Shadow on the Wall Cast by an Abrikosov Vortex

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At the surface of a d-wave superconductor, a zero-energy peak in the quasiparticle spectrum can be observed. This peak appears due to Andreev bound states and is maximal if the nodal direction of the d-wave pairing potential is perpendicular to the boundary. We examine the effect of a single Abrikosov vortex in front of a reflecting boundary on the zero-energy density of states. We can clearly see a splitting of the low-energy peak and therefore a suppression of the zero-energy density of states in a shadowlike region extending from the vortex to the boundary. This effect is stable for different models of the single Abrikosov vortex, for different mean free paths and also for different distances between the vortex center and the boundary. This observation promises to have also a substantial influence on the differential conductance and the tunneling characteristics for low excitation energies.

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Today, there is common agreement that most high-T_c superconductors exhibit d-wave symmetry. An important characteristic of d-wave superconductors is the possible existence of Andreev bound states at their surface [1–3]. This increase of the local zero-energy quasiparticle density of states at the surface can clearly be observed in the differential tunneling conductance as a pronounced zero-bias conductance peak [4–6]. For specular boundaries, this peak reaches maximum height if the surface is perpendicular to the nodal direction of the d wave. The effect shrinks if the orientation is changed [2,4]. For an angle of 45° between the nodal direction and the surface the bound states have vanished completely. However, it has been pointed out that for rough surfaces a similar shape of the zero-bias conductance peak is obtained which is independent of the boundary orientation [7]. If a magnetic field is applied, the spectral weight of the zero-bias peak decreases and a splitting of the peak is observed [8–10]. It has been shown that surface screening currents along the boundary can lead to such a splitting [7]. Also, interaction of the bound states either with impurity states or with localized states in a neighboring barrier can lead to a suppression and broadening of the zero-bias conductance peak [11,12].

In this Letter, we study a single Abrikosov vortex in front of a specular surface, and we investigate the effect of the vortex on the local quasiparticle density of states along the boundary. All interesting phenomena of this problem are described within the quasiclassical theory, which is valid if the coherence length is much larger than the Fermi wavelength. To calculate the local density of states in the vicinity of the boundary it is necessary to find numerically stable solutions of the Eilenberger equations [13,14] that fulfill the appropriate boundary conditions at the specular surface. For this purpose we use the Riccati parametrization of the quasiclassical propagator [15]. Along a trajectory of the kind $\boldsymbol{r}(x) = \boldsymbol{r}_0 + x\boldsymbol{v}_F$, the Eilenberger equations of superconductivity reduce to a set of two decoupled differential equations of the Riccati type for the functions $a(x)$ and $b(x)$:

$$\begin{aligned} \hbar v_F \partial_x a(x) + [2\tilde{\epsilon}_n + \Delta^\dagger a(x)]a(x) - \Delta &= 0, \\ \hbar v_F \partial_x b(x) - [2\tilde{\epsilon}_n + \Delta b(x)]b(x) + \Delta^\dagger &= 0, \end{aligned} \tag{1}$$

where $i\tilde{\epsilon}_n = i\epsilon_n + \boldsymbol{v}_F \cdot \frac{e}{c}\boldsymbol{A}$ are shifted Matsubara frequencies. For the simple case of a cylindrical Fermi surface, the Fermi velocity can be written as $\boldsymbol{v}_F = v_F(\boldsymbol{e}_1 \cos\theta + \boldsymbol{e}_2 \sin\theta)$. The θ and $\boldsymbol{r}$ dependence of the pairing potential Δ can be factorized in the form $\Delta(\boldsymbol{r}, \theta) = \Delta_0 \chi(\theta)\Psi(\boldsymbol{r})$. For a $d_{x^2-y^2}$-wave superconductor the symmetry function takes the form $\chi(\theta) = \cos(2\theta)$, and for s-wave symmetry it becomes constant $\chi(\theta) = 1$. For $\epsilon_n > 0$ the Riccati equations have to be solved using the bulk values as initial values at $x = \pm\infty$:

$$\begin{aligned} a(-\infty) &= \frac{\Delta(-\infty)}{\epsilon_n + \sqrt{\epsilon_n^2 + |\Delta(-\infty)|^2}}, \\ b(+\infty) &= \frac{\Delta^\dagger(+\infty)}{\epsilon_n + \sqrt{\epsilon_n^2 + |\Delta(+\infty)|^2}}. \end{aligned} \tag{2}$$

