Local density of states of an isolated vortex in an extreme type-II superconductor

Salman Ullah and Alan T. Dorsey
Department of Physics, University of Virginia, McCormick Road, Charlottesville, Virginia 22901

Louis J. Buchholtz
Department of Physics, California State University, Chico, Chico, California 95926
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We use Eilenberger's quasiclassical equations to compute the self-consistent local density of states of an isolated vortex in an extreme type-II superconductor. We include the contributions from both the scattering states and the bound states and consider a two-dimensional Fermi surface. The local density of states as a function of energy shows a double-peak structure: (a) there is one peak at $E=\Delta$ at *all* distances from the vortex core and (b) a second peak at lower energies due to bound states in the core. This low-energy peak appears at successively lower energy as one moves closer to the core, giving rise to the enhancement of the zero-bias differential conductivity at the vortex core reported by Hess *et al.*

I. INTRODUCTION

Hess and co-workers[1] have recently measured the position-dependent differential conductance $\sigma(r,V)=dI/dV$ near the vortex cores in $NbSe_2$ (an extreme type-II superconductor) using a scanning tunneling microscope (STM). The STM provides a *local* spectroscopy of the vortex, and thus gives detailed information on the core structure. The surprising experimental result was that the differential conductance at the core $\sigma(r=0,V)$ exhibited a large peak at small bias V, approximately a factor of 2 greater than the normal-state conductance. This result is at odds with the commonly held view that the vortex core is "normal."

This work has lead several authors[2,3] to compute the local density of states (LDOS) for an isolated vortex using the Bogoliubov–de Gennes equations. They find that the zero-bias anomaly could be explained by the presence of low-energy ($E<\Delta$) quasiparticle states which are bound to the vortex. Unfortunately, the Bogoliubov–de Gennes equations are very difficult to solve for the scattered states ($E>\Delta$) and indeed only the scattered states at the core have been computed.[3] Moreover, far from the core it becomes increasingly inefficient to solve the Bogoliubov–de Gennes equations for the LDOS because the important contribution from the high-angular-momentum states becomes difficult to compute.[4]

An alternative method, that of the quasiclassical Green's functions,[5] has been used by Klein[6] to compute the *direction-dependent* local density of states for a vortex lattice. However, Klein has used a spherical Fermi surface rather than a cylindrical [two-dimensional (2D)] Fermi surface which more closely models $NbSe_2$. In a more recent paper, Klein[7] has computed the LDOS for a spherical Fermi surface but has not considered the contribution from the scattering states. In this paper we solve numerically the quasiclassical equations to obtain a self-consistent local density of states for an isolated vortex in the limit that the magnetic field can be neglected: $\lambda \gg \xi$, where λ is the penetration depth and ξ is the coherence length. The plan of the paper is as follows. In Sec. II we introduce the quasiclassical equations and discuss their solutions for an isolated vortex. Next, in Sec. III, we outline the computation of the LDOS from the direct solution of the analytically continued quasiclassical equations for the cylindrical (2D) Fermi surface which is appropriate for $NbSe_2$.[8] Section III also contains the main quantitative results of this paper: the LDOS as a function of energy and the local differential conductivity as a function of bias voltage.

II. THE QUASICLASSICAL EQUATIONS

The quasiclassical equations for an s-wave superconductor consist of a transport equation for the quasiclassical Green's function $\hat{q}$, a normalization condition, and a self-consistency equation (the gap equation)—see, for example, Serene and Rainer.[9] Essentially, the quasiclassical equations exploit the fact that the Green's function is peaked at the Fermi surface and that quantities of interest vary on a length scale set by the coherence length ξ rather than the atomic length k_F^{-1}. The quasiclassical equations may be obtained from Gorkov's equations[10] by (1) integrating over the energy variable $E=v_F(p-p_F)$ in the region $p_F r_{12} \gg \hbar$, where the variable $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$ may be though of as the separation of the quasiparticles forming a pair, and (2) eliminating terms of order $1/k_F\xi$ from the energy-integrated Gorkov equations.[11]

