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Electronic tunneling into an isolated vortex in a clean type-II superconductor

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The electronic structure of a type-II superconductor is investigated in the vicinity of an isolated vortex line by solving the Bogoliubov–de Gennes equations for the quasiparticle amplitudes. The tunneling differential conductance as a function of bias voltage is calculated at the center of the vortex; it shows a pronounced peak near zero bias originating from the lowest quasiparticle bound state. This explains recent scanning-tunneling-microscopy observations by Hess *et al.* [Phys. Rev. Lett. **62**, 214 (1989)]. Quantitative agreement with these experiments can be obtained by considering several intrinsic and extrinsic broadening effects.

Theoretical attempts at understanding the electronic properties of vortex lines in type-II superconductors have recently been revived by a beautiful scanning-tunneling-microscopy (STM) experiment by Hess *et al.* on $NbSe_2$.[1] In addition to vortex imaging, a strong enhancement of the tunneling differential conductance was observed at zero bias with the tip at the center of a vortex core. The naive picture describing the vortices as cylindrical domains having the properties of a normal metal cannot account for this effect. A simple model was recently proposed by Overhauser and Daemen[2] which describes the change in the density of states of such a cylinder of normal metal induced by coupling to a superconducting background. It predicts an enhancement in the density of one-electron states at the Fermi energy in qualitative agreement with the observations. A more complete understanding of the electronic properties of vortex lines, however, requires a microscopic approach such as, e.g., given by the Bogoliubov–de Gennes theory.[3,4] Within this framework, and parallel with our own work, Shore *et al.*[5] have estimated the contributions of quasiparticle bound states to the local density of states, and deduced that the resulting tunneling conductance should have a peak at the Fermi level. However, since their analysis did not include the quasiparticle scattering states, no explicit complete conductance spectrum was obtained and no direct comparison with experiment was possible.

In this paper, we study the electronic properties of a vortex line in the framework of the Bogoliubov–de Gennes theory, for both bound and scattering quasiparticle states, analyze the tunneling process in terms of these states, and show that the differential conductance observed in Ref. 1 can be well reproduced in an energy range of $E_F \pm 3\Delta_0$. We also study the dependence of the tunneling differential conductance on various parameters, such as the coherence length and the anisotropy of the Fermi surface. We find that for a quantitative explanation of the data, additional extrinsic effects have to be invoked.

The electronic properties of a superconductor are determined in the mean-field picture by the solutions of the Gor'kov equations.[3,4] A closed solution of these equations, however, has only been obtained in the homogeneous case and appears to be beyond reach in the presence of a magnetic field where the translational symmetry is broken by the appearance of vortex lines. Within the quasiparticle approximation, the Gor'kov equations reduce to the simpler Bogoliubov–de Gennes equations from which one can obtain the properties of the lowest fermionlike excitations of the system.

The Bogoliubov–de Gennes equations for the quasiparticle amplitudes $\tilde{u}(\mathbf{r})$ and $\tilde{v}(\mathbf{r})$ read

$$[(\mathbf{p}-e\mathbf{A})^2-(E_F+E)]\tilde{u}(\mathbf{r})+\Delta(\mathbf{r})\tilde{v}(\mathbf{r})=0\,, \quad (1a)$$

$$[(\mathbf{p}+e\mathbf{A})^2-(E_F-E)]\tilde{v}(\mathbf{r})-\Delta^*(\mathbf{r})\tilde{u}(\mathbf{r})=0\,. \quad (1b)$$

We consider here the case of an isolated vortex carrying one flux quantum. Following Caroli and co-worker[6] we choose the gauge in which the order parameter $\Delta(\mathbf{r})$ is real so that the solutions can be written (in cylindrical coordinates)

$$\tilde{u}(r,\theta,z)=u_{\mu n k_z}(r)e^{-i\mu\theta}e^{ik_z z}\,, \quad (2a)$$

$$\tilde{v}(r,\theta,z)=v_{\mu n k_z}(r)e^{i\mu\theta}e^{ik_z z}\,, \quad (2b)$$

where μ is half an odd integer, n a radial quantum number, and $u_{\mu n k_z}(r)$ and $v_{\mu n k_z}(r)$ are solutions of the radial equations

$$-\frac{\partial^2}{\partial r^2}u_{\mu n k_z}(r)-\frac{1}{r}\frac{\partial}{\partial r}u_{\mu n k_z}(r)+\left[\frac{(\mu-\frac{1}{2})^2}{r^2}-\left(E_F-\frac{k_z^2}{m_z}+E_{\mu n k_z}\right)\right]u_{\mu n k_z}(r)+\Delta(r)v_{\mu n k_z}(r)=0\,, \quad (3a)$$

$$-\frac{\partial^2}{\partial r^2}v_{\mu n k_z}(r)-\frac{1}{r}\frac{\partial}{\partial r}v_{\mu n k_z}(r)+\left[\frac{(\mu+\frac{1}{2})^2}{r^2}-\left(E_F-\frac{k_z^2}{m_z}-E_{\mu n k_z}\right)\right]v_{\mu n k_z}(r)-\Delta(r)u_{\mu n k_z}(r)=0\,. \quad (3b)$$

