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The electronic structure of normal metal–superconductor bilayers

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Abstract

We study the electronic properties of ballistic thin normal metal–bulk superconductor heterojunctions by solving the Bogoliubov–de Gennes equations in the quasiclassical and microscopic 'exact' regimes. In particular, the significance of the proximity effect is examined through a series of self-consistent calculations of the space-dependent pair potential $\Delta(\boldsymbol{r})$. It is found that self-consistency cannot be neglected for normal metal layer widths smaller than the superconducting coherence length ξ_0, revealing its importance through discernible features in the subgap density of states. Furthermore, the exact self-consistent treatment yields a proximity-induced gap in the normal metal spectrum, which vanishes monotonically when the normal metal length exceeds ξ_0. Through a careful analysis of the excitation spectra, we find that quasiparticle trajectories with wavevectors oriented mainly along the interface play a critical role in the destruction of the energy gap.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Due to progressive advancements in the areas of materials growth and sample fabrication techniques, the study of artificial structures consisting of normal metal–superconductor (N/S) bilayers has undergone a considerable resurgence. In particular, refined material deposition methods can yield reproducible and clean N/S layers with highly transparent interfaces. These heterostructures have potential uses in a variety of applications, including logic elements and rf devices.

The physical mechanism behind the proximity effect, i.e. the existence of superconducting correlations in the normal metal, was investigated long ago [1] and is now known to be due to Andreev reflection [1]. In this process, a superconductor in contact with a normal metal induces phase coherence between the particle and hole wavefunctions in the metal, even in the absence of a pairing interaction in the normal metal. The associated superconducting correlations give rise to a finite value of the pair amplitude, $F(\boldsymbol{r})$, which is the probability amplitude for finding

a Cooper pair at the point $\boldsymbol{r}$. Although the pair potential, $\Delta(\boldsymbol{r})$, gives essentially the same information in the superconductor as $F(\boldsymbol{r})$, the quantity $\Delta(\boldsymbol{r})$ vanishes in the normal metal in the absence of attractive coupling. For a bulk, homogenous superconductor, Δ is a constant that corresponds to the minimum excitation energy in the spectrum or the energy gap E_{g}. It is well known that E_{g} is the binding energy of a Cooper pair, and its existence affects most thermodynamic measurements. For inhomogenous N/S systems, $\Delta(\boldsymbol{r})$ naturally depends on position, and thus the association between E_{g} and $\Delta(\boldsymbol{r})$ is then nontrivial. An analogous property is exhibited in elementary quantum mechanics, whereby the Schrödinger equation contains potentials that can vary in space yet the eigenvalues are spatially independent.

Over the years several quasiclassical works involving N/S hybrid structures have been presented [2–12]. The self-consistent pair potential was calculated for a finite-width, double-layer system with a finite reflection coefficient at the interface [3]. A numerical self-consistent study of a system consisting of a finite normal metal layer adjacent to a bulk superconductor indicated that a properly adjusted step-function model for the pair potential yields satisfactory results [4]. Geometric resonance effects [5, 6] in finite N/S sandwiches were investigated through tunnelling density of states (DOS) calculations. The existence of an energy gap in the excitation spectrum has also been purported in various contexts [7–11]. Interface quality and surface roughness have both been shown to reduce the overall gap [12].

For other types of systems, quasiclassical methods are inapplicable. In particular, there are geometric configurations in which the structure under consideration has dimensions that are smaller than the mean free path, or in which the interaction potentials vary over atomic length scales. In this case, it is more appropriate to solve the problem within the ballistic regime and to use a 'microscopic method', which implies that all length scales have been retained in the respective equations. Unfortunately, solving the relevant equations from a microscopic standpoint can be very demanding computationally, especially if the pair potential is treated in a proper self-consistent way. Some recent works, however, have overcome some of these difficulties. A microscopic recursion method [13] that uses a tight-binding model Hamiltonian was presented for calculating the local spectral densities in hybrid N/S and ferromagnet–superconductor nanostructures. A study of layered N/S layered structures [14] involved numerical self-consistent solutions to the microscopic Gor'kov equations, and the DOS revealed a gap structure in the normal metal layer. A particularly interesting restriction of the quasiclassical approximation that is not found in the exact formalism is demonstrated in the Andreev [1] equations, whereby values of the quasiparticle momentum parallel to the interface—and comparable to the Fermi momentum—are crudely approximated. This point has been discussed previously [15] in the context of superconductor–normal metal–superconductor junctions, where it was shown that normal reflections can dominate the Andreev reflection process. Recently, Andreev bound states have also been numerically calculated [16] exactly and self-consistently for clean bulk N/S junctions. It was found that the quasiclassical approximation fails for certain transverse junction widths.

