

# Bound States in the Vortex Core

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## Abstract

The quasiparticle excitation spectrum of isolated vortices in clean layered  $d$ -wave superconductors is calculated. A large peak in the density of states in the "pancake" vortex core is found, in an agreement with the recent experimental data for high-temperature superconductors.

## 1 Introduction

The vortex core in classical type-II superconductors can be treated as the normal metal area with radius of the order of the coherence length  $\xi(0) \sim 10$  nm.[1, 2] The spectrum of the bound states near the Fermi surface, formed by the constructive interference between the incident and the Andreev reflected quasiparticles,[3] is quasicontinuous (gapless). High-temperature superconductors (HTS) are layered, having a cylindrical Fermi surface, the superconductivity is of the strong and  $d$ -wave coupling type, and the vortex core radius is much smaller,  $\xi(0) \sim 1$  nm.

For a two-dimensional (2D) vortex and  $s$ -pairing, Rainer *et al.* have shown, using the Andreev quasiclassical theory in the analytical, and Eilenberger's in the numerical part of their study, that bound states exist in the vortex core.[4] Similar conclusions have also been obtained by Maki and coworkers for  $d$ -pairing, within the Bogoliubov-de Gennes approach.[5]

In this paper, the Eilenberger quasiclassical equations [6], in the case of both  $s$  and  $d$ -pairing, are solved analytically, within the model considering the spatial variation of the order parameter in the vortex core as for a normal metal cylinder of radius  $r_c \sim \xi$ . A crucial difference is found in the quasiparticle spectra below the bulk energy gap, between the classical superconductors with spherical Fermi surface,  $s$ -pairing, large  $\xi$ , and HTS with cylindrical Fermi surface,  $d$ -pairing, small  $\xi$ . Our results confirm that the quasiparticle density of states (DOS) has one large maximum, recently observed in YBCO by scanning tunneling microscopy.[7]

## 2 Model of the Vortex Core

An efficient method for calculating local spectral properties is the quasiclassical theory of superconductivity, which gives the Eilenberger equations

$$\left[ 2\hbar\omega_n + \hbar\mathbf{v} \cdot \left( \nabla - i\frac{2e}{\hbar c}\mathbf{A} \right) \right] f = 2\Delta g, \quad \left[ 2\hbar\omega_n - \hbar\mathbf{v} \cdot \left( \nabla + i\frac{2e}{\hbar c}\mathbf{A} \right) \right] f^\dagger = 2\Delta^* g, \quad (1)$$

$$\hbar\mathbf{v} \cdot \nabla g = \Delta^* f - f^\dagger \Delta. \quad (2)$$

Here  $g = g_{\downarrow\downarrow}(\mathbf{r}, \mathbf{v}, \omega_n)$  and  $f = f_{\downarrow\uparrow}(\mathbf{r}, \mathbf{v}, \omega_n)$  represent the normal and the anomalous Green function respectively,  $\Delta = \Delta(\mathbf{r}, \mathbf{v})$  is the gap function,  $\omega_n = \pi k_B T (2n + 1)$ ,  $n = 0, \pm 1, \pm 2, \dots$ , are the Matsubara's frequencies, and  $\mathbf{v}$  is the Fermi velocity vector. The function  $f^\dagger$  is defined by  $f_{\uparrow\downarrow}^\dagger(\mathbf{r}, \mathbf{v}, \omega_n) = f_{\downarrow\uparrow}^*(\mathbf{r}, -\mathbf{v}, \omega_n)$ .  $\Delta$  and  $f$  are connected by the self-consistency equation.

For a homogeneous and isotropic superconductor, solutions of the Eilenberger equations are

$$\langle f \rangle = \frac{\Delta}{\varepsilon_n}, \quad \langle f^\dagger \rangle = \frac{\Delta^*}{\varepsilon_n}, \quad \langle g \rangle = \frac{\hbar\omega_n}{\varepsilon_n} \quad (\varepsilon_n^2 = |\Delta|^2 + (\hbar\omega_n)^2). \quad (3)$$

In the cylindrical coordinates  $(r, \varphi, z)$ , with the origin situated on the vortex axis, the vortex magnetic field is  $\mathbf{h} = h\mathbf{e}_z$ . At distances  $r \sim \xi \ll \lambda$  from the vortex axis,  $h$  is approximately constant, and the gauge can be chosen in the form  $\mathbf{A} = (\mathbf{h} \times \mathbf{r})/2$ . Taking the same vortex gap function as for a normal metal cylinder embedded in a superconductor

$$\Delta = \Delta(r, \theta)e^{-i\varphi}, \quad \Delta(r, \theta) = \begin{cases} 0, & r \leq r_c \\ \Delta(\theta), & r > r_c \end{cases}. \quad (4)$$

Here,  $r_c$  is the vortex core radius, and  $\theta$  is the polar angle in  $\mathbf{k}$ -space. For  $d$ -pairing  $\Delta(\theta) = \Delta_0 \cos 2\theta$ , and for  $s$ -pairing  $\Delta(\theta) = \Delta_0$ . The gauge in Eq. (4) is due to the flux quantization.