The order parameter $\Delta(r)$ must be determined self-consistently by

$$\Delta(r)=2V\sum_{\mu n k_z}u_{\mu n k_z}(r)v^*_{\mu n k_z}(r)[1-2f(E_{\mu n k_z})]\,, \quad (4)$$

where $f(E)$ is the Fermi function and V is the electron-electron attractive coupling constant. The Ginzburg-Landau parameter is assumed to be large ($\kappa_{\parallel}\sim 9$ in $NbSe_2$),[7] so that the spatial dependence of the magnetic field can be ignored.

Equation (3) admits two types of solutions:[6] bound states which are exponentially localized within a radius of order ξ of the vortex center with corresponding eigenvalues $E_{\mu n k_z} < \Delta_0$, and extended scattering states, which are associated with eigenvalues $E_{\mu n k_z} > \Delta_0$. The quantity of interest for a comparison to a tunneling experiment is the local density of one-particle excitations in the superconductor. This information is contained in the one-particle spectral function, which in the quasiparticle approximation is given by

$$A_S(\mathbf{r},E) = 2\pi \sum_{\mu n k_z} [u^2_{\mu n k_z}(\mathbf{r})\delta(E-E_{\mu n k_z}) + v^2_{\mu n k_z}(\mathbf{r})\delta(E+E_{\mu n k_z})] . \quad (5)$$

In the normal metal, the corresponding quantity is

$$A_N(\mathbf{r},E) = 2\pi \sum_{\mathbf{k}} \delta(E-E_{\mathbf{k}}) . \quad (6)$$

Assuming the tip to be small compared to ξ and centered at $\mathbf{r}$, the tunneling current due to an applied voltage V is then

$$I(\mathbf{r},V) \propto \int \frac{dE}{2\pi} A_S(\mathbf{r},E) A_N(\mathbf{r},E+eV) . \quad (7)$$

The differential conductance is then given by

$$\frac{\partial I(\mathbf{r},V)}{\partial V} \propto -\sum_{\mu n k_z} [u^2_{\mu n k_z}(\mathbf{r}) f'(E_{\mu n k_z}-eV) + v^2_{\mu n k_z}(\mathbf{r}) f'(E_{\mu n k_z}+eV)] , \quad (8)$$

where f' is the derivative of the Fermi function.

The tunneling process involves states near the Fermi surface, which in $NbSe_2$ consists of undulating cylinders oriented along the k_z direction and centered on the H-K axis of the hexagonal Brillouin zone.[8] Its precise shape is not well known, since it is modified by the onset of a charge-density wave (CDW) below $T=32$ K. It can be assumed, however, that the portions of the Fermi surface which subsist in the presence of the CDW remain approximately cylindrical.[7,9] In the case of a perfectly cylindrical Fermi surface ($m_z \to \infty$) Eq. (3) is independent of k_z. Deviations from a cylindrical Fermi surface will introduce a finite dispersion as a function of k_z, which will tend to broaden any structure in the density of states.

The matrix element which usually appears in the definition of the tunneling current is described in detail by Tersoff and Hamann.[10] A detailed analysis shows that the tunneling matrix element is maximal for states with large k_z. In the limit of a cylindrical Fermi surface, however, this will not have any effect on the spectral distribution, since the eigenvalues $E_{\mu n k_z}$ are independent of k_z and the tunneling current will be given by Eq. (7).