In this paper, we perform the first systematic investigation of the *self-consistent* quasiparticle spectra of clean N/S heterojunctions using an efficient numerical algorithm to solve, without approximations, the microscopic Bogoliubov–de Gennes equations within the continuum. The method therefore permits all length scales in the problem to be accounted for equally. Our geometry is a bilayer 'sandwich' structure, where the normal layer is thin ($d_{\mathrm{N}} \leqslant \xi_0$) and the superconductor is in the bulk limit. Our study includes comparisons with analytical solutions to the so-called (quasiclassical) Andreev equations. In the microscopic regime, we find the energy gap variation as a function of the normal metal thickness parameter. The role that self-consistency, and particular quasiparticle trajectories, play in the calculated electronic structure is also carefully discussed.

2. Method and results

We consider a three-dimensional semi-infinite system comprising a thin normal metal (of width $d_N \lesssim \xi_0$) in electrical contact with a superconductor of width $d_S \gg \xi_0$. The system has a total length of d in the z-direction, with the planar interface located at the point $z = d_N$. The free surfaces at $z = 0$ and d are specularly reflective. After taking into account the translational invariance in the x–y plane, the electronic structure of the N/S system is given in terms of the quasiparticle amplitudes $\Psi(z)^T = (u_n(z), v_n(z))$, which are solutions to the microscopic Bogoliubov–de Gennes equations [17]:

$$[\hat{\sigma}_z(-\nabla_z^2/2m + \varepsilon_\parallel - E_F) + \hat{\sigma}_x\Delta(z) - \epsilon_n]\Psi(z) = 0, \tag{1}$$

where $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are the usual Pauli spin matrices, $\varepsilon_\parallel \equiv 1/2m(k_x^2 + k_y^2)^{1/2}$ is the kinetic energy of the quasiparticles parallel to the interface, E_F is the Fermi energy, ϵ_n are the quasiparticle energy eigenvalues, and $\Delta(z)$ is the pair potential. The coupled set of equations (1) are completed by the self-consistency condition for the pair potential

$$\Delta(z) = g(z)\sum_{0<\epsilon_n\leqslant\omega_D} u_n(z)v_n(z)[1 - 2f(\epsilon_n)], \tag{2}$$

where $g(z)$ is the effective coupling constant that describes the electron–electron interaction, ω_D is the Debye energy, and f is the Fermi function. Here, $g(z) = 0$ in the normal metal and $g(z) = g$ in the superconductor.

For thin normal metal layers, the proximity effect plays a crucial role in the determination of electronic properties. Thus a self-consistent pair potential is required. For the exact solutions to equation (1), a numerical method is implemented to achieve this. We begin by expanding the quasiparticle amplitudes in terms of a finite subset of orthonormal basis vectors:

$$u_n(z) = \sum_q^N u_{nq}\phi_q(z), \qquad v_n(z) = \sum_q^N v_{nq}\phi_q(z). \tag{3}$$

We use the complete set of eigenfunctions $\phi_q(z) = \langle z|q\rangle = (2/d)^{1/2}\sin(k_q z)$, where $k_q = q/\pi d$ and q is a positive integer. Due to the finite range of the pairing interaction, we can write the cut-off number N as the integer value of $N = k_F d/\pi(1 + \omega_D/E_F)^{1/2}$ [18]. Once this is done, we arrive at the following $2N \times 2N$ matrix eigensystem:

$$\begin{pmatrix} \mathcal{H} & \mathcal{D} \\ \mathcal{D} & -\mathcal{H} \end{pmatrix}\Psi_n = \epsilon_n\Psi_n, \tag{4}$$

where $\Psi_n^T = (u_{n1}, \ldots, u_{nN}, v_{n1}, \ldots, v_{nN})$. The matrix elements $\mathcal{H}_{qq'}$ connecting ϕ_q to $\phi_{q'}$ are constructed from the term found in brackets in equation (1):

$$\mathcal{H}_{qq'} = \langle q|[-\nabla_z^2/2m + \varepsilon_\parallel - E_F]|q'\rangle = [k_q^2/2m + \varepsilon_\parallel - E_F]\delta_{qq'}. \tag{5}$$

The off-diagonal matrix elements $\mathcal{D}_{qq'}$ are given as

$$\mathcal{D}_{qq'} = \langle q|\Delta(z)|q'\rangle = \int_{d_N}^{d} \mathrm{d}z\,\phi_q(z)\Delta(z)\phi_{q'}(z). \tag{6}$$

Solving equation (4) yields the eigenvectors and eigenvalues required for the calculation of physically relevant quantities performed below.