For convenience we shall introduce dimensionless lengths and energies as follows: all lengths are measured in terms of the temperature-dependent coherence length $\xi(T)=\hbar v_F/\Delta_{BCS}(T)$ (this coherence length is larger by a factor of π than the usual BCS temperature-dependent coherence length) and all energies are measured in units of the bulk BCS temperature-dependent gap $\Delta_{BCS}(T)$. In addition, we set $\hbar=1$. Then the quasiclassical equation

for an s-wave superconductor is

$$\hat{\mathbf{k}}\cdot\nabla\hat{q}+[\hat{M},\hat{q}]=0\ , \tag{1}$$

where the 2×2 self-energy matrix is

$$\hat{M}=\begin{bmatrix}\omega_n & \Delta\\ \Delta^* & -\omega_n\end{bmatrix} \tag{2}$$

and $\omega_n=\pi(2n+1)k_BT/\Delta_{\rm BCS}(T)$ is the dimensionless Matsubara frequency. The unit vector $\hat{\mathbf{k}}$ is the direction of the momentum of a quasiparticle on the Fermi surface: in dimensionful units it is simply the Fermi velocity $\mathbf{v}_F$. Next, the normalization condition

$$\hat{q}^2=\hat{1} \tag{3}$$

requires that $\hat{q}(\hat{\mathbf{k}},\mathbf{R},\omega_n)$ have the form

$$\hat{q}=\begin{bmatrix}a & d\\ e & -a\end{bmatrix}\ , \tag{4}$$

where a, d, e are functions of the coordinate $\mathbf{R}$, the unit vector $\hat{\mathbf{k}}$, and the Matsubara frequency ω_n. Finally, the self-consistency equation is

$$\Delta(\mathbf{R})=\frac{\pi gT}{\Delta_{\rm BCS}(T)}\sum_{\omega_n>0}{}'\int\frac{d^2\hat{k}\,'}{2\pi}(d+e^*)\ . \tag{5}$$

The prime on the frequency sum denotes a high-energy cutoff; this cutoff dependence is absorbed into the coupling constant g. And also, the angular integration is over half of all $\hat{\mathbf{k}}$ directions.

For an isolated vortex we can exploit the cylindrical symmetry of the problem and adopt cylindrical coordinates: ρ is the radial distance from the vortex core and ϕ is the azimuthal angle. Then the derivative term in Eq. (1) has the following form for the 3D case:

$$\hat{\mathbf{k}}\cdot\nabla=\cos\theta_K\partial_z+\sin\theta_K\left[\cos\psi\frac{\partial}{\partial\rho}+\frac{1}{\rho}\sin\psi\frac{\partial}{\partial\phi}\right]\ , \tag{6}$$

where the subscript K refers to the $\hat{\mathbf{k}}$ coordinate system and $\psi\equiv\phi_K-\phi$. The 2D expression is obtained by setting $\theta_K=\pi/2$.[12]

Unfortunately, we cannot use the cylindrical coordinate system because, despite its simplicity, it is pathological for the following reason. We have found that only quasiparticle trajectories which do not pass through the point $\rho=0$ give rise to the peak in the "core" DOS where "core" refers to all points near the vortex center except the single point $\rho=0$. However, in the cylindrical coordinate system *all* the quasiparticle trajectories pass through the vortex core $\rho=0$. This point is singular in that the quasiparticles passing through this point see an infinite centrifugal barrier and so the wave function of these quasiparticles must vanish at the core. (As a direct consequence, the LDOS at the core is equal to the normal-state value.) Therefore, we transform (6) to a Cartesian coordinate system[6] defined by

$$r_\parallel=\rho\cos\psi,\quad r_\perp=\rho\sin\psi\ . \tag{7}$$

Then, the derivative term in Eq. (1) becomes

$$\hat{\mathbf{k}}\cdot\nabla=\sin\theta_K\partial_{r_\parallel}\ . \tag{8}$$

In Fig. 1 we show the coordinates (ϕ,ρ) and the $\hat{\mathbf{k}}_\perp$-dependent coordinates $(r_\parallel,r_\perp)$—$\hat{\mathbf{k}}_\perp$ is the projection in the x-y plane of the unit vector $\hat{\mathbf{k}}$ of Eq. (1). In this Cartesian coordinate system, the trajectories are straight lines parallel to the $r_\parallel$ axis.

