

Aharonov-Bohm Effect for Quasiparticles around a Vortex Line in a d -Wave Superconductor

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On the basis of the Bogoliubov–de Gennes theory we develop an analytical description of low-energy extended quasiparticle states around an isolated flux line in a superconductor with gap nodes. The wave functions of these excitations and the corresponding density of states are shown to be strongly influenced by the interaction with a pure gauge potential due to the Aharonov-Bohm scenario.

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Understanding the nature of low-energy quasiparticle (QP) states in isolated vortices and vortex lattices of type-II superconductors is of considerable importance since for low temperatures T these states impact on various static and dynamic properties. The flux lines affect the QP excitations through the following mechanisms: (i) QP scattering on the gap inhomogeneity in vortex cores (which results in formation of localized core states in s -wave compounds) [1]; (ii) QP scattering on the potential proportional to the superfluid velocity \mathbf{V}_s [2]; (iii) long-range magnetic field effects which are responsible for a finite curvature of a quasiclassical trajectory in a vortex lattice [3]; (iv) interaction with a pure gauge potential due to the Aharonov-Bohm (AB) scenario [2,4–8] which is known to describe the action of the enclosed fluxes on the quantum interference of charged particles [9]. For conventional s -wave superconductors these mechanisms have been studied for several decades, and now one may conclude that the physical picture of the electronic structure of the mixed state in s -wave systems is rather clear. The situation is dramatically different in superconductors with gap nodes where the vanishing pair potential in the nodal directions results in qualitative changes in quantum mechanical motion of QPs. The interest to these fundamental issues is stimulated by recent experimental observations of unconventional behavior of QP excitations in the mixed state of high- T_c compounds [10,11] where the dominating order parameter (OP) is believed to be of d -wave symmetry.

In this Letter we focus on the quantum mechanical effects caused by the interaction of QPs with pure gauge potentials induced by flux lines. The AB scattering of electronic excitations by singly quantized vortices in s -wave superconductors was analyzed by Cleary [2] in 1968. The importance of the AB mechanism for the understanding of the origin of the Iordanskii force acting on a moving vortex line in a superfluid has been pointed out in [5]. Recently the significance of the AB effect was addressed in a number of papers devoted to the calculations of the QP band spectrum [6,7] and thermal conductivity [8] in the mixed state ($H_{c1} \ll H \ll H_{c2}$) of high- T_c cuprates. The main goal of our theoretical analysis is to show that contrary to the s -wave case the AB effect plays a crucial role in the behavior of low-lying QP states in d -wave compounds.

Let us consider a single isolated vortex line which carries the flux quantum $\phi_0 = \pi\hbar c/|e|$. Because of the Meissner effect a magnetic field \mathbf{H} is screened at the London penetration depth λ_L and at large distances from the vortex center $r \gg \lambda_L$ the vector potential takes the form $\mathbf{A} = \phi_0[\mathbf{z}_0, \mathbf{r}]/(2\pi r^2)$, where $[\mathbf{z}_0, \mathbf{r}]$ is a vector product of vectors \mathbf{z}_0 and \mathbf{r} , and \mathbf{z}_0 is a unit vector chosen along the vortex axis. Such a vector potential cannot be excluded from the Bogoliubov–de Gennes (BdG) equations (describing the quantum mechanics of QPs) using any single-valued gauge transformation. Note that within the standard Schrödinger theory for a particle with a charge e an AB solenoid with a magnetic flux $\Phi = \phi_0$ is known to be the most effective scatterer [9]. However, for s -wave superconductors the effect of the AB potentials on the QP density of states (DOS) should be rather small. The point is that the size of the semiclassical wave packet propagating outside the flux tube (i.e., in the region $r \gg \lambda_L$) appears to be much less than the impact parameter. As a result, the interference effects are small and can be neglected. As we see below, such a conclusion is no more valid if we consider superconductors with gap nodes. Hereafter we assume Fermi surface (FS) to be two-dimensional (2D), which is appropriate to high- T_c superconductors, and take the gap function in the general form $\Delta_d = 2\Delta_0 F(\mathbf{k})k_x k_y / k_F^2$, where the real function $F(\mathbf{k})$ has the tetragonal symmetry of the normal metal, Δ_0 is the gap maximum, the x axis is taken along the [110] crystal direction. In contrast to conventional superconductors, the DOS at low energies ε in d -wave systems is dominated by contributions which come from the regions far from the cores [12] and associated with extended QP states with momenta close to the nodal directions. This conclusion based on the semiclassical approach has been confirmed by the recent numerical analysis [13] of the BdG equations for a single isolated vortex line (in the limit $\lambda_L \rightarrow \infty$). Note that the calculations presented in [13] also point to the absence of truly localized core states or any resonant levels in the pure d -wave case though such states were observed in numerical simulations [14].