The Bogoliubov–de Gennes equations were solved using the following approximate form for the order parameter:

$$\Delta(r) = \Delta_0 \tanh\frac{r}{\xi} , \quad (9)$$

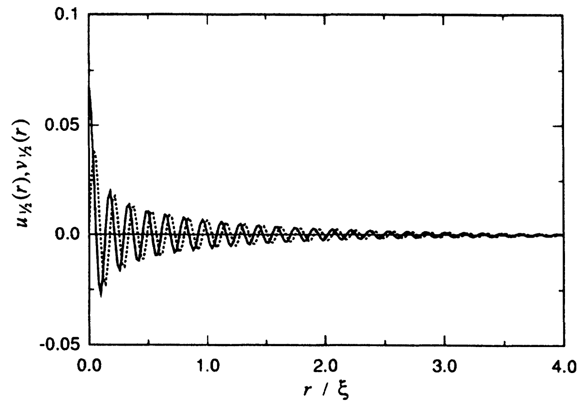

FIG. 1. Quasiparticle amplitudes $u(r)$ (solid line) and $v(r)$ (dotted line) of the lowest bound state for $k_F\xi=40$, $E_F/\Delta_0=32$, and $T/T_c=0.3$.

which has the appropriate behavior in the limits $r\to 0$ and $r\to\infty$. The dimensionless parameter $k_F\xi$ was estimated to be 40, which is consistent[1,8] with a value of k_F of about 0.5 Å^{-1} and a coherence length ξ of 80 Å. We solve Eq. (3) in a cylinder of radius $R \gg \xi$, with Dirichlet boundary conditions at $r=R$. The dimensionless ratio E_F/Δ_0 was chosen to obey the relation[3,4]

$$k_F\xi \gtrsim \frac{E_F}{\Delta_0} ,$$

which for given ξ, Δ_0 can be used, e.g., to define the in-plane effective mass.

The lowest bound-state eigenvalues ($E_{\mu n} < \Delta_0$) are in good agreement with the values predicted by Caroli and co-worker[6]

$$E_\mu \sim \mu\frac{\Delta_0}{k_F\xi} \sim \mu\frac{\Delta_0^2}{E_F} . \quad (10)$$

The quasiparticle amplitudes corresponding to the lowest bound state are shown in Fig. 1. They are exponentially localized on a distance of order ξ near the vortex center. Note the finite value of $u_{1/2}(r)$ at the origin, which is a characteristic of s-like states ($\mu=\frac{1}{2}$) only. There are no other bound states with $\mu=\frac{1}{2}$ for $k_F\xi \lesssim 80$. States with higher angular momentum are successively more extended and have zero amplitude at $r=0$. Scattering states are found at energies larger than Δ_0. At energies larger than $2\Delta_0$, the energy spacing between successive eigenvalues becomes identical to that of free electron states contained in a cylinder of radius R.

The complete tunneling differential conductance at the center of the vortex core, shown in Fig. 2, was calculated using Eq. (8) with $k_F\xi=40$, $m_z\to\infty$, $E_F/\Delta_0=32$, and $T/T_c=0.3$, which corresponds to the experimental conditions of Ref. 1. The pronounced peak at zero bias arises from the lowest bound state ($\mu=\frac{1}{2}$) which, as mentioned, is the only bound state that has a nonzero amplitude at the origin. For $V>\Delta_0$, the contributions from scattering states become dominant, giving the spectrum its characteristic peak-dip structure. The calculation of the full spectrum allows for a direct comparison with experimen-

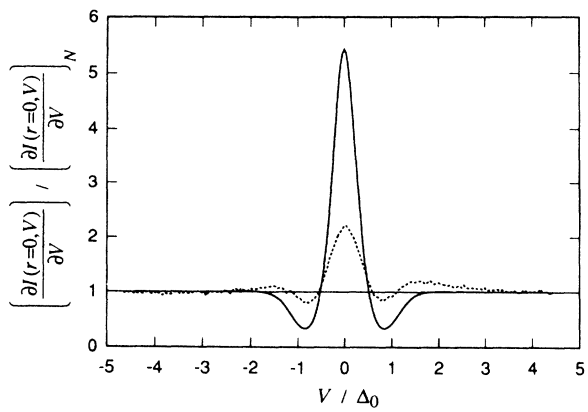

FIG. 2. Tunneling differential conductance calculated at the center of the vortex using parameters $k_F\xi$, E_F/Δ_0, and T/T_c corresponding to the nominal experimental conditions (solid line), compared to the experimental curve (dotted line).

tal data, also shown in Fig. 2 for reference. The calculated zero-bias differential conductance is larger than the experimental one by a factor of 2 to 3. Various effects reduce the magnitude of the zero-bias peak. First, we expect the peak height to be affected by the presence of impurities or defects. In fact, the height of the experimental peak shows considerable variations from sample to sample, which indicates that the purity of the sample is an important parameter.[11] Second, any rise of the tip temperature above that of the sample, broadens the features of the differential conductance and reduces the height of the zero-bias peak which is strongly temperature dependent. The peak height also decreases with increasing $k_F\xi$ for given E_F/Δ_0. Calculations done with various values of $k_F\xi$ show that in the limit of large $k_F\xi$, the differential conductance at $r=0$ loses its structure and becomes a constant, as expected for a normal metal. This does not exclude, however, the possibility that the differential conductance may exhibit some structure at a distance of order ξ from the vortex center.

In an attempt to reproduce more closely the experimental data, we have performed calculations with various values of the parameters $k_F\xi$, E_F/Δ_0, and T/T_c. The differential conductance calculated with $k_F\xi=60$, $E_F/\Delta_0=16$, and $T/T_c=0.5$ (i.e., about twice the nominal experimental temperature) is shown on Fig. 3 (top). The height and width of the zero-bias peak are now in good agreement with the experimental curve. This in principle offers the possibility of extracting materials parameters from such a line-shape analysis. However, the enhancement of the differential conductance beyond $V\approx\pm\Delta_0$ can never be reproduced in this fashion. Since this feature was not observed in all the samples measured,[11] we attribute it to extrinsic effects. For instance, the presence of a secondary tip would in some cases add contributions to the differential conductance from tunneling events into superconducting regions away from the vortex core. The differential conductance in these regions has peaks near $V=\pm\Delta_0$ corresponding to the singularities in the density of states of a homogeneous superconductor. The differential conductance arising from such a double-tip configuration, represented by an equal combination of the differential conductance at the vortex center and at large distance from the vortex is shown in Fig. 3 (bottom), along with the experimental curve. In addition, the structure of the underlying density of states of $NbSe_2$ can begin to appear in the differential conductance on an energy scale of several Δ_0.

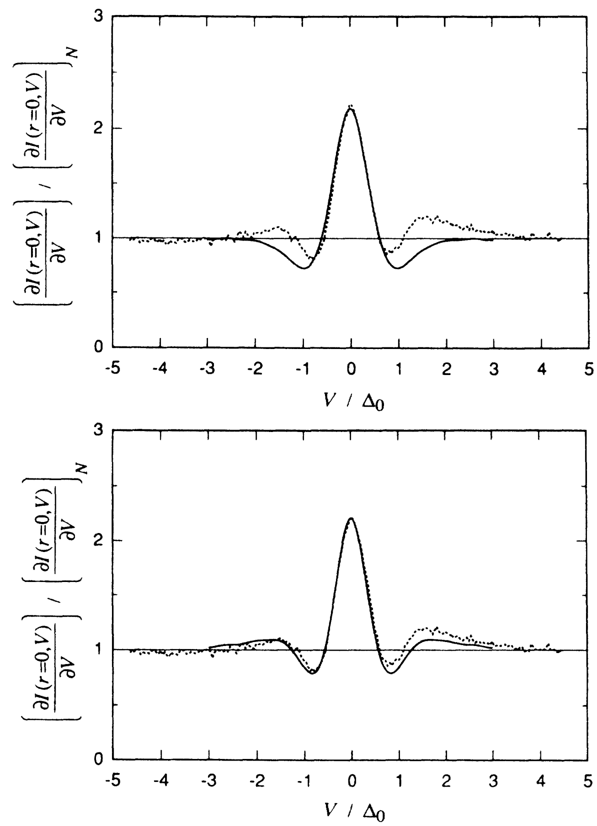

FIG. 3. Top part: tunneling differential conductance calculated with adjusted $k_F\xi$, E_F/Δ_0, and T/T_c values (see text). Bottom part: theoretical results for $k_F\xi=40$, $E_F/\Delta_0=32$, and $T/T_c=0.45$, with inclusion of the contributions of a secondary tip. The experimental data are shown as a dotted line.

In conclusion, we have investigated the electronic properties of a clean type-II superconductor in the vicinity of an isolated vortex line by solving the Bogoliubov–de Gennes equations for both bound and scattering quasiparticle states. The complete tunneling differential conductance was calculated for the first time. At the center of the vortex core, it shows a strong zero-bias enhancement arising from the lowest quasiparticle bound state. This yields the characteristic observed peak-dip conductance spectrum. However, quantitative agreement with experiment can only be obtained by using an increased effective temperature and in some cases by assuming extrinsic effects, such as the presence of a secondary tip contributing to the tunneling current. The solution of the Bogoliubov–de Gennes equations in a vortex *lattice* geometry is the next step towards a more complete understanding of the electronic properties of type-II superconductors in a magnetic field, and will be the subject of forthcoming studies.

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