Next, we have to make a gauge choice for the gap function. In the real gauge the Green's functions and the gap functions are written as

$$\begin{aligned}&\Delta\rightarrow\Delta(\rho)\exp(i\psi)\ ,\\ &d\rightarrow d(\rho)\exp(i\psi)\ ,\\ &e\rightarrow e(\rho)\exp(-i\psi)\ ,\end{aligned} \tag{9}$$

for a singly quantized vortex and $\Delta(\rho)$ is real. This gauge choice is useful for analytic work since then the Green's functions are symmetric about $r_\parallel=0$ (see the Appendix), but it is not suitable for numerical solution near $r_\perp=0$. For our purposes it is more useful to adopt a gauge in which the gap function is complex:

$$\begin{aligned}\Delta&=\bar{\Delta}(r_\parallel,r_\perp)\exp(i\psi)\\ &=\bar{\Delta}(r_\parallel,r_\perp)\left[\frac{r_\parallel}{(r_\parallel^2+r_\perp^2)^{1/2}}+i\frac{r_\perp}{(r_\parallel^2+r_\perp^2)^{1/2}}\right]\ ,\end{aligned} \tag{10}$$

where the function $\bar{\Delta}(r_\parallel,r_\perp)$ is real. As a check on the numerical method, we solved for the LDOS using both gauges and found identical results except near $r_\perp=0$ where the real gauge becomes inappropriate for numerical solution.

In order to compute the LDOS we have to first solve the quasiclassical equations self-consistently for the gap function $\Delta(\rho)$. The transport equation (1) is difficult to solve numerically because the finite (physical) solution tends to get subsumed by exponentially exploding (unphysical) solutions. One method which overcomes this

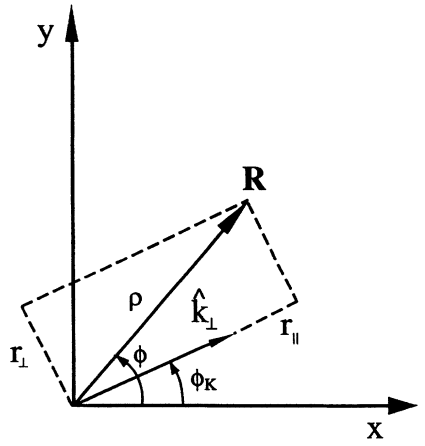

FIG. 1. The vector $\mathbf{R}$ denotes the position of the center of mass of a Cooper pair and $\hat{\mathbf{k}}_\perp$ is the projection in the x-y plane of the unit vector $\hat{\mathbf{k}}$ of Eq. (1). The $\hat{\mathbf{k}}_\perp$-dependent coordinates $(r_\perp,r_\parallel)$ are used in this paper. The z axis is out of the paper.

problem, the "explosion method," is extensively discussed in Ref. 13. We use an alternative algorithm in which we eliminate the exploding solutions by computing a function orthogonal to the Green's function rather than the Green's function itself. Our algorithm is rather complex and Ref. 14 contains a brief explanation of the method of solution. A fuller discussion will be presented in a future paper.[15] We find that the reduced gap function

$$\Delta(\rho)=\Delta_{\rm true}(\rho)/\Delta_{\rm BCS}(T)$$

is accurately given by $\Delta(\rho)=\tanh(\rho)$ for temperatures greater than $T/T_c=0.2$. This functional form is somewhat surprising in that, in dimensionful units,