Let us start with some qualitative arguments which indicate a significance of pure gauge potentials in the quantum mechanics of extended QP excitations. In the homogeneous state the low-energy excitations (confined to

one of the gap nodes) are described by a Dirac-like spectrum, $\varepsilon^\pm = \pm \hbar \sqrt{V_F^2 q_\perp^2 + V_\Delta^2 q_\parallel^2}$, where V_F is the Fermi velocity, and (q_\parallel, q_\perp) defines a coordinate system whose origin is at the node, with q_\perp (q_\parallel) normal (tangential) to the FS. The V_Δ value characterizes the gap slope near the node. For the simplest gap function with $F(\mathbf{k}) \equiv 1$ the Dirac cone anisotropy $\alpha = V_F/V_\Delta$ is determined only by the ratio of the coherence length $\xi = \hbar V_F/\Delta_0$ to the Fermi wavelength ($\alpha = k_F \xi/2$) while for a more general case the parameter α depends also on the $F(\mathbf{k})$ value at the node. One can separate the following length scales for QP wave functions: an atomic length scale k_F^{-1} and two characteristic wavelengths of a slowly varying envelope $l_\perp \sim q_\perp^{-1} \sim \hbar V_F/\varepsilon$, $l_\parallel \sim q_\parallel^{-1} \sim \hbar V_\Delta/\varepsilon$. The length scales l_\perp and l_\parallel determine the size of the semiclassical wave packet, which appears to diverge in the low-energy limit. Such a divergence is responsible for a crucial role of quantum mechanical effects in QP motion and, in particular, for the extremely large AB scattering amplitude.