The numerical solution of the Riccati equations can be done with minor effort and leads to rapidly converging results. For the calculation of the local density of states, the imaginary part of the quasiclassical propagator has to be integrated over the angle θ that defines the direction of the Fermi velocity. In terms of a and b, we have

$$N(\boldsymbol{r}_0, E) = \int_0^{2\pi} \frac{d\theta}{2\pi} \mathrm{Re}\left[\frac{1 - ab}{1 + ab}\right]_{i\epsilon_n \to E + i\delta}, \tag{3}$$

where E denotes the quasiparticle energy with respect to the Fermi level and δ is an effective scattering parameter that corresponds to an inverse mean free path. As is well known, the localized zero-energy state in a $d_{x^2-y^2}$-wave superconductor at a specular 110 boundary arises from the sign change in the pairing potential on a quasiparticle trajectory that is reflected at the surface. The outgoing particles are Andreev reflected at this potential step and interfere with the incident quasiparticles. This interference process leads to stable zero-energy trapped states in the vicinity of the boundary, called Andreev bound states. The same sign change in the order parameter is found on a trajectory that passes near the center of a vortex and therefore leads to similar localized Andreev bound states inside the vortex core. The suppression of the amplitude of the pairing potential around the vortex center gives only a small quantitative correction in the calculation of the trapped state, as we already pointed out before [16]. The influence of the boundary for anisotropic superconductors is included within the quasiclassical theory if the nonlinear boundary conditions for the quasiparticle propagator are applied [17,18]. For the Riccati parametrization, a substantial simplification occurs, and an explicit solution of the nonlinear boundary conditions can be found [19].

In the following, we assume a totally reflecting surface where the transparency $\mathcal{T}$ equals zero while the reflectivity $\mathcal{R}$ becomes one. In this special case the boundary conditions reduce to $a^{l/r}_{\rm out} = a^{l/r}_{\rm in}$ and $b^{l/r}_{\rm in} = b^{l/r}_{\rm out}$. Then, we try to find an appropriate model that describes the pairing potential associated with the single vortex in front of the reflecting boundary. With the condition that there are no currents flowing across the boundary, we have to find a phase of the order parameter where the phase gradient vanishes perpendicular to the boundary. In analogy to the classical boundary value problem of electrostatics with a point charge in front of a conducting surface, we introduce an image vortex on the opposite site of the reflecting boundary. The pairing potential around a vortex at position $\boldsymbol{r}_V$ can be written as $\Psi(\boldsymbol{r}) = f(\boldsymbol{r} - \boldsymbol{r}_V)e^{i\Phi(\boldsymbol{r})}$ (see also [20]). The function $f(\boldsymbol{r} - \boldsymbol{r}_V)$ characterizes the amplitude of the pairing potential of the single vortex. Since we consider a vortex-antivortex pair, the phase $\Phi(\boldsymbol{r})$ is given as $\Phi(\boldsymbol{r}) = \arg(\boldsymbol{r} - \boldsymbol{r}_V) - \arg(\boldsymbol{r} - \bar{\boldsymbol{r}}_V)$. The location of the image vortex behind the boundary is defined by $\bar{\boldsymbol{r}}_V = \boldsymbol{r}_V - 2\hat{\boldsymbol{n}}\langle\hat{\boldsymbol{n}}, \boldsymbol{r}_V\rangle$. The normal unit vector is given as $\hat{\boldsymbol{n}} = 1/\sqrt{2}(\boldsymbol{e}_1 + \boldsymbol{e}_2)$ for a 110 boundary. The origin $\mathcal{O}$ of our coordinate system is placed at the boundary right between the vortex and the image vortex. The y axis is oriented parallel to the boundary. x_V denotes the vortex position on the x axis and also measures the vortex to boundary distance. Furthermore, it is useful to introduce the coherence length $\xi = \frac{\hbar v_F}{\Delta_0}$ as our length scale. We performed calculations of the local density of states for both a fully self-consistently determined pairing potential and a constant modulus $f(\boldsymbol{r} - \boldsymbol{r}_V) = 1$. The latter corresponds to a pure phase vortex. The self-consistent results show some quantitative differences, the vortex core states and surface states being somewhat more extended in space and the peak height reduced. However, the main qualitative effect we want to present here, the shadow on the zero-energy density of states, exists independently. Thus, we will restrict our following considerations to the simpler second model. In Fig. 1 we show the zero-energy local density of states in the vicinity of the reflecting boundary. In the upper part of the image, the local density of states is shown as a three-dimensional surface; in the projection below, we show the same quantity as a density plot. A phase vortex is placed two coherence lengths $x_V = 2\xi$ away from the surface. We assume a $d_{x^2-y^2}$ symmetry of the order parameter and set the boundary with an angle of 45° to the b axis of the crystal. First, we notice that the fourfold symmetry of the local density of states around the vortex is broken. We also observe a shadowlike suppression of the zero-energy density of states in a triangular region between the vortex and the boundary. The picture for an s-wave superconductor is totally different. As shown in Fig. 2, the vortex has little influence on the boundary density of states. Here, the high zero-energy