For the non-self-consistent solutions to equation (1), the pair potential is taken to be a step function $\Delta(z) = \Delta_0\Theta(z - d_N)$. Furthermore, to emphasize the existence of a gap,

we consider here excitations in the energy range $\epsilon_n/\Delta_0 \leqslant 1$. The solutions to equation (1) then take the form

$$\Psi(z) = \begin{cases} a(\epsilon_n, \varepsilon_\parallel)\sin(k^+ z)\begin{pmatrix}1\\0\end{pmatrix} + b(\epsilon_n, \varepsilon_\parallel)\sin(k^- z)\begin{pmatrix}0\\1\end{pmatrix}, & \text{for } 0 \leqslant z \leqslant d_{\mathrm{N}} \\ c(\epsilon_n, \varepsilon_\parallel)\mathrm{e}^{\mathrm{i}q^+ z}\begin{pmatrix}1\\ \mathrm{e}^{-\mathrm{i}\varphi}\end{pmatrix} + d(\epsilon_n, \varepsilon_\parallel)\mathrm{e}^{-\mathrm{i}q^- z}\begin{pmatrix}1\\ \mathrm{e}^{\mathrm{i}\varphi}\end{pmatrix}, & \text{for } z \geqslant d_{\mathrm{N}} \end{cases} \tag{7}$$

where

$$\mathrm{e}^{\pm\mathrm{i}\varphi} \equiv \epsilon_n/\Delta_0 \pm \mathrm{i}\sqrt{1-(\epsilon_n/\Delta_0)^2}. \tag{8}$$

Here the wavevectors in the normal metal layer are given as

$$k^\pm = k_{\mathrm{F}}[1 - \varepsilon_\parallel/E_{\mathrm{F}} \pm \epsilon_n/E_{\mathrm{F}}]^{1/2}, \tag{9}$$

while the wavevectors in the superconductor are

$$q^\pm = k_{\mathrm{F}}\left[1 - \varepsilon_\parallel/E_{\mathrm{F}} \pm \mathrm{i}\sqrt{(\Delta_0/E_{\mathrm{F}})^2 - (\epsilon_n/E_{\mathrm{F}})^2}\right]^{1/2}. \tag{10}$$

The constants a, b, c and d are determined by invoking the continuity of $\Psi(z)$ and $\partial\Psi(z)/\partial z$ at the interface. After incorporating the boundary conditions, a relatively straightforward calculation gives the following dispersion relation or eigenvalue equation [19]:

$$\frac{2d_{\mathrm{N}}}{\pi\xi_0}(\epsilon_n/\Delta_0) - [n\pi + \arccos(\epsilon_n/\Delta_0)]\sqrt{1-\varepsilon_\parallel/E_{\mathrm{F}}} = 0, \qquad n = 0, \pm1, \pm2, \ldots, \tag{11}$$

where $\xi_0 \equiv k_{\mathrm{F}}/(\pi m\Delta_0)$ and, in accordance with the quasiclassical approximation, we have retained only the leading-order terms in the small parameter Δ_0/E_{F}. For each fixed parallel mode $\varepsilon_\parallel$, equation (11) gives the allowed energies ϵ_n. Furthermore, as the ratio of d_{N}/ξ_0 is reduced, the number n of energy excitation branches decreases. In figure 1 we show the calculated eigenvalues as a function of $\varepsilon_\parallel$. The figure illustrates a nonzero minimum in ϵ_n only for the cases calculated exactly, and occurs for quasiparticles with in-plane momenta close to the Fermi level ($\varepsilon_\parallel/E_{\mathrm{F}} \simeq 1$). This is due in part to the quasiparticles not coupling to those states responsible for superconductivity. It is therefore those trajectories with a significant momentum component parallel to the interface that are significant in contributing to the filling in of the gap. In the Andreev or quasiclassical approximation scheme, these trajectories are not treated accurately, and those with $\varepsilon_\parallel/E_{\mathrm{F}} > 1$ are neglected altogether. This discrepancy is illustrated in the figure, where we see the quasiclassical result diverges from the exact cases for sufficiently large $\epsilon_\parallel$. Figure 1 also illustrates that a self-consistent $\Delta(z)$ serves to reduce E_{g} and contributes to additional localized bound states in the vicinity of $\epsilon_n = \Delta_0$.