Our further consideration of the low-energy QP states ($|\varepsilon| \ll \Delta_0$) with momenta locked to the nodes is based on the essentially 2D quantum mechanical model proposed by Simon and Lee [15]. For QPs with momenta close to a certain gap node direction [e.g., $\mathbf{k}_1 = (k_F, 0)$] one can divide out the fast oscillations on a scale k_F^{-1} in the particlelike and holelike parts of the wave function $(u, v) = (\tilde{u}, \tilde{v}) \exp(i\mathbf{k}_1 \mathbf{r})$ and simplify the nonlocal off-diagonal terms in BdG equations (see [6–8,15,16] for details). Let us introduce the gap function describing the mixed state in the form $\Delta(\mathbf{k}, \mathbf{R}) = \Delta_d(\mathbf{k})\Psi(\mathbf{R})$, where $\Psi(\mathbf{R}) = f \exp(i\chi)$ is the OP used in the Ginzburg-Landau theory. The BdG equations for QP wave functions $\hat{g} = (\tilde{u} \exp(-i\chi), \tilde{v})$ read $\hat{H}_{SL} \hat{g} = \varepsilon \hat{g}$ [17]. Outside the cores the Hamiltonian \hat{H}_{SL} linearized in gradient terms takes the form $\hat{H}_{SL} = \hat{H}_0 + |e|\varphi$, where $\hat{H}_0 = V_F \hat{\sigma}_z \hat{p}_x + V_\Delta \hat{\sigma}_x \hat{p}_y$, $\hat{\mathbf{p}} = -i\hbar \nabla + \hbar \nabla \chi/2$, $\hat{\sigma}_x, \hat{\sigma}_z$ are the Pauli matrices, $\varphi = M V_F V_{sx}/|e|$ is the Doppler shift of the QP energy, M is the electron effective mass, $\mathbf{V}_s = V_{sx} \mathbf{x}_0 + V_{sy} \mathbf{y}_0$, $\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0$ are the unit vectors of the coordinate system with \mathbf{z}_0 chosen along the c axis. The \mathbf{V}_s field can be written as a superposition of contributions from individual vortices situated at points \mathbf{r}_i : $\mathbf{V}_s(\mathbf{r}) = \hbar \sum_i K_1(|\mathbf{d}_i|) \times [\mathbf{z}_0, \mathbf{e}_i]/(2M\lambda_L)$, where $\mathbf{d}_i = (\mathbf{r} - \mathbf{r}_i)/\lambda_L$, K_1 is the McDonald (modified Bessel) function of the first order, $\mathbf{e}_i = \mathbf{d}_i/|\mathbf{d}_i|$. In this expression we neglect the effects of nonlocal electrodynamics [19] which are known to be small far away from the core. Our equations are analogous to the ones describing the quantum mechanical motion of a massless Dirac particle with a charge $|e|$ in the “vector potential” $\mathbf{a} = -\phi_0 \nabla \chi/(2\pi)$ of AB solenoids and the scalar potential φ of 2D “electrical dipoles” screened at a length scale λ_L . Both the solenoids and the dipoles are positioned at \mathbf{r}_i . Each solenoid carries the flux quantum ϕ_0 . The expression for a dipole moment reads $\mathbf{P} = -0.5\hbar V_F \mathbf{y}_0/|e|$. The Hamiltonian \hat{H}_{SL} provides a simple tool for the study of 2D quantum mechanical

effects in the QP motion and has recently been used as a starting point for the analysis of the band spectrum in regular vortex arrays with a rather small intervortex distance $R_v \ll \lambda_L$ [6,7,16].

Isotropic Dirac cone.—Let us focus on the case of a single isolated vortex line. We start our analysis from the simplest isotropic limit $V_F = V_\Delta = V$ (isotropic Dirac cone) and show that the low-energy QP states near each node are strongly influenced by the pure gauge potential \mathbf{a} due to the AB scenario. Indeed, if we neglect the potential of a 2D electric dipole in \hat{H}_{SL} , the scattering cross section of a Dirac fermion in the AB potential appears to diverge for $\varepsilon \rightarrow 0$: $\frac{d\sigma}{d\theta} \propto \varepsilon^{-1}$ [20]. Introducing a polar coordinate system (r, θ) with the origin at the vortex center and taking the OP phase in the form $\chi = \theta$ one can obtain the eigenfunctions of the Hamiltonian \hat{H}_0 in the angular momentum representation:

$$\hat{g}_m^{(1)} \propto (1 + i\hat{\sigma}_x) \sqrt{\frac{k}{L}} \begin{pmatrix} e^{im\theta} J_{m+1/2}(kr) \\ \text{sgn}\varepsilon e^{i(m+1)\theta} J_{m+3/2}(kr) \end{pmatrix}, \quad (1)$$

$$\hat{g}_m^{(2)} \propto i\hat{\sigma}_y e^{-i\theta} (\hat{g}_m^{(1)})^*, \quad (2)$$

where J_ν is the ν th Bessel function, m is an integer, $|\varepsilon| = \varepsilon_k = \hbar V k$, and L is the system size. Note that a full QP wave function $(u, v) = (\tilde{u}_m^{(1,2)}, \tilde{v}_m^{(1,2)}) \exp(i\mathbf{k}_1 \mathbf{r})$ [with the envelopes $\tilde{u}_m^{(1,2)}, \tilde{v}_m^{(1,2)}$ determined by Eqs. (1) and (2)] is not an eigenfunction of the angular momentum operator, which is an obvious consequence of the noncommutability of the angular momentum and the d -wave gap operators. QP states confined near each node provide the following contribution to the local DOS:

$$N = \sum_m \frac{L}{2\pi} \int dk [|\tilde{u}_m|^2 \delta(\varepsilon - \varepsilon_k) + |\tilde{v}_m|^2 \delta(\varepsilon + \varepsilon_k)]. \quad (3)$$