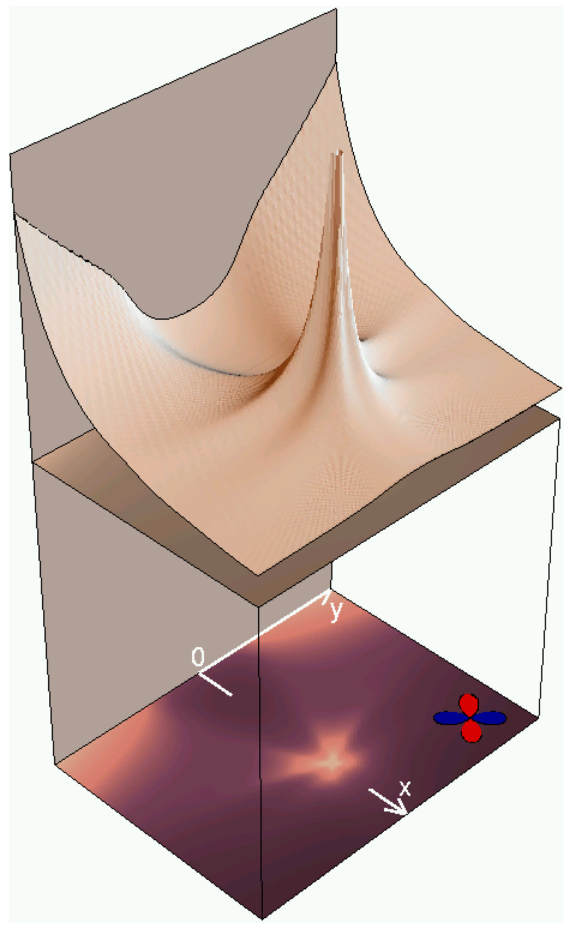

FIG. 1 (color online). Zero-energy local density of states of a $d_{x^2-y^2}$-wave superconductor. A reflecting 110 boundary is situated at the back of the image; the single Abrikosov vortex can be found at a distance of two coherence lengths $x_V = 2\xi$ in front of it. The Andreev bound states at the boundary are seen as the bright regions along the y axis, and as the high values in the three-dimensional plot. The localized states in the vortex center are seen as the peak in the upper image and as the bright spot in the image below. One can clearly identify the distinct shadow that emanates from the vortex center to the boundary. An effective scattering parameter of $\delta = 0.1\Delta_0$ has been used for the calculations.

