Andreev bound states for a superconducting-ferromagnetic box

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Within the microscopic Bogoliubov–de Gennes formalism an exact quantization condition for Andreev bound states of the ferromagnetic-superconducting hybrid systems of box geometry is derived and a semiclassical formula for the density of states is obtained. The semiclassical formula is shown to agree with the exact result, even when the exchange field $h$ is much larger than the superconductor order parameter, provided $h$ is small compared with the Fermi energy.

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Mesoscopic hybrid systems formed from ferromagnets (F) in contact with superconductors (S) exhibit interesting transport properties resulting from the suppression of the electron-hole correlation in the ferromagnets.1–8 These transport phenomena are intimately related to the influence of an exchange field on the density of states (DOS) of clean ferromagnetic films in contact with superconductor, which has been investigated both experimentally9 and theoretically.10,11 In FS systems, Andreev bound states below the bulk superconducting gap are spin split by the exchange field of the ferromagnet. In a quasiclassical treatment of a system with rough boundaries it was shown that subgap features in the DOS of FS hybrids can be understood from the behavior of the length distribution of the classical trajectories existing in the ferromagnetic region, which depends purely on the geometry and the boundaries of the ferromagnetic region.10–12

In this work we calculate the Andreev levels of a FS box consisting of a clean ferromagnetic region with a superconductor attached to one side, as shown in Fig. 1. This geometrical arrangement is a generalization of that investigated in Ref. 10, where the size of the system along the FS interface was infinite. The discrete energy spectrum of the FS box system is obtained by solving the microscopic Bogoliubov–de Gennes (BdG) equation.1,13 We derive an exact quantization condition without using the frequently applied Andreev’s approximation. Our exact quantum description of the FS hybrid is an extension of the commonly used model developed by Blonder et al.14 and by Saint-James and de Gennes15 for normal-superconducting systems. To get the exact energy levels of the system the mismatch in the effective masses and Fermi energies of the ferromagnet and the superconductor are taken into account in our calculations and the tunnel barrier at the interface is modeled using a Dirac delta potential. The treatment of the problem is based on an adaptation of a method developed in our previous work16 to the case of FS systems. However, to obtain an analytical expression of the density of states in our semiclassical calculations no mismatch and tunnel barrier is assumed.

Starting from this exact quantization condition, we give a semiclassical expression for the subgap DOS for exchange fields which are much less than the Fermi energy. The semiclassical DOS is expressed in terms of the classical return probability of the electrons which depends only on the geometry of the F region and its boundaries. Besides the DOS, from our derivation an explicit expression for this return probability is also found. Based on the quasiclassical Green’s function approach a similar expression has been derived for the DOS of ferromagnetic layers in contact with clean superconductor in Ref. 10. Our DOS expression for FS systems can be regarded as an extension of the Bohr-Sommerfeld formula developed for normal-superconducting hybrids.17 In this work we compare the DOS obtained from the exact quantum calculations with that found from our semiclassical formula. We show that a good agreement between the two calculations can be expected only for small enough exchange fields (much less than the Fermi energy).

The BdG equation for the FS systems can be written as

$$
\begin{align*}
H_0 - \sigma h(r) & \Delta \\
\Delta^{\ast} & -H_0 - \sigma h(r)
\end{align*}
$$

where $H_0 = p^2/2m_{\text{eff}} + V(r) - \mu$ is the single-particle Hamiltonian, $\mu = E_{F}^{(F)}, E_{S}^{(S)}$ are the Fermi energies, $m_{\text{eff}} = m_{F}, m_{S}$ are the effective masses in the F/S regions, $\Psi_{\sigma}$ is a two-component wave function for a given spin state $\sigma$ (here $\sigma = \pm \uparrow$ for spin up/down states), $E$ is the quasiparticle energy measured from the Fermi energy $E_{F}^{(F)}$. The tunnel barrier $V(r)$ at the FS interface and the exchange energy $h(r)$ are modeled in a usual way by $V(x,y) = U_0 \delta(x)$ and $h(x,y) = h \Theta(x)$, where $\Theta$ is the unit step function. We also adopt the usual step-function model18 for the pair potential and take $\Delta(r) = \Delta \Theta(x)$. It is easy to see that the Hamiltonian is separable and the ansatz for the wave functions in the F region can be written as

$\Psi_{\sigma} = E \Psi_{\sigma}$.

FIG. 1. A rectangular shape of ferromagnetic dot (F) in contact with a superconductor (S).
\[
\Psi_{m,\sigma}(x,y) = \begin{cases} 
    a_e \sin[k_m^{(e)}(x-d)] \\
    a_h \sin[k_m^{(h)}(x-d)] 
\end{cases} \chi_m(y),
\] (2a)

while in the S region the wave functions have the form
\[
\Psi_{m,\sigma}(x,y) = \begin{cases} 
    c_e \gamma \left( e^{-i q^{(e)}_{m,\sigma} y} + c_h \gamma e^{i q^{(h)}_{m,\sigma} y} \right) \\
    c_e \left( e^{-i q^{(e)}_{m,\sigma} y} + c_h e^{i q^{(h)}_{m,\sigma} y} \right) \chi_m(y),
\end{cases}
\] (2b)

where
\[
k_{m,\sigma}^{(e,h)} = k_F^{(F)} \sqrt{1 \pm \frac{E + \sigma \hbar}{k_F^{(F)}^2} - \left( \frac{m \pi}{k_F^{(F)} W} \right)^2},
\] (2c)
\[
d_{m,\sigma}^{(e,h)} = k_F^{(S)} \sqrt{1 \pm \frac{\Delta^2 - E^2}{k_F^{(S)} W} - \left( \frac{m \pi}{k_F^{(S)} W} \right)^2},
\] (2d)
\[
\chi_m(y) = \sqrt{2/W} \sin(m \pi y/W),
\] (2e)
\[
\gamma_{e,h} = e^{\pm i \arccos(\Delta/E)}.
\] (2f)

Here \(m\) is a fixed integer and the Fermi wave numbers in the F/S regions are given by \(k_F^{(F)} = \sqrt{2 m_F E_F^2/\hbar^2}\) and \(k_F^{(S)} = \sqrt{2 m_S E_S^2/\hbar^2}\) and \(\epsilon/\hbar\) in Eqs. (2) refer to the electron/hole-like quasiparticle excitations, corresponding to +/− signs in Eqs. (2c), (2d), and (2f). The wave functions satisfy the Dirichlet boundary conditions at the boundary of the F region except for the FS interface where the matching conditions16 should be applied. The four coefficients \(a_e, a_h, c_e, c_h\) in Eqs. (2a) and (2b) are determined from these matching conditions. One can find the following secular equation for the eigenvalues \(E\) of the FS system for fixed mode index \(m\) and spin state \(\sigma\)
\[