 6. Angular dependence of the local density of states. (a) $E = 0$, (b) $E/\Delta = 0.5$, and (c) $E/\Delta = 0.7$. They are normalized by the density of states of normal state $N_0$.

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[1] P. I. Soininen, C. Kallin, and A. J. Berlinsky, Phys. Rev. B 50, 13883 (1994).
[2] K. Maki, N. Schopohl, and H. Won, Physica B 204, 214 (1995); N. Schopohl and K. Maki, Phys. Rev. B 52, 490 (1995).
[3] Y. Wang and A. H. MacDonald, Phys. Rev. B 52, R3876 (1995).
[4] D. J. Van Harlingen, Rev. Mod. Phys. 67, 515 (1995).
[5] C. C. Tsuei and J. R. Kirtley, Physica B 282-287, 4 (1997).
[6] C. C. Tsuei and J. R. Kirtley, Phys. Rev. Lett. 85, 182 (2000).
[7] J. D. Kokales et al., Phys. Rev. Lett. 85, 3696 (2000).
[8] R. Prozorov, R. W. Giannetta, P. Fournier, and R. L. Greene, Phys. Rev. Lett. 85, 3700 (2000).
[9] I. Maggio-Aprile, Ch. Renner, A. Erb, E. Walker, and O. Fischer, Phys. Rev. Lett. 75, 2754 (1995).
[10] Ch. Renner, B. Bevaz, K. Kadawaki, I. Maggio-Aprile, and O. Fischer, Phys. Rev. Lett. 80, 3606 (1998).
[11] S. H. Pan, E. W. Hudson, A. K. Gupta, K. W. Ng, H. Eisaki, S. Uchida, and J. C. Davis, Phys. Rev. Lett. 85, 1536 (2000);
[12] Y. Morita, M. Kohmoto, and K. Maki, Phys. Rev. Lett. 78, 4841 (1997); 79, 4514 (1997); Europhys. Lett. 40, 207 (1997).
[13] C. Caroli, P. G. de Gennes, and J. Matricon, Phys. Lett. 9, 307 (1999).
[14] M. Franz and Z. Tešanović, Phys. Rev. Lett. 80, 4763 (1998).
[15] K. Yasui and T. Kita, Phys. Rev. Lett. 80, 4168 (1999).
[16] M. Takigawa, M. Ichioka, and K. Machida, Phys. Rev. Lett. 83, 3057 (1999).
[17] M. Kato and K. Maki, Physica B 284-288, 739 (2000); *ibid* 281 & 282, 942 (2000).
[18] F. Gygi and M. Schlüter, Phys. Rev. B 41, 822 (1990); Phys. Rev. B 43, 7609 (1991).
[19] G. E. Volovik, JETP Lett. 58, 496 (1993).
[20] K. A. Moler, D. J. Boer, J. S. Urbach, R. Liang, W. N. Hardy, and K. Zhang, Phys. Rev. Lett. 73, 2744 (1994).
[21] C. Kübert and P. J. Hirschfeld, Solid State Comm. 105, 459 (1998); Phys. Rev. Lett. 80, 4963 (1998).
[22] May Chiao, R. W. Hill, C. Lupien, B. Popić, R. Gagnon, and L. Taillefer, Phys. Rev. Lett. 82, 2943 (1999); May Chiao, R. W. Hill, C. Lupien, L. Taillefer, P. Lambert, R. Gagnon, and P. Fourrier, Phys. Rev. B 62, 3554 (2000).
[23] M. Kato and K. Maki, Prog. Theor. Phys., 103, 867 (2000).