For a pancake vortex in  $(r, \varphi)$  plane, denoting the coordinate along  $\mathbf{v}$  by  $s$ , and along  $\mathbf{h} \times \mathbf{v}$  by  $p$  (Fig.1.), in the gauge with real gap, Eqs. (1) and (2) can be rewritten in the form

$$\left[ 2\hbar\omega_n + \hbar v \left( \frac{\partial}{\partial s} + i\frac{p}{l_H^2} + i\frac{p}{r^2} \right) \right] f = 2\Delta(r, \theta)g, \quad (5)$$

$$\left[ 2\hbar\omega_n - \hbar v \left( \frac{\partial}{\partial s} - i\frac{p}{l_H^2} - i\frac{p}{r^2} \right) \right] f^\dagger = 2\Delta(r, \theta)g, \quad (6)$$

$$\hbar v \frac{\partial}{\partial s} g = \Delta(r, \theta)(f - f^\dagger), \quad (7)$$

where  $r^2 = p^2 + s^2$  and  $l_H^2 = \hbar c / eh$ .

For a normal metal cylinder and zero magnetic field, Eqs. (5)-(7) with  $p = 0$ , the solution is of the form

$$f = \sum_i f_i(p) e^{\kappa_i s}, \quad g = \sum_i g_i(p) e^{\kappa_i s}. \quad (8)$$

For  $r \leq r_c$ , with  $\kappa_0 = 2\omega_n/v$ ,

$$f = F e^{-\kappa_0 s}, \quad g = G. \quad (9)$$

For  $r > r_c$  and  $\kappa = 2\varepsilon_n/\hbar v$ ,

$$f = \langle f \rangle + \Phi_1 e^{-\kappa s}, \quad g = \langle g \rangle + \Gamma_1 e^{-\kappa s}, \quad \text{for } s > 0, \quad (10)$$

$$f = \langle f \rangle + \Phi_2 e^{\kappa s}, \quad g = \langle g \rangle + \Gamma_2 e^{\kappa s}, \quad \text{for } s \leq 0. \quad (11)$$

Eqs. (5)-(7) imply

$$\frac{\Phi_1}{\Gamma_1} = \frac{\Delta(\theta)}{\hbar\omega_n - \varepsilon_n}, \quad \frac{\Phi_2}{\Gamma_2} = \frac{\Delta(\theta)}{\hbar\omega_n + \varepsilon_n}. \quad (12)$$

Using the continuity condition for  $f$  and  $g$  at  $\pm s_0 = \pm \sqrt{r_c^2 - p^2}$ , for  $r < r_c$  the normal Green function is

$$G = \frac{\hbar\omega_n \cosh(\kappa_0 s_0) + \varepsilon_n \sinh(\kappa_0 s_0)}{\hbar\omega_n \sinh(\kappa_0 s_0) + \varepsilon_n \cosh(\kappa_0 s_0)}. \quad (13)$$

For a vortex, approximating  $p/r^2$  by  $p/r_c^2$ , the solution of Eq. (5)-(7) can be obtained from Eq. (13), by changing  $\omega_n \rightarrow \omega_n'$ ,

$$G \approx \frac{\hbar\omega_n' \cosh(\kappa_0' s_0) + \varepsilon_n' \sinh(\kappa_0' s_0)}{\hbar\omega_n' \sinh(\kappa_0' s_0) + \varepsilon_n' \cosh(\kappa_0' s_0)}, \quad (14)$$

where

$$\omega_n' = \omega_n + i\frac{pv}{2} \left( \frac{1}{r_c^2} + \frac{1}{l_H^2} \right), \quad (15)$$

and  $\kappa_0' = 2\omega_n'/v$ . In this case, the magnetic flux quantization leads to [1, 5]

$$p_i = \left( i + \frac{1}{2} \right) \frac{\hbar}{mv}, \quad i = 0, \pm 1, \pm 2, \dots \quad (16)$$

Since for an isolated vortex  $l_H \gg r_c$ , the direct influence of the field can be neglected, and the only relevant contribution is due to the screening supercurrent flow,  $ipv/2r_c^2$  term in Eq. (15).