$$\Delta(\rho)=\Delta_{\rm BCS}(T)\tanh[\rho/\xi(T)]\ ,$$

where $\xi(T)=\pi\xi_{\rm BCS}(T)$; that is, the relevant coherence length is, in fact, π times as large as the BCS coherence length. For slightly lower temperatures it differs by less than 5% from this value (we performed a simple least-squares comparison of the numerical results for $T/T_c=0.2$ and $T/T_c=0.1$ with the hyperbolic tangent), and we expect that even at the lowest temperatures the spatial dependence of the gap function is essentially unchanged from this form.[16] However, we would like to mention that earlier work by Kramer and Pesch[17] on the structure of the vortex core near H_{c1} shows a significant decrease in the vortex core as the temperature is reduced. (The inclusion of the magnetic field and its associated consequences is not responsible for the reduction in the size of the core.) We hope to investigate this important issue in a future paper. We have not attempted to solve for the gap function for much lower temperatures simply because this requires a very substantial increase in CPU time. We shall take $\Delta(\rho)=\tanh(\rho)$ for all subsequent calculations. Now that we have determined the gap function we can solve the quasiclassical equations (1) and (3) for the LDOS.

III. DENSITY OF STATES

The LDOS is given by

$$N(\rho,\omega)=N(E_F)\int\frac{d^2k}{4\pi}\mathrm{Re}[a(\hat{\mathbf{k}},\rho:i\omega_n\rightarrow\omega+i\eta)]\ , \quad (11)$$

where the analytic continuation $i\omega_n\rightarrow\omega+i\eta$ is written explicitly and $N(E_F)$ is the normal-state DOS. Therefore, in order to compute the LDOS we have to solve the analytically continued version of the quasiclassical equation (1) for the Green's function $\hat{q}(\hat{\mathbf{k}},\rho:\omega+i\eta)$ for all directions of $\hat{\mathbf{k}}$ and frequencies. We used 200 values of $r_\perp$ in the range $-3<r_\perp<3$.

We have solved the equation for values of the frequency in the range $0<\omega<2.0$ and a step size $\delta\omega=0.05$. A smaller step size does not reveal any additional bound states. The value of the infinitesimal η is chosen simply so that the peaks in the LDOS are sharp on the scale $\delta\omega$. For $\omega<1$ we chose $\eta=0.005$. For the scattered states $\omega>1$ we had to increase the infinitesimal to $\eta=0.08$ in order to damp out spurious oscillations in the Green's functions away from the core. This change in η is responsible for the non-square-root singular behavior of the LDOS at $\omega=1$: for comparison we include in Fig. 2 our result for the LDOS at the core with $\eta=0.005$ for all ω. We use the terms "energy" and "frequency" interchangeably.

We remind the reader that any enhancement in the LDOS is due to a pole in the Green's function and, therefore, the actual peak height depends on how closely one approaches this pole in the frequency domain and, in this sense, is arbitrary. We remark that our results are independent of the starting point of the integration, provided we begin the integration of the differential equations at a distance greater than approximately 4ξ—the distance at which the gap assumes its bulk value. Finally, we note that our algorithm is rather efficient: the total CPU time was only a few hours on a workstation.

There are several features worth mentioning.

(1) There is a pronounced peak in the LDOS at the core $\rho=0$ for both $\omega=0$ and 1. The zero-frequency peak is due to the lowest-lying bound state in the vortex core[2,18] and gives rise to the zero-bias peak in the differential conductivity reported by Hess *et al.*[1] Next, the peak at $\omega=1$ is the familiar peak in the DOS for a bulk superconductor. Of course, the surprise is that this peak persists even at the core, although its weight in the frequency-integrated LDOS is substantially reduced from the bulk case.

(2) As one moves away from the core, the low-frequency peak gets shifted to higher frequencies and the weight of the $\omega=1$ peak increases. For $\rho=3$ the two peaks are almost coincident, and indeed, for $\rho\approx4$ there remains only one peak at $\omega=1$—the bulk result. For high frequencies the LDOS quickly approach 1, the normal-state value. Note that the small bump at $\omega\approx1.2$ is due to numerical error: increasing η removes this feature. Furthermore, the small wiggles for low frequencies are an artifact of the angular integration in Eq. (11).