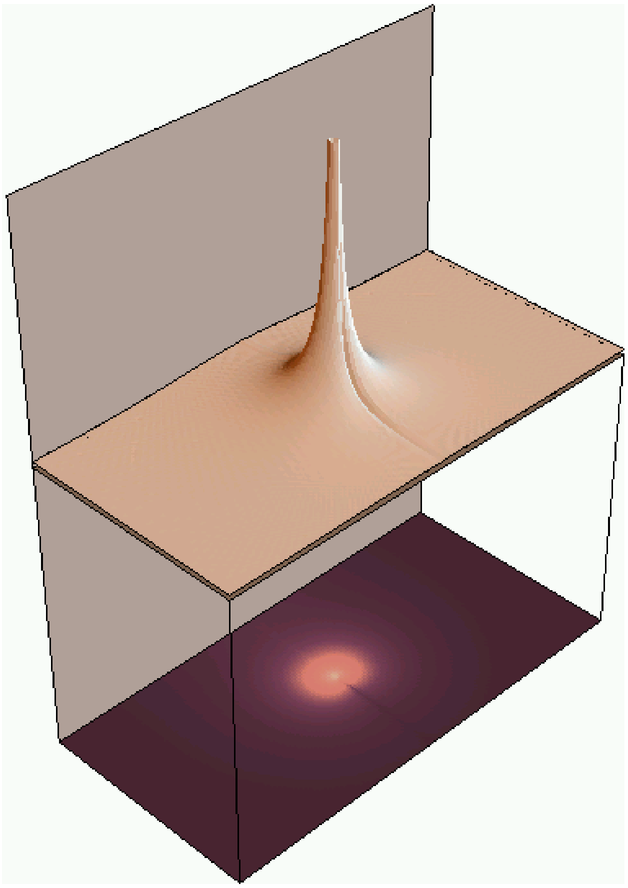

FIG. 2 (color online). Zero-energy local density of states of an s-wave superconductor. Again, the reflecting boundary is situated at the back of the image, while the single Abrikosov vortex can be found at a distance of one coherence length $x_V = \xi$ in front of it. The high zero-energy density of states of the s-wave vortex slightly illuminates the boundary. An effective scattering parameter of $\delta = 0.1\Delta_0$ has been used for the calculations.

density of states of the vortex rather illuminates the boundary. The small shadow on the right-hand side of the vortex and the slight line between the vortex and the boundary are due to quasiparticles with an inclination angle of 90° that are trapped between the reflecting boundary and the potential step in the vortex core. Below, we will focus on a $d_{x^2-y^2}$-wave superconductor with a 110 boundary. For a 100 boundary the result is very similar to the s-wave case. More details with an arbitrary orientation of the boundary will be discussed in a following work. In Fig. 3 we show the zero-energy density of states along the 110 boundary. The different curves correspond to different vortex positions x_V. The calculations have been done using a value of $\delta = 0.1\Delta_0$. For increasing vortex to boundary distances x_V we find a decrease of the shadow depth, while the width increases visibly. Apparently, the shadow effect exists for a wide range of vortex to boundary distances x_V even larger than 10ξ. For distances smaller than 1 coherence length ξ, a self-

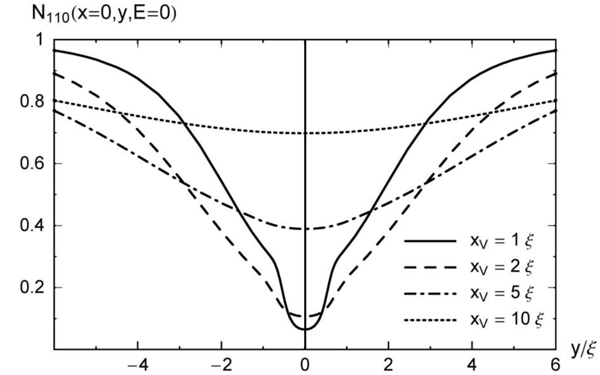

FIG. 3. Zero-energy density of states of a $d_{x^2-y^2}$-wave superconductor along a 110 boundary for different vortex positions x_V. The curves are normalized to the local density of states at the boundary without vortex ($x_V \to \infty$). The effective scattering parameter is chosen to be $\delta = 0.1\Delta_0$.

consistent calculation of the pairing potential around the vortex might become necessary.

In the following, we want to obtain a more detailed impression of the vortex shadow at the point $\mathcal{O}$. We also want to study the influence of the effective quasiparticle scattering parameter δ introduced in Eq. (3) on the local density of states. Without vortex, the value of the zero-energy density of states at the boundary shows a sensitive dependence on the decoherence parameter δ. With decreasing δ, the value of the zero-energy peak at the boundary increases rapidly. In Fig. 4 we show the zero-energy density of states at the point $\mathcal{O}$ as a function of the vortex to boundary distance x_V for different values of δ. The curves are normalized to the particular values of the zero-energy boundary density of states without a vortex or far away from the vortex center. We find that both the range and the relative depth of the shadow increase, if we decrease the scattering rate δ. We want to point out that