### 3 Bound States

Performing an analytical continuation of  $G$  by  $\hbar\omega_n \rightarrow -iE + \eta$ ,  $E$  being the quasiparticle energy with respect to the Fermi level, the retarded propagator  $g^R(E, p, \theta)$  is obtained. In terms of reduced variables  $E/\Delta_0 \rightarrow E$ ,  $\sqrt{\Delta^2(\theta) - E^2}/\Delta_0 \rightarrow \varepsilon$ ,  $\sqrt{E^2 - \Delta^2(\theta)}/\Delta_0 \rightarrow e$ ,  $p/r_c \rightarrow p$ ,  $2s_0/\pi\xi_0 \rightarrow s_0$ ,  $\xi_0 = \hbar v/\pi\Delta_0$  being the BCS coherence length, angle resolved partial DOS (PDOS) is obtained from  $N(E, p, \theta) = \text{Reg}^R(E, p, \theta)$ .

For the normal metal cylinder

$$\begin{aligned} N(E, p, \theta)/N(0) &= \Theta(e^2) \frac{|E|e}{e^2 \cos^2(Es_0) + E^2 \sin^2(Es_0)} + \\ &+ \Theta(\varepsilon^2) \frac{\pi|\Delta(\theta)|}{\Delta_0} \delta(E \sin(Es_0) - \varepsilon \cos(Es_0)), \end{aligned} \quad (17)$$

where  $\delta$  is the Dirac function,  $\Theta$  is the step-function, and  $N(0) = m/2\pi\hbar^2$  is the normal metal density of states at the Fermi surface for one spin orientation. For  $s$ -wave pairing, PDOS does not depend on  $\theta$ , while for  $d$ -wave pairing, averaging over the cylindrical Fermi surface leads to

$$\begin{aligned} N(E, p)/N(0) &= \frac{1}{2\pi} \int_0^{2\pi} N(E, p, \theta)/N(0) d\theta = \\ &= \frac{2}{\pi} \int_{\sqrt{\max\{0, E^2-1\}}}^{|E|} \frac{|E|e^2 de}{\sqrt{E^2 - e^2} \sqrt{1 - E^2 + e^2} (e^2 \cos^2(Es_0) + E^2 \sin^2(Es_0))} + \\ &+ \frac{(E \tan(Es_0) + |E \tan(Es_0)|)}{\sqrt{\cos^2(Es_0) - E^2}} \Theta(\cos^2(Es_0) - E^2). \end{aligned} \quad (18)$$

Finally, after spatial averaging over the cylinder area  $\pi r_c^2$ , DOS is

$$N(E) = \frac{4}{\pi} \int_0^1 N(E, p) \sqrt{1 - p^2} dp. \quad (19)$$

For the vortex, in Eqs. (17) and (18),  $E \rightarrow E + E_0 \text{sign } E$ ,  $E_0 = \hbar|p_i|v/2\Delta_0 r_c^2$ , Eq. (15), with  $p_i$  from Eq. (16), and  $\sum_{p_i}$  instead of integration in Eq. (19). Here, signs of  $p$  and  $E$  are connected, because the magnetic field causes a difference in propagation of particles and holes.

For small radius vortices in HTS,  $\xi_0 mv/\hbar \sim 1$  ( $\sim 10$  in classical superconductors), only one trajectory through the vortex core is allowed, with  $p = p_0$ , Eq. (16). Taking for YBCO  $r_c = \xi_0$ ,  $p_0 = 1/3$ ,  $\Delta_0/E_F = 0.424$ , only one peak in DOS in the vortex core around  $E/\Delta_0 \approx 0.3$  is obtained (Fig. 2). For comparison, DOS of normal metal cylinder embedded in the same superconductor and with the same radius  $r_c = \xi_0$ , but in the zero magnetic field, is shown. In this case, a large energy gap is found in DOS, due to formation of lowest bound state at high energy, of the order of  $\Delta_0$ . This is not the case in classical superconductors, where  $\Delta_0/E_F \ll 1$ .