(3) We also computed the core LDOS for the 3D case and found no qualitative difference: the $\omega=1$ peak is broadened somewhat for $\omega<1$ while the low-frequency peak is essentially unchanged. The broadening of the $\omega=1$ peak is due to the observation that quasiparticles moving along the vortex axis see no gap at all. In order to see this explicitly, one merely has to rescale the $r_\parallel$ coordinate in the quasiclassical equations by $r_\parallel\rightarrow\sin\theta_K r_\parallel$ and notice that $\Delta\rightarrow0$ as $\sin\theta_K\rightarrow0$.

(4) The value of the infinitesimal η determines the width and height of the peaks in the LDOS. Although we have neglected all impurity scattering effects [the self-energy matrix (2) is correct for the clean limit only] we could follow Klein[7] and treat η as a dirt parameter[19] and fit it to the experimentally determined zero-field density of states and then use this value for all subsequent calculations of the vortex LDOS. We find that such an approach does not fit the experimental results.[20]

(5) The differential conductivity is given by

$$\frac{\sigma(\rho,V)}{\sigma_N}=\frac{1}{\sigma_N}\frac{dI}{dV}=\int_{-\infty}^{\infty}dE\frac{N_S(\rho,E)}{N(E_F)}\left[\frac{-\partial f(E+eV)}{\partial(eV)}\right]\ , \quad (12)$$