The wave functions $\hat{g}_m^{(1)}$ and $\hat{g}_m^{(2)}$ with $m \geq 0$ are regular at the origin. The local DOS corresponding to a set of these regular solutions vanishes in the region $r < \hbar V/|\varepsilon|$ and approaches the value $N_\infty \propto |\varepsilon|$ for $r \gg \hbar V/|\varepsilon|$ (N_∞ is the DOS in the absence of vortices). The solutions with negative m diverge at the origin and are responsible for the formation of the nonzero DOS near the vortex inside the domain $r < \hbar V/|\varepsilon|$. Thus, the residual DOS $N_0 = N(\varepsilon = 0)$ is also determined by the states with $m < 0$. The crucial role in the formation of the residual DOS is played by the states $g_{-1}^{(1)}$ and $g_{-1}^{(2)}$ which appear to decay most slowly from the vortex center (as $r^{-1/2}$) in the limit $\varepsilon \rightarrow 0$. Using (3) one can obtain $N_0 \sim (\hbar V r)^{-1}$. Let us emphasize that this contribution appears to be nonzero even in the large- \mathbf{r} domain ($r > \lambda_L$) in sharp contrast to the behavior expected on the basis of the semiclassical model which takes account of the Doppler term $|e|\varphi$ and neglects the AB effect.

We now proceed with the analysis of the effect of the Doppler term in the Hamiltonian \hat{H}_{SL} on the behavior of

wave functions in the small- \mathbf{r} domain ($r < \lambda_L$). For low energies $\varepsilon \ll \hbar V/\lambda_L$ the regular solutions (1) and (2) with $m \geq 0$ are only weakly influenced by the φ potential. On the contrary, for the wave functions (1) and (2) with negative m the potential φ cannot be considered as a small perturbation. In the limit $\varepsilon \ll \hbar V/\lambda_L$ the solutions in the domain $r < \lambda_L$ can be written in the form

$$\hat{g}_\mu = (1 + i\hat{\sigma}_x)r^{\mu+1/2} \exp[-i\theta(1 + \hat{\sigma}_z)/2]\hat{G}_\mu(\theta), \quad (4)$$

where the equation for $\hat{G}_\mu(\theta)$ reads

$$i\frac{\partial}{\partial\theta}\hat{G}_\mu + (1 + \mu)\hat{\sigma}_z\hat{G}_\mu + \frac{\sin\theta}{2}\hat{\sigma}_x\hat{G}_\mu = 0. \quad (5)$$

A set of discrete quantum numbers μ is determined by the condition $\hat{G}_\mu(\theta) = \hat{G}_\mu(\theta + 2\pi)$. In the large- $|\mu|$ limit the μ values can be calculated using the quasiclassical quantization rule, $\int_0^{2\pi} \sqrt{(1 + \mu)^2 + \frac{1}{4}\sin^2\theta} d\theta = 2\pi n$, where n is an integer. The residual DOS near the vortex center is dominated by the states (4) with $\mu < -1/2$, which are characterized by the power divergence at $r \rightarrow 0$. The divergence should be cut off due to the matching with the solution inside the core, which results in a mixing of QP wave functions characterized by different μ values and corresponding to all four nodes. Outside the core the most slowly decaying wave functions correspond to the value $\mu = -1$ and can be found exactly using Eq. (5):

$$\hat{G}_{-1}^{(1)} = C(\cos\gamma, -i\sin\gamma), \quad \hat{G}_{-1}^{(2)} = i\hat{\sigma}_y(\hat{G}_{-1}^{(1)})^*, \quad (6)$$