**Fig.1.** Trajectory passing at distance  $p$  from the vortex center.

**Fig.2.** Quasiparticle DOS in the vortex core (solid curve), and in the normal metal cylinder (dashed curve), for clean layered  $d$ -wave superconductor.  $r_c/\xi_0 = 1$ ,  $\Delta_0/E_F = 0.424$ .

In conclusion, cylindrical Fermi surface,  $d$ -wave pairing and small  $\xi_0$ , large  $\Delta_0/E_F \sim 0.1$ , make DOS of a normal metal cylinder embedded in HTS and a pancake vortex different from DOS of a normal cylinder and a vortex in classical superconductors. Since the Andreev bound states can transport charge currents, unlike the bound states in a potential well, supercurrents can flow through the vortex without losses, strongly influencing its dynamics. This could be very important for transport properties of HTS, especially for understanding the unusual magnetic-field dependence of the electrothermal conductivity, which was observed experimentally and awaits explanation.[8]

## References

- [1] C. Caroli, P. G. de Gennes and J. Matricon, Phys. Lett. **9**, 307 (1964).
- [2] J. Bardeen and M. J. Stephen, Phys. Rev. **140**, 1197 (1965).; *ibid* **187**, 556 (1969).
- [3] A. F. Andreev, Sov. Phys. JETP **19**, 1228 (1964).
- [4] D. Rainer, J. A. Sauls and D. Waxman, Phys. Rev. B **54**, 10094 (1996).
- [5] N. Schopohl and K. Maki, Phys. Rev. B **52**, 490 (1995).; Y. Morita, M. Kohmoto and K. Maki, Phys. Rev. Lett. **78**, 4841 (1997).
- [6] G. Eilenberger, Z. Phys. **190**, 142 (1966); *ibid* **214**, 195 (1968).
- [7] I. Maggio-Aprile *et al.*, Phys. Rev. Lett. **75**, 2754 (1995).
- [8] J. A. Clayhold, Y. Y. Xue, C. W. Chu, J. N. Eckstein and I. Bozovic, Phys. Rev. Lett. **53**, 8681 (1996).