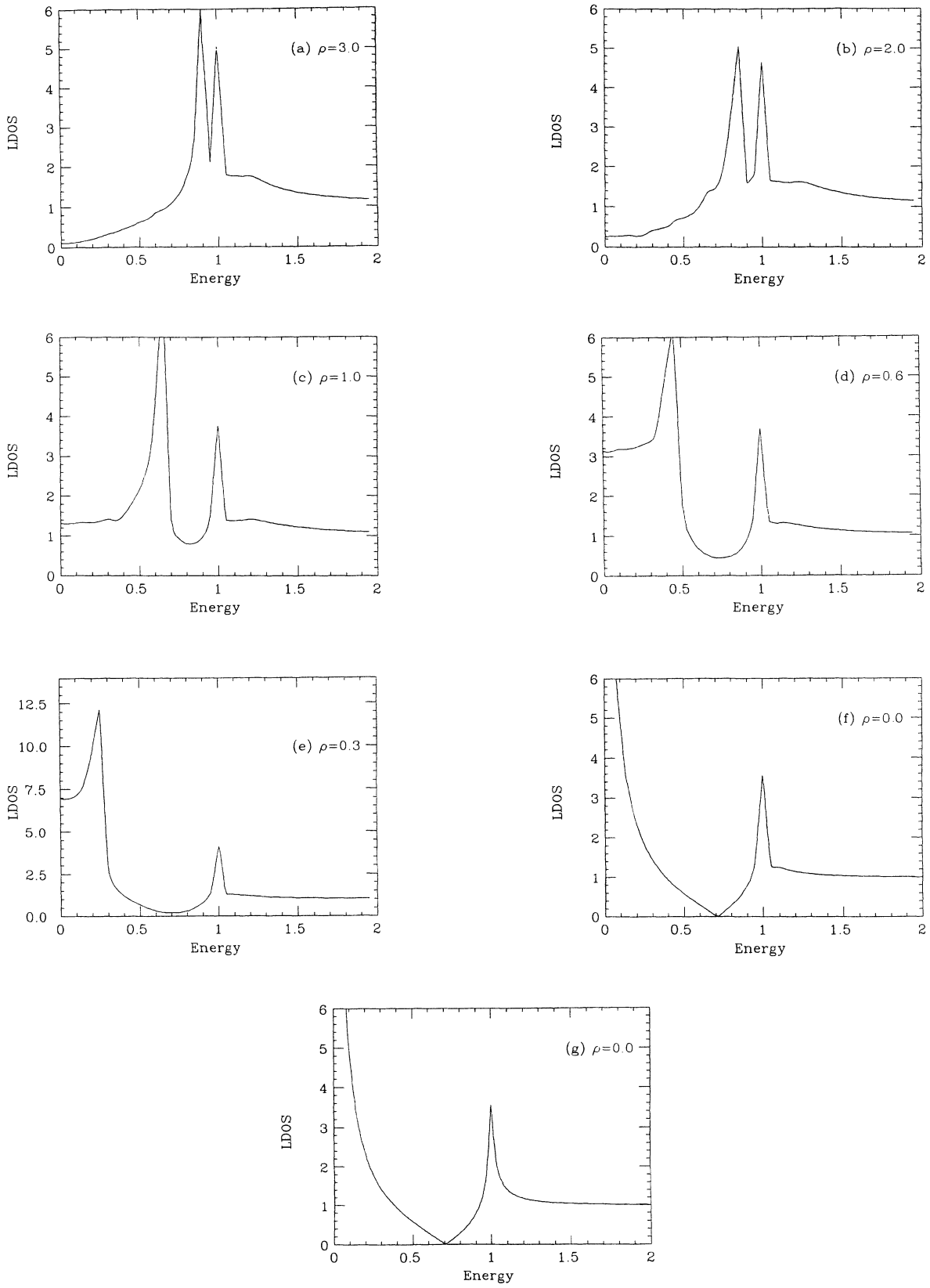

FIG. 2. The local density of states as a function of energy for a cylindrical (2D) Fermi surface. The distance from the core ρ is in units of $\xi(T)=\pi\xi_{BCS}(T)$ and for $\omega<1$, $\eta=0.005$ while for $\omega>1$, $\eta=0.08$ (see text): (a) $\rho=3.0$, (b) $\rho=2.0$, (c) $\rho=1.0$, (d) $\rho=0.6$, (e) $\rho=0.3$, (f) $\rho=0.0$, (g) $\rho=0.0$ but $\eta=0.005$ for all ω. The LDOS is normalized to the normal-state value and the energy is in units of $\Delta_{BCS}(T)$.

where V is the bias voltage and e is the electron charge. Figure 3 shows the differential conductivity (normalized by the normal-state value) for $T/T_c=0.2$; that is, approximately the experimental temperature in Ref. 1. The differential conductivity does not show the sharp features of the corresponding LDOS because it is smeared out by the Fermi function; the small weight of the $\omega=1$ peak is lost in the integration. Recently, Hess *et al.*[20] have repeated the experiment at a much lower temperature of $T=140$ mK. However, at such low temperatures, dirt effects dominate and smear out the differential conductivity.