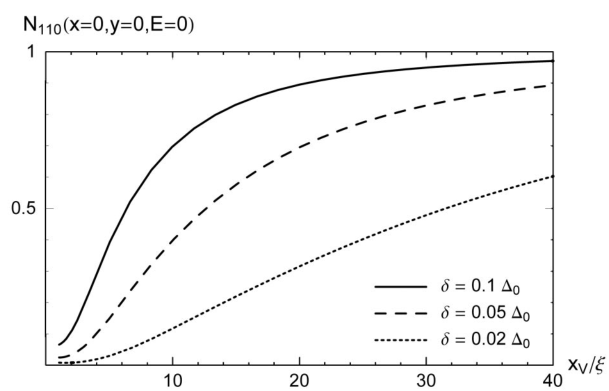

FIG. 4. Zero-energy quasiparticle density of states of a $d_{x^2-y^2}$-wave superconductor at the boundary as a function of the vortex position x_V. The different curves correspond to different mean free paths related to the inverse of δ. The density of states of each curve is normalized to the corresponding boundary density of states without vortex.

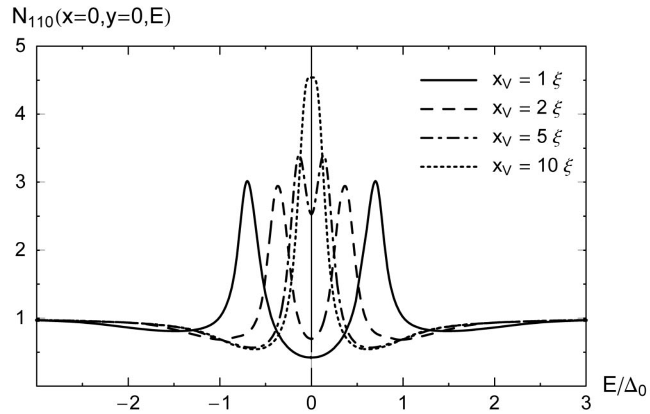

FIG. 5. Quasiparticle spectrum of a $d_{x^2-y^2}$-wave superconductor taken at a 110 boundary at the point adjacent to the vortex center ($\mathcal{O}$). The curves are calculated for different vortex distances x_V from the boundary. The effective scattering parameter is chosen to be $\delta = 0.1\Delta_0$.

this shadow effect can be observed in clean superconductors with a long mean free path as well as in superconductors with higher scattering rates.

In order to explain the suppression of the local zero-energy density of states at the surface, we now concentrate on a given point in the shadow region. In order to find the quasiparticle spectrum there, the angular integration in Eq. (3) has to be done. For each angle, the integrand corresponds to the contribution of a quasiparticle trajectory with the direction specified by θ. Because of the phase gradient of the order parameter, the energy "seen" by a quasiparticle flying along a trajectory is shifted. Additionally, this shift itself changes locally along the trajectory. Thus, for most of the angles, the Riccati equations [Eq. (1)] are not evaluated at zero energy. This is sufficient, however, to miss the sharp zero-energy peak of the bound state at the surface. As a consequence, the zero-energy density of states is reduced. In the quasiparticle spectrum, the spectral weight of the bound states is shifted from the Fermi level towards higher energies. In the limit $x_V \to \infty$, this effect corresponds to the splitting of the zero-bias peak due to surface currents [7].

In Fig. 5 we show the local density of states at the point $\mathcal{O}$ for different vortex to boundary distances x_V as a function of energy. If the Abrikosov vortex is placed in the vicinity of the boundary, we observe a distinct splitting of the zero-energy peak. With increasing distance between vortex and boundary the splitting is reduced. At $x_V = 10\xi$ a splitting is no longer visible, while the height of the zero-energy peak is still considerably reduced.

The strong reduction of the zero-energy density of states at the 110 boundary of a $d_{x^2-y^2}$-wave superconductor has of course an important influence on the zero-bias anomaly in the tunneling conductance. Even in zero magnetic field, vortices can remain in the high-T_c materials by pinning defects. In the vicinity of grain boundaries the shadow effect of these pinned vortices will play an important role for the grain boundary tunneling due to the local reduction of the zero-energy density of states and provide a natural explanation for the experimental observation of zero-bias conductance peak splitting in the absence of an external magnetic field [10] as well as hysteresis [9]. The shadow shown in Fig. 1 might also be observable directly by an STM tunneling experiment. We have checked that the vortex shadow effect reported here remains for a self-consistently determined pairing potential and even in the presence of rough surfaces, which we will present in a future work.

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