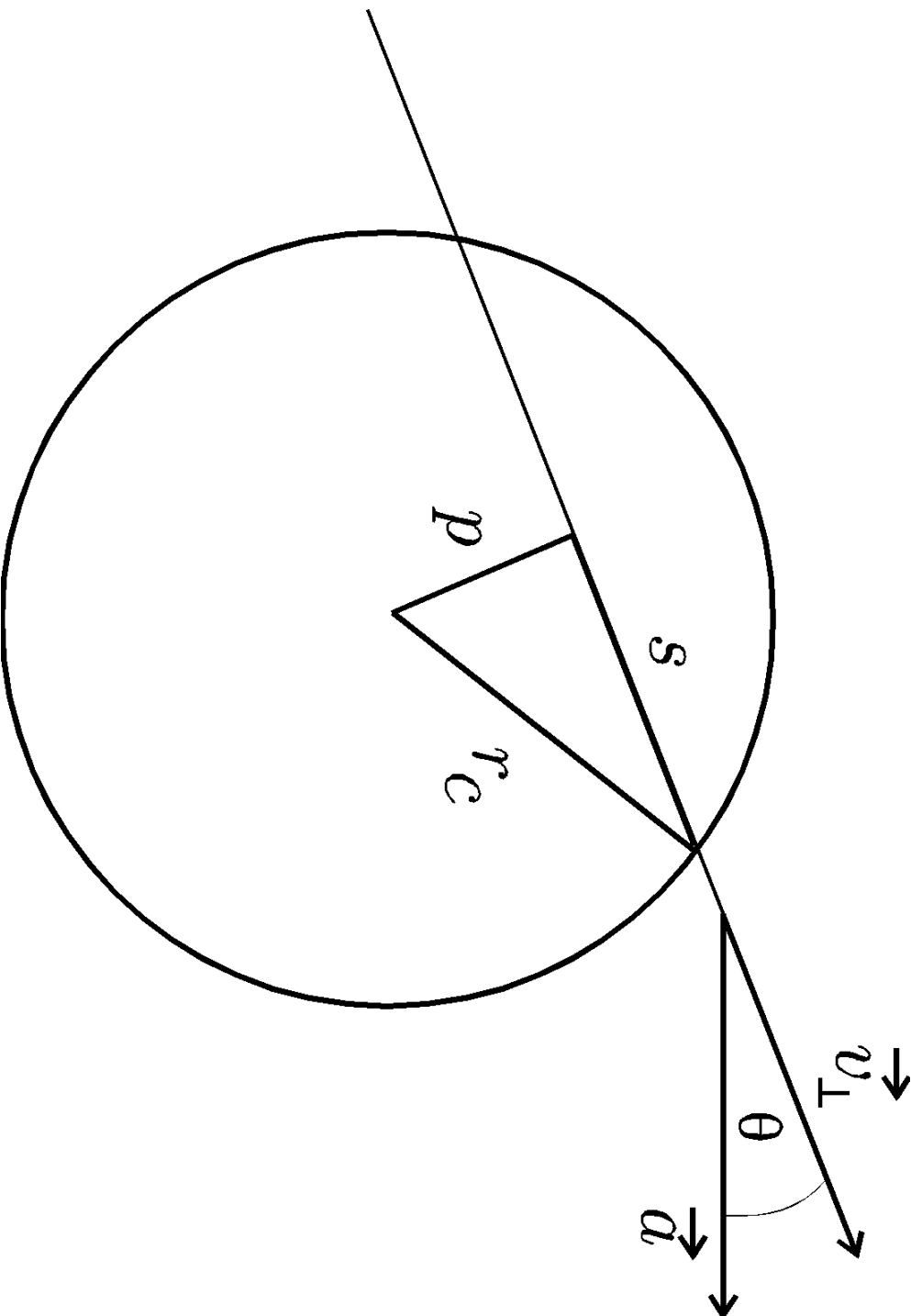


Figure 1

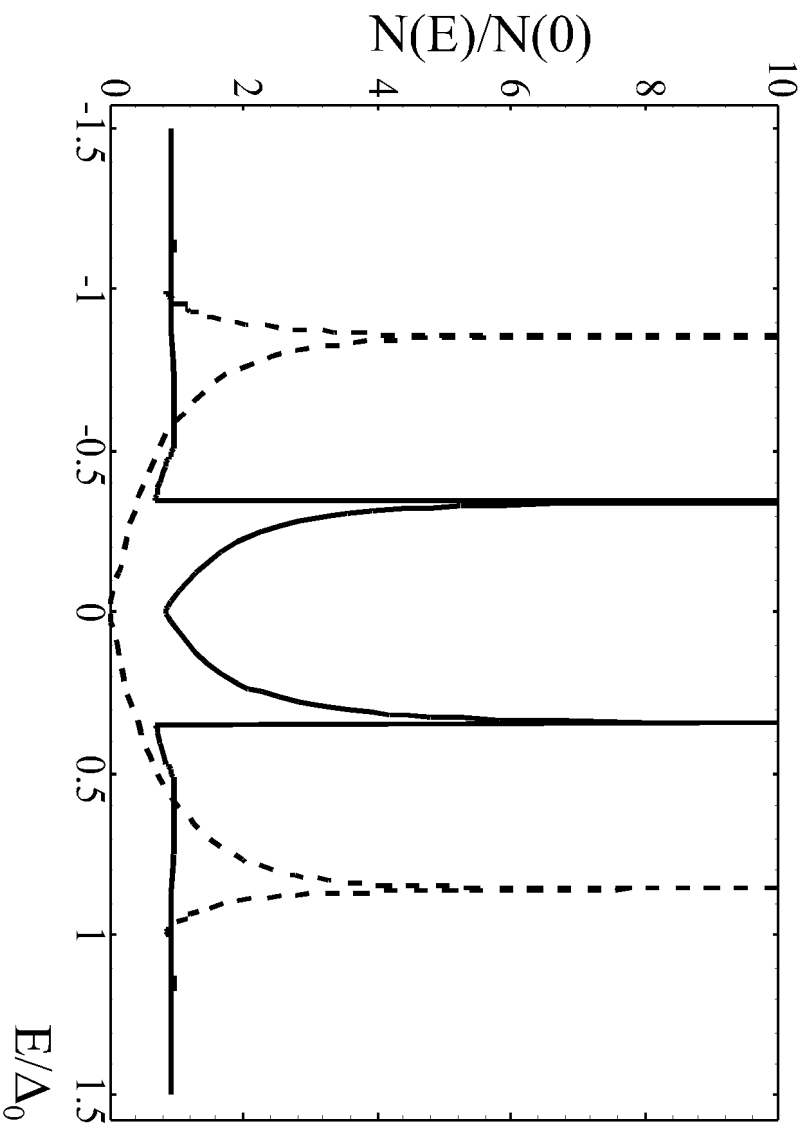


Figure 2