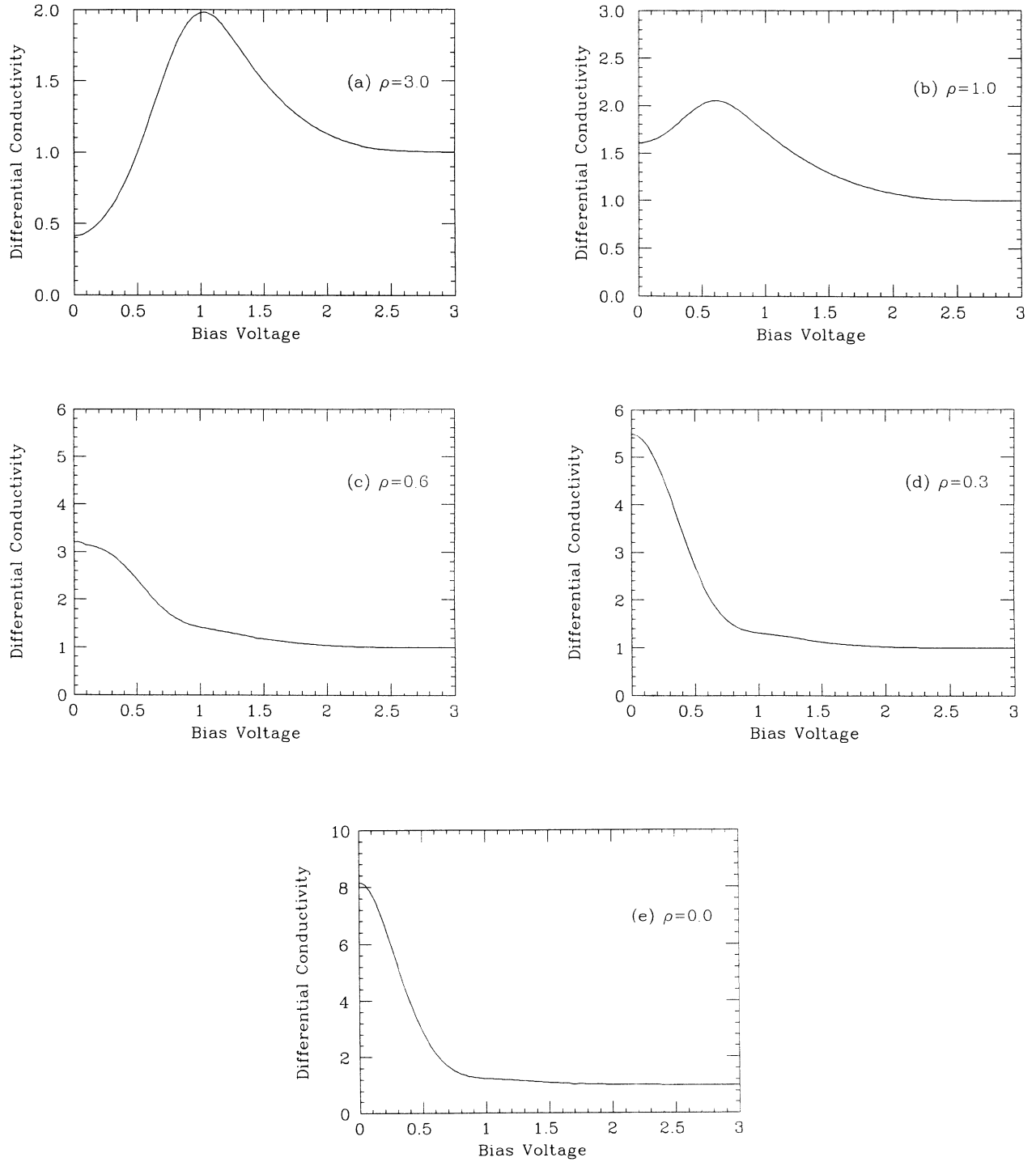

FIG. 3. The differential conductivity vs bias voltage for a 2D Fermi surface at $T/T_c=0.2$. The differential conductivity is normalized by the normal-state value and the bias voltage is in units of $\Delta_{BCS}(T)$: (a) $\rho=3.0$, (b) $\rho=1.0$, (c) $\rho=0.6$, (d) $\rho=0.3$, and (e) $\rho=0.0$.

IV. CONCLUSIONS

We have presented the results of a self-consistent calculation of the LDOS for an isolated vortex. There are two main conclusions: (1) The relevant coherence length for the gap function is π times as large as the BCS coherence length. (2) The LDOS is a double-peaked function in frequency with the position of the low-frequency peak dependent on the distance from the vortex core, and the second peak is always at $\omega=1$.

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APPENDIX

In this appendix we reproduce for completeness the analytic calculation of the LDOS for small ω and $r_\perp$ found in Refs. 6 and 21. The quasiclassical equations are

$$\begin{aligned} a' &= -\mu(e\Delta - d\Delta^*) , \\ d' &= -2\mu(-a\Delta + \Omega d) , \\ e' &= -2\mu(a\Delta^* - \Omega e) , \\ a &= (1-de)^{1/2} , \end{aligned} \tag{A1}$$

where $\mu=(\sin\theta_K)^{-1}$ and $\Omega=-i\omega+\eta$, and the prime denotes differentiation with respect to $r_\parallel$. For a singly quantized vortex we see from Eq. (10) that the gap function has the following symmetries:

$$\begin{aligned} \Delta(r_\parallel) &= -\Delta(-r_\parallel) , \\ \Delta(r_\perp)^* &= \Delta(-r_\perp) . \end{aligned} \tag{A2}$$

Therefore, under the transformation $r_\parallel \to -r_\parallel$, the equations remain self-consistent if the following relations hold: $d(-r_\parallel)=e(r_\parallel)$ and $a(r_\parallel)=a(-r_\parallel)$.