The dependence of E_{g} on the thickness of the normal layer is illustrated for the exact self-consistent case in figure 2. The curve originates at $E_{\mathrm{g}} = \Delta_0$ for $d_{\mathrm{N}} = 0$, corresponding to a single superconductor in the bulk limit. As d_{N} increases, E_{g} declines monotonically towards a gapless superconducting state [20]. The gap decays over the length scale ξ_0. It should be noted that, for the quasiclassical case, equation (11) admits a finite number of states for arbitrary d_{N}/ξ_0, thus precluding the possibility of an energy gap. It can be concluded from figure 2 that the length scale at which E_{g} is destroyed is much smaller than the characteristic length scale describing the decay of the pair amplitude in the metal.

The quasiparticle amplitudes are contained partly within the normal metal region for subgap energies. As an example, in figure 3 we show the normalized function $|u_n(z)|^2$ at the energy $\epsilon_n = 0.8\Delta_0$ for both the self-consistent and non-self-consistent exact cases. The wavefunctions undergo damped oscillations with a period of the order of the Fermi wavelength. Their envelope decays over the length scale given by ξ_0. As expected, for positions deep within the superconductor, the quasiparticle amplitudes vanish at the given subgap energy. It is evident

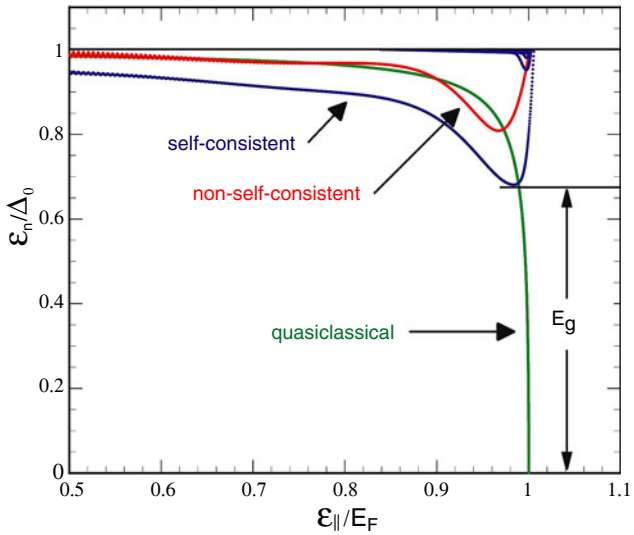

Figure 1. The normalized self-consistent quasiparticle spectrum as a function of the normalized energy $\varepsilon_\parallel/E_F$. The dimensionless parameters are $k_F d_N = 10$ and $k_F\xi_0 = 50$.

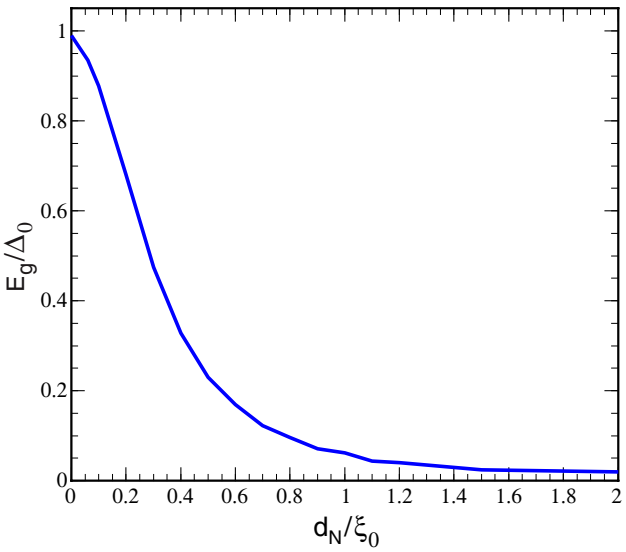

Figure 2. The variation of the dimensionless energy gap in the normal metal as a function of d_N/ξ_0. The curve follows from the exact self-consistent spectra.

that, for the self-consistent case, this quasiparticle state has a much greater extent within the superconductor region. This follows from the inherent reduction in $\Delta(z)$ near the interface and further demonstrates the importance of self-consistency for this configuration.

The previous results in figure 2 revealed the particular influence that the normal metal width has on E_g. We now focus our attention on the one-particle excitations within the bilayer.

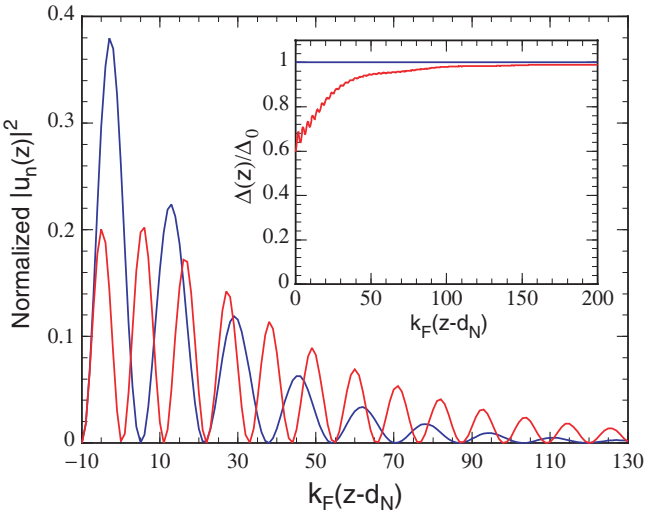

Figure 3. Normalized quasiparticle amplitudes, $|u_n(z)|^2$, as a function of dimensionless position $k_{\rm F}(z-d_{\rm N})$. The highest peaked (blue) curve corresponds to the non-self-consistent result; the other (red) curve is the self-consistent case. The fixed parameters are $d_{\rm N}/\xi_0 = 0.2$ and $\epsilon_n/\Delta_0 = 0.8$. The inset depicts the corresponding spatially varying pair potential contrasted with the non-self-consistent case. As the main plot illustrates, the self-consistent pair potential allows greater subgap quasiparticle propagation within the superconductor.

To this end, we calculate the DOS, which can be expressed as [21]

$$N(\varepsilon) = \frac{1}{(2\pi)^2}\frac{1}{d}\sum_n \int {\rm d}^2 k_\parallel \delta(\epsilon - \epsilon_n), \tag{12}$$

where $k_\parallel = (k_x^2 + k_y^2)^{1/2}$. For the quasiclassical case, equation (12) can be written analytically as

$$N(\epsilon) = \frac{2d_{\rm N}}{\xi_0} N(0) \sum_n \left[\frac{\epsilon/\Delta_0}{[n\pi + \arccos(\epsilon/\Delta_0)]^2} + \frac{(\epsilon/\Delta_0)^2}{\sqrt{1-(\epsilon/\Delta_0)^2}[n\pi + \arccos(\epsilon/\Delta_0)]^3} \right], \tag{13}$$

where $N(0)$ is the normal DOS for both spins at the Fermi surface. In figure 4 we show $N(\epsilon)$ for two different normal metal widths. Focusing on the non-self-consistent cases first, the larger normal metal width (upper panel) shows some agreement between the exact and quasiclassical DOS for most energies. The DOS rises approximately linearly from the Fermi level and then increases rapidly to form a rather pronounced peak. The location of this first peak is found from equation (11) and occurs at the energy ϵ, satisfying

$$\frac{\epsilon}{\Delta_0} = \cos\left(\frac{2d_{\rm N}}{\pi\xi_0}\frac{\epsilon}{\Delta_0}\right). \tag{14}$$

For the case $d_{\rm N}/\xi_0 = 1.5$, this corresponds to $\epsilon/\Delta_0 \approx 0.75$. It is readily deduced that the self-consistent pair potential serves to shift the relative positions of the peaks. Within the neighbourhood of the main peaks, the disparity between the different cases is much more evident. Moreover, we found that, besides oscillations on the atomic scale, there are no discernible differences between the quasiclassical and exact cases in the limit $d_{\rm N} \gg \xi_0$, as expected. For the very thin metal layer (bottom panel), however, the curves have minimal correlation, thus emphasizing that the Andreev approximation is not applicable in the regime $d_{\rm N} \ll \xi_0$. This holds similarly for the self-consistent case, whereby the differences in the

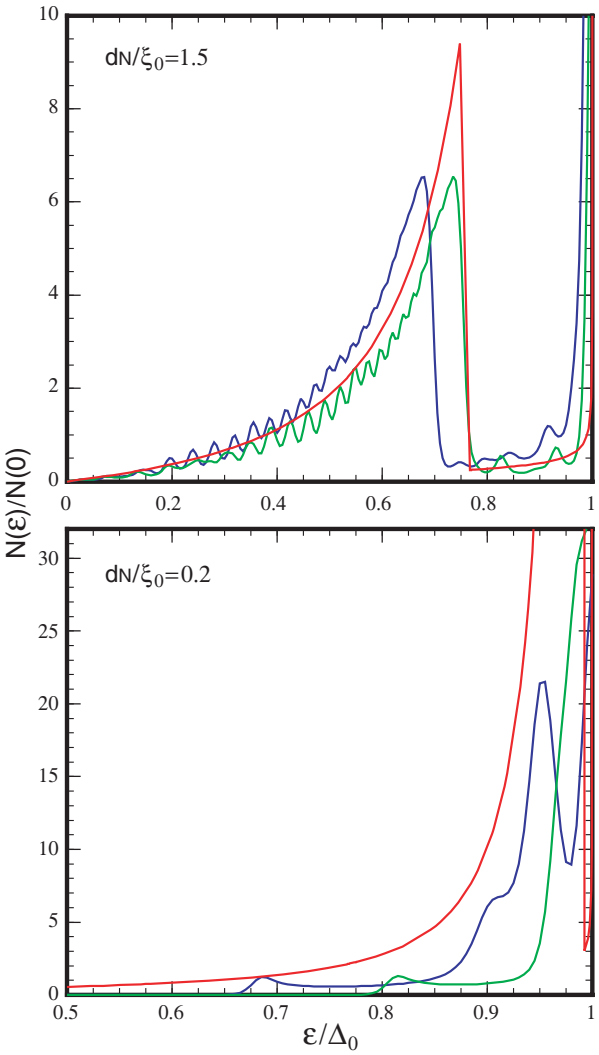

Figure 4. DOS for two different d_N, labelled in the figure. In the top panel, the quasiclassical result is the upper (red) curve sharply peaked at $\epsilon/\Delta_0 \approx 0.75$. The self-consistently calculated DOS is shifted towards lower energies relative to the exact non-self-consistent DOS (dark grey (blue) and light grey (green) curves, respectively). For smaller d_N (lower panel), all three cases differ significantly. The uppermost quasiclassical curve lacks the same subgap structure exhibited by the exact results, and the self consistent dark grey (blue) curve clearly shows a reduction in the gap relative to the non-self-consistent case. To facilitate comparisons, the exact results have been convolved with a Gaussian of width $0.01\Delta_0$.

curves are not merely an overall shift. Thus, self-consistency is increasingly important for thin normal metal layers. Finally, it is evident that the energy gap shown in figure 2 for $d_N = 0.2\xi_0$ is consistent with the value of the gap seen in the bottom panel of figure 4.

3. Conclusions

In conclusion, we have systematically and self-consistently calculated the electronic structure of N/S heterostructures consisting of a thin normal metal layer adjoining a bulk superconductor.

Both exact and quasiclassical results were obtained. The exact solutions revealed that the energy gap decays monotonically at a rate that depends on the dimensionless normal metal width $k_F d_N$. This measure of length is smaller than the characteristic length scale that describes the decay of the pair amplitude in the normal metal, indicating that E_g is suppressed more rapidly than the pair amplitude. The quasiclassical results, as expected, did not permit a gap in the normal metal. The DOS in the normal metal was consistent with the above observations. The exact quasiparticle spectra revealed that the gap onset is due to quasiparticle trajectories with a large momentum component parallel to the interface, and that such states are not accounted for accurately within the Andreev approximation. In addition, the modification to the number of bound states and peaks in the DOS indicated that self-consistency should not be neglected. We have focused here on the spectral properties of a thin normal metal adjacent to a superconductor in the clean limit, which is clearly appropriate for layers whose dimensions do not exceed the mean free path. It is known that elastic impurity scattering in the bulk does not affect the gap. However, for situations where inelastic effects may be important, a finite DOS at low energies is likely to arise.

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