where $\gamma = \cos\theta/2$, and the constant $C \propto L^{-1/2}$ is determined from the matching with the solution in the large- \mathbf{r} domain ($r > \lambda_L$). One can see that for intermediate distances $\xi \ll r \ll \lambda_L$ these states provide a dominating contribution to the residual DOS $N_0 \sim (\hbar Vr)^{-1}$, which coincides with the one predicted on the basis of the semiclassical model [12]. The admixture of the solutions decaying more rapidly from the vortex axis becomes substantial near the core, and can result in a narrow DOS peak similar to the one observed in high- T_c compounds [11]. Despite a possible formation of such a peak structure the resulting low-energy states are not truly localized. The wave functions $\hat{g}_{-1}^{(1)}$ and $\hat{g}_{-1}^{(2)}$ can be considered as leading terms in a large distance ($r \gg \xi$) asymptotic expansion for the low-lying states and, thus, are responsible for the escape of QPs from the core. For these functions the generalized inverse participation ratio, defined as [13] $\beta \propto \langle |\tilde{u}|^4 + |\tilde{v}|^4 \rangle \cdot \langle |\tilde{u}|^2 + |\tilde{v}|^2 \rangle^{-2}$ (angular brackets stand for spatial averages), appears to grow logarithmically with an increase in L . The $\beta \propto L^2$ divergence expected for localized states is absent in a good agreement with the numerical analysis [13] carried out in the limit $L \ll \lambda_L$.

Anisotropic Dirac cone.—The physical picture suggested above can be generalized for the case of an anisotropic spectrum $V_F \neq V_\Delta$. Such a generalization is of particular importance for high- T_c cuprates, where

estimates based on the results of thermal conductivity measurements [21] give us rather large anisotropy parameters: $\alpha \sim 14$ for YBaCuO and $\alpha \sim 19$ for BiSrCaCuO. Taking an appropriate gauge transformation $\hat{g} = e^{iS}\hat{f}$ one can choose the vector potential \mathbf{a} in the Hamiltonian \hat{H}_0 in the form $\mathbf{a} = \phi_0\alpha[\mathbf{r}, \mathbf{z}_0]/(2\pi\tilde{r}^2)$, where $\tilde{r}^2 = x^2 + (\alpha y)^2$. Using the scale transformation ($\alpha y = \tilde{y}$, $x = \tilde{x}$) the Hamiltonian \hat{H}_0 can be reduced to the isotropic one with $V = V_F$. In the new coordinates the solution \hat{f} in the large- \tilde{r} domain (where the Doppler shift is negligible) can be written in the form (1) and (2). The small distance asymptotic expansion can be analyzed analogously to the isotropic case. The most slowly decaying solutions can be obtained from (4) and (6) if we replace θ and r by $\tilde{\theta} = \tan^{-1}(\tilde{y}/\tilde{x})$ and \tilde{r} , respectively, and take $\gamma = 0.5\alpha\tau^{-1}\tan^{-1}(\tau\cos\tilde{\theta})$, where $\tau = \sqrt{\alpha^2 - 1}$. Outside the core the expression for the residual DOS (taking account of the contributions from all four nodes) reads

$$\hbar N_0 \sim (V_\Delta^2 x^2 + V_F^2 y^2)^{-1/2} + (V_\Delta^2 y^2 + V_F^2 x^2)^{-1/2}. \quad (7)$$

The angular dependence (7) is strongly determined by the Dirac cone anisotropy. For $\alpha \neq 1$ the local DOS exhibits a fourfold symmetry with maxima along the nodal directions (see Fig. 1).