We may now reduce the problem to the solution of one differential equation, say the equation for d in (13) and the normalization

$$a=[1+d(r_\parallel)d(-r_\parallel)]^{1/2} .$$

First, we decompose the anomalous Green's function d into symmetric and antisymmetric functions

$$d = S + A \tag{A3}$$

such that $S(r_\parallel)=S(-r_\parallel)$ and $A(r_\parallel)=-A(-r_\parallel)$. Then the problem reduces to solving the equations

$$\begin{aligned} S' &= 2\mu(a\bar{\Delta}\cos\psi - 2\Omega A) , \\ A' &= 2\mu(i2a\bar{\Delta}\sin\psi - 2\Omega S) , \\ a &= (1+S^2+A^2)^{1/2} . \end{aligned} \tag{A4}$$

We shall solve these equations for small ω and $r_\perp$. We may assume $S \gg (1-A^2)^{1/2}$ for $r_\parallel$ not too large, as we shall presently verify. The normalization gives $a=-|S|$ (fixing the sign to give a convergent solution), so that the solution of (16) for small $\omega, r_\perp$ is

$$\begin{aligned} S &= B\exp[-u(r_\parallel)] , \\ A &= -2\mu B\int^{r_\parallel} dr'_\parallel (i\bar{\Delta}\sin\psi+\Omega)\exp[-u(r'_\parallel)] , \\ u &= 2\mu\int^{|r_\parallel|} dr'_\parallel \bar{\Delta}(r'_\parallel, r_\perp) . \end{aligned} \tag{A5}$$

In order to determine the constant B we have to solve for d in bulk, say at $r_\parallel=r_0$. In the real gauge

$$\begin{aligned} d_R(r_\parallel=r_0) &= \frac{\bar{\Delta}}{(\bar{\Delta}^2-\Omega^2)^{1/2}} \\ &= d_R(r_\parallel=-r_0) \end{aligned} \tag{A6}$$

and $d=\exp(i\psi)d_R$. Thus,

$$A(r_0)=i\frac{r_0}{r_\perp}S(r_0) . \tag{A7}$$

That is, far away from the vortex core, for $r_0 \gg r_\perp$, $A \gg S$, so that the Green's function at $r_\parallel=r_0$ is

$$a(r_0)=[1-A^2(r_0)]^{1/2} . \tag{A8}$$

However, for $r_\perp=0$ and $\omega=0$, Eq. (17) gives

$$a(r_\parallel)=-S(r_\parallel) . \tag{A9}$$

Finally, equating (20) and (21) at $r_\parallel=r_0$ gives

$$S^2(r_0)+A^2(r_0)=1 \tag{A10}$$

which determines the constant B:

$$B=\left[\exp[-2u(r_0)] + \left[2\mu\int^{r_0} dr'_\parallel \exp[-u(r'_\parallel)] \times(i\bar{\Delta}\sin\psi+\Omega)\right]^2\right]^{-1/2} . \tag{A11}$$

We can now determine the LDOS for small ω and $r_\perp$. For simplicity, take the limit $r_0\to\infty$ in Eq. (A11) and notice that near resonance $\omega\approx\bar{\Delta}\sin\psi$, the antisymmetric function $A\approx 0$ [see Eq. (17)], so that

$$a = B\exp[-u(r_\parallel)] . \tag{A12}$$

Next, using the identity

$$1/(z+i\eta)=\mathcal{P}(1/z)-i\pi\delta(z)$$

we immediately obtain the real part of a:

$$\rho_{\mathrm{LDOS}} \propto \mathrm{Re}(a)$$

$$= \pi \exp[-u(r_{\parallel})]\delta(\Xi) , \tag{A13}$$

where ρ_{LDOS} represents the LDOS and

$$\Xi = 2\mu \int^{\infty} dr'_{\parallel} \exp[-u(r'_{\parallel})](\bar{\Delta}\sin\psi - \omega) . \tag{A14}$$

Thus, we see that the bound-state energy is proportional to $r_{\perp}$ and independent of $\mu = \sin\theta_K$, in agreement with our numerical results.

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