Density of States in a Vortex Core and the Zero-Bias Tunneling Peak

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Scanning-tunneling-microscope measurements by Hess *et al.* of the tunneling conductance into a superconducting vortex core show a pronounced peak at small bias. We show that this peak is due to the quasiparticle bound states in the core. A numerical (and approximately self-consistent) solution of the Bogoliubov–de Gennes equations yields the *local* density of states in the core, which resembles the tunneling conductance once we account for thermal broadening effects. We find additional structure in the local density of states which should be observable at lower temperatures.

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Recently, Hess *et al.*[1] have used a scanning-tunneling microscope (STM) to study the properties of excitations in the vortex cores of the type-II superconductor $NbSe_2$. By measuring the differential conductance dI/dV as a function of the bias voltage V, they were able to map out the *local* density of states in the vicinity of a single vortex.[2] Far from the center of a vortex they reproduce the standard BCS form for the *bulk* density of states in the absence of an applied field. However, when the STM tip is scanned over the center of a vortex a rather pronounced peak in dI/dV is observed at small bias. In this Letter we present an explanation of this anomaly based on an approximately self-consistent numerical solution of the Bogoliubov–de Gennes equations[3] for the quasiparticle bound states in the presence of a single vortex, for parameters relevant to $NbSe_2$. From this numerical solution we obtain the quasiparticle amplitudes $u(r)$ and $v(r)$ explicitly, unlike previous approaches which have relied on various analytical approximations.[4–7] In contrast to previous work,[5] we find that the local density of states at the vortex core exhibits a remarkable amount of structure, which may be resolved by repeating the experiment at sufficiently low temperatures. The details of these calculations will be provided in a future publication.[8]

We begin by reviewing the experiments of Hess *et al.*[1] $NbSe_2$ was chosen for its excellent surface quality; atomically clean surfaces were observed over the 6000-Å scan range of the STM. The material is a layered crystal which undergoes a charge-density-wave (CDW) transition at 33 K, with a CDW gap of 35 meV, and a superconducting transition at 7.2 K, with a superconducting gap Δ_0 of 1.11 meV. The upper critical field $H_{c2\perp}$ for a field applied perpendicular to the planes is 5 T. The coherence length $\xi_\parallel$ in the plane is 77 Å. The Ginzburg-Landau parameter $\kappa_\parallel = \lambda_\parallel/\xi_\parallel = 30$,[9] so that $NbSe_2$ is an extreme type-II superconductor. The experiment is performed by applying a field $H > H_{c1}$ perpendicular to the surface, so that an Abrikosov flux lattice is formed. The dI/dV vs V curves are obtained by imposing a small dither voltage of 0.1 mV on top of the sample voltage, while a constant sample to tip distance is maintained. We have included a reproduction of the data of Ref. 1 in Fig. 1. Far from a vortex, the dI/dV vs V agrees with the usual BCS form (once one accounts for smearing due to thermal effects). However, at the center of the vortex a rather pronounced peak appears at small bias. The height of this peak is quite sensitive to the position of the tip relative to the center of the vortex. It is this enhanced conductance near zero bias which is the puzzling feature of these data.

Before embarking upon a discussion of the technical details of our calculation, we would like to first provide an intuitive explanation of our results. In the presence of a *single* vortex, the pair potential $\Delta(r)$ is zero at the center of the vortex and asymptotically approaches its zero-field value Δ_0 at a distance of several coherence lengths from the center of the vortex. In some respects, this spatial variation of the pair potential is analogous to a potential well for the quasiparticles, of depth Δ_0 and

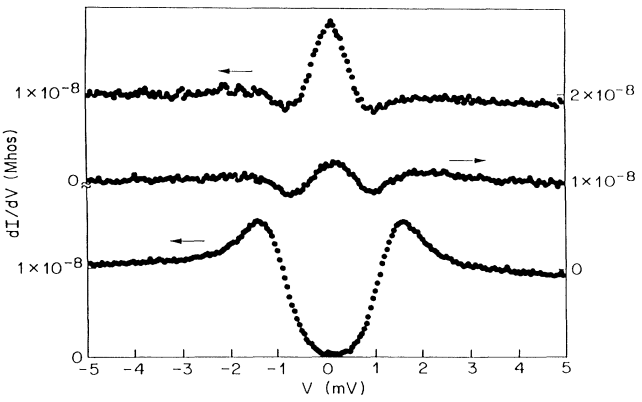

FIG. 1. Data of Hess *et al.* (Ref. 1) showing dI/dV vs V for $NbSe_2$ in a 0.02-T field and at a temperature of 1.85 K. The data give results for three STM tip positions; at the vortex center (top), about 75 Å ($\approx \xi_\parallel$) away from the vortex center (middle), and 2000 Å away (bottom). Note the different zero for each curve.

radius $\sim\xi_{\parallel}$.[10] Quasiparticles with energies $E<\Delta_0$ will form bound states in the radial direction in this well, with an energy spacing of order $\hbar^2/2m\xi_{\parallel}^2\sim\Delta_0^2/E_F\ll\Delta_0$, where E_F is the Fermi energy (in this paper energies are measured relative to the Fermi energy). Quasiparticles with energies $E>\Delta_0$ will be scattered from the vortex. It is the bound states which yield a nonzero *total* density of states for energies $E<\Delta_0$, as demonstrated in Refs. 4–7. The *local* density of states, on the other hand, reflects the spatial behavior of the quasiparticle wave functions. Since there is a cylindrical symmetry about the axis of the vortex, the wave functions can be labeled by an angular-momentum quantum number μ (μ must be half integral[3]). As shown in Fig. 2, the lowest-energy bound states (those with small μ) will have wave functions which are peaked closer to the axis of the vortex (just as the low-angular-momentum states of the hydrogen atom are peaked closer to the origin). Therefore, a measurement of the local density of states at the vortex core would find an enhancement at small bias since the low-energy bound states have a *much* greater probability of being close to the center of the vortex. Farther from the center of the vortex the bound-state wave functions have diminished weight, and the local density of states will be dominated by the high-energy scattering states. Thus, sufficiently far from the center of the vortex the local density of states will assume its zero-field BCS form. This is precisely the behavior observed in the experiment.

In order to make a quantitative comparison to the experiment, it is necessary to solve the Bogoliubov–de Gennes (BdG) equations for the quasiparticle amplitudes $u(\mathbf{r})$ and $v(\mathbf{r})$ in the presence of a single vortex.[3] We first note that for $NbSe_2$ $2\Delta_0/k_BT_c=3.58$, close to the BCS value of 3.53, justifying the weak-coupling approximation. Second, de Haas–van Alphen measurements indicate that these materials have extremely long mean free paths,[11] so that it is possible to work in the "clean" limit. In cylindrical coordinates, $\mathbf{r}=(r,\theta,z)$, the order parameter is of the form $\Delta(\mathbf{r})=\exp(-i\theta)\Delta(r)$ with $\Delta(r)$ real. By taking advantage of the cylindrical symmetry, the quasiparticle amplitudes may be written as[4]

$$\begin{pmatrix}u(\mathbf{r})\\ v(\mathbf{r})\end{pmatrix}=e^{ik_zz}e^{i\mu\theta}e^{-i\sigma_z\theta/2}\begin{pmatrix}g^+(r)\\ g^-(r)\end{pmatrix} \tag{1}$$

(the σ's are the usual Pauli matrices). The BdG equations then take the form

$$\sigma_z\frac{\hbar^2}{2m_{\parallel}}\left\{-\frac{d^2}{dr^2}-\frac{1}{r}\frac{d}{dr}+\left[\mu-\sigma_z\left(\frac{1}{2}+\frac{eA_\theta r}{\hbar}\right)\right]^2\times\frac{1}{r^2}-k_\rho^2\right\}\hat{g}(r)+\sigma_x\Delta(r)\hat{g}(r)=E\hat{g}(r)\,, \tag{2}$$

where $\hat{g}$ is a two-component spinor. We have assumed different effective masses $m_{\parallel}$ in the plane and m_z along the z direction, and defined a radial wave number k_ρ by

$$\frac{\hbar^2k_\rho^2}{2m_{\parallel}}=E_F-\frac{\hbar^2k_z^2}{2m_z}\,. \tag{3}$$

Since $NbSe_2$ is an extreme type-II superconductor, the vector potential in Eq. (2) may be ignored in subsequent calculations. The pair potential $\Delta(r)$ is to be determined self-consistently from

$$\Delta(r)=V\sum_n g_n^+(r)g_n^-(r)[1-2f(E_n)]\,, \tag{4}$$

where the sum on the states n is restricted to positive-energy states (with energies less than the Debye energy), V is the attractive coupling, and $f(E)$ is the Fermi function. Finally, the quantity of interest is the local density of states, defined as

$$N(r,E)=\sum_n[|g_n^+(r)|^2\delta(E-E_n)+|g_n^-(r)|^2\delta(E+E_n)]\,. \tag{5}$$

In these last two equations the summation includes an integration over the scattering states.

Our numerical procedure consists of determining the eigenvalues by using a "shooting" method. We first factor out the asymptotic oscillatory behavior of the wave functions $\hat{g}(r)$, and then solve the resulting differential equation for a fixed μ and k_z by integrating far from the vortex axis to the axis. The requirement that the wave functions be well behaved at the axis determines the eigenvalues and corresponding eigenfunctions. For the pair potential, we choose the form

$$\Delta(r)=\Delta_0\tanh(dr/\xi_{\parallel})\,. \tag{6}$$

We initially guess a value for d, and after the wave func-

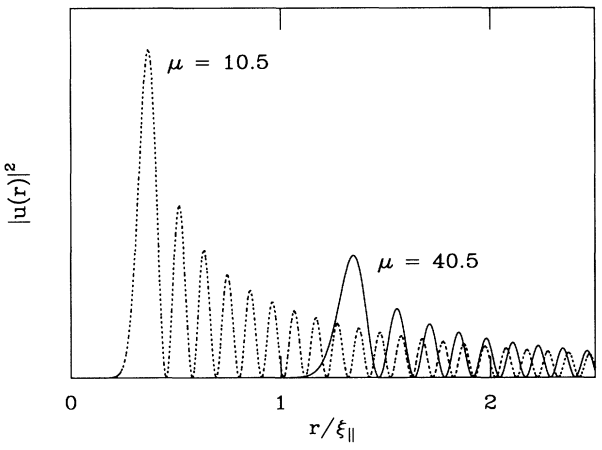

FIG. 2. Quasiparticle amplitude $|u(r)|^2$ vs the distance r from the vortex center for two different values of angular momentum μ, demonstrating that the first peak in the amplitude occurs further away from the center for larger μ (and hence larger energy). The parameters used here are $k_z=0$, $E_F/\Delta_0=250$, and $d=1.0$ [see Eq. (6)].

tions are determined we can then solve for $\Delta(r)$ from Eq. (4) in order to obtain a better estimate of d, if we assume that the shape of $\Delta(r)$ is accurately determined by only the bound states. This allows us to obtain an approximately self-consistent solution.

Our numerical results are shown in Figs. 2–4. We have assumed an isotropic three-dimensional material ($m_{\parallel}=m_z$) and chosen parameters appropriate to $NbSe_2$.[12] The eigenvalues for small μ and k_z agree to better than 1% with the results of Caroli *et al.*[4] [see their Eq. (10), valid in the limit $\mu \ll E_F/\Delta_0$ and small k_z]. Our *total* density of states has a minimum at zero energy and a form in agreement with that found by previous theoretical and experimental investigations.[13] Figure 3 shows the *local* density of states at $r=0$ and $r=\xi_{\parallel}$, while Fig. 4 shows the thermally broadened local density of states (which is proportional to the experimentally measured differential conductance dI/dV) at a temperature of 1.9 K. The thermal broadening is due to the finite temperature of the STM tip, and is determined by convoluting the results in Fig. 3 with the absolute value of the derivative of the Fermi function. Note that at $r=\xi_{\parallel}$, the local density of states displays considerable structure, but that this structure is smeared into one large peak once we account for the broadening. We do find that at somewhat lower temperatures or further from the vortex center, a double peak (with a dip in the differential conductance at zero bias) persists after thermal broadening (although at large distances it will be washed out by the thermal broadening of the scattering states into the gap region).

Our results for the differential conductance are in satisfactory agreement with the experimental results of Hess *et al.*,[1] although the peaks we obtain are about 2.5 times higher and somewhat narrower than theirs. We believe this discrepancy has two sources: (1) intrinsic effects, e.g., pair-breaking and dirt effects in the sample (Hess *et al.* do find some sample dependence in the height of the peaks[14]); and (2) probe resolution, e.g., the spatial resolution of the tip, and uncertainty in the tip temperature due to lack of tip equilibration with the bath. We could imagine accounting for broadening due to probe resolution by using an *effective* tip temperature of 3.5 K, which is obtained by fitting the energy width of the experimental peak at $r=0$. Using this effective temperature would reduce the peaks in Fig. 4 by about 40%.

Overhauser and Daemen[15] have recently published an alternative calculation of the zero-bias tunneling peak (valid only for the center of the vortex). Their intuitive approach is rather different from our systematic solution: They perturbatively couple normal core electrons to the superconducting excitations outside the core. We have duplicated their calculation; their results differ qualitatively from ours (even after correcting for their use of the measured dI/dV curve, which includes thermal broadening, as the superconducting density of states out-

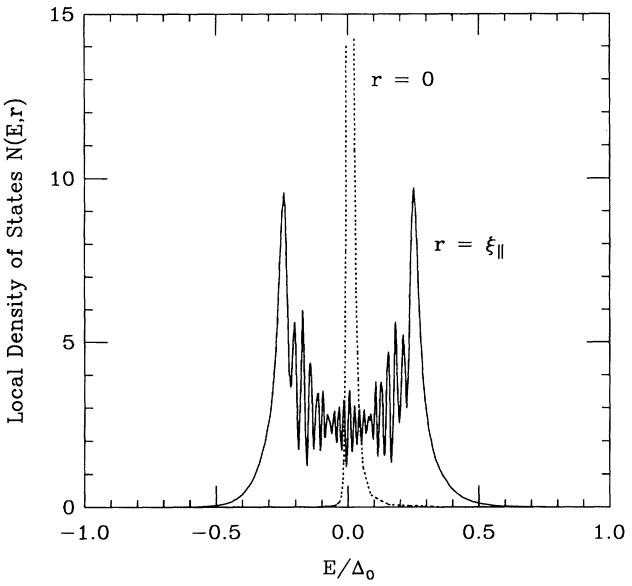

FIG. 3. Calculated *local* electron density of states vs energy, normalized by the Fermi-level density of states in the normal metal, for $r=0$ and $r=\xi_{\parallel}$. For $r=0$, the peak is at $N(E,r)\approx 180$ (off scale). The parameters are $E_F/\Delta_0=250$ and $d=1.0$. These parameter values yield a nearly self-consistent result for $\Delta(r)$ when $T=1.9$ K.

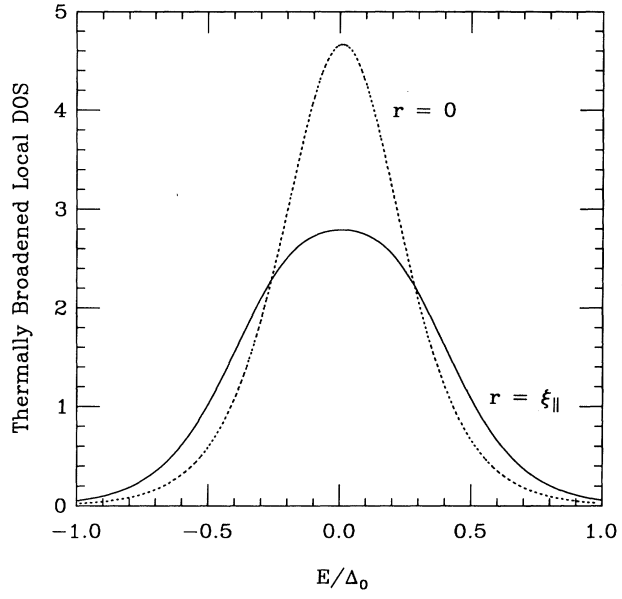

FIG. 4. The same data shown in Fig. 3 after convolution with the derivative of the Fermi function for a temperature of 1.9 K, in order to simulate the differential conductance that would be observed in the experiment. Note that in this and the previous figure, $\xi_{\parallel}$ has been set so that the spatial width of the peak at zero bias approximately matches that seen in the experiment.

side the core). On the other hand, we believe that the basic underlying physics we are describing is the same as that of Overhauser and Daemen.

In conclusion, we have solved the Bogoliubov–de Gennes equations numerically for the quasiparticle bound-state energies and wave functions in the core of a vortex, and have found that we can satisfactorily reproduce the zero-bias tunneling peak seen by Hess *et al.*[1] We find additional structure in the local density of states, and on the basis of this, we predict that if the tunneling experiment is performed at lower temperatures, the zero-bias peak will split into a double peak (with a dip at zero bias) as the STM tip is moved away from the vortex center.[16] Future work includes solving for the scattering states, in order to obtain a complete description of the local density of states and to allow us to incorporate the scattering states into the self-consistent solution for the pair potential $\Delta(r)$. The effects of impurities and of magnetic fields (important for materials with $\kappa \sim 1$) also warrant further investigation. We are also considering the implications for the high-T_c materials, where the small coherence lengths and large superconducting gaps will make the energy spacing of the bound states fairly large. Finally, we are investigating the effect of quasiparticle tunneling between the vortices, which will become important in higher magnetic fields.

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