Neither the power law decay of $N_0(r)$ nor the fourfold anisotropy (which should be rather strong for α values mentioned above) have been observed within the experimental resolution in scanning tunneling microscopy (STM) studies of high- T_c compounds [11]. Such a conflict with the existing STM data is probably explained by the following reasons: (i) at large distances r from the vortex center the contribution of the extended states to the tunneling

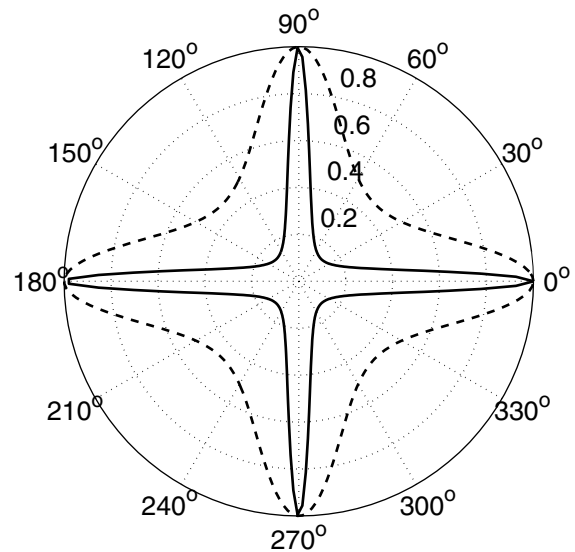


FIG. 1. The angular dependence of the residual DOS $N_0(\theta)/N_0(\theta = 0)$ in polar coordinates for $\alpha = 5$ (dashed line) and $\alpha = 20$ (solid line).

conductance may be suppressed due to the finite lifetime effects and the anisotropy of the tunneling matrix element [22]; (ii) at rather small distances r a partial suppression of the DOS contributions from nodal QP states and a resulting reduction of the DOS anisotropy is probably caused by the generation of a secondary OP component (see [23] and references therein). The relative phase between the coexisting OP components (s and d or $d_{x^2-y^2}$ and d_{xy}) is spatially dependent. As a consequence, four \mathbf{k} -space nodes of the local pair potential $\Delta(\mathbf{k}, \mathbf{r})$ are removed into the extended (\mathbf{k}, \mathbf{r}) space (see also [24]) with the formation of pointlike zeros at $\mathbf{r}_i(\mathbf{k}_F)$ in $\Delta(\mathbf{k}, \mathbf{r})$. The resulting OP $\Delta(\mathbf{k}, \mathbf{r})$ appears to be nodeless over most of the vortex core [23] (and, in particular, along the x and y axes). Obviously, such an OP structure near the core should partially suppress the DOS contribution (7) (which comes from the nodal QP states in a pure d -wave case) and can result in a reduction of the DOS anisotropy. However, the secondary OP component is known to decay rapidly outside the core [23] and, as a consequence, we can conclude that the anisotropic DOS contributions discussed above might become observable in the domain $r \gg \xi$ in the cleanest samples.

Multiquanta flux structures.—For a vortex carrying an odd number M_ϕ of the flux quanta the effect of the AB potential on the local DOS outside the flux tube ($r > \lambda_L$) is the same as for a singly quantized vortex. On the contrary, a vortex with an even winding number M_ϕ does not cause the AB interference and, thus, cannot provide the slowly decaying DOS contribution ($N_0 \propto r^{-1}$). The most direct way to observe this odd-even effect is to consider a hollow cylinder with a trapped magnetic flux Φ . The AB mechanism is the cause of an oscillating dependence $N_0(\Phi)$, which should be observable by any experimental technique sensitive to the residual DOS. The amplitude of these oscillations in the DOS integrated over the sample is proportional to the system size L . The large odd-even effect in the DOS is specific for superconductors with gap nodes and can be considered as a test for d -wave pairing. Obviously, the magnitude of such odd-even effect is strongly influenced by finite lifetime and temperature effects which should suppress the DOS contribution (7) in the domain $r > \hbar V_F / \max[\Gamma, T]$, where Γ is a scattering rate.

To summarize, we developed a 2D quantum mechanical description of extended QP states for an isolated flux line in a superconductor with gap nodes, taking account of both the Doppler shift of the QP energy and the AB effect. It is hoped that the physical picture considered in this Letter

can provide a starting point for the analysis of static and dynamic properties of the mixed state in various d -wave systems, including, probably, high- T_c copper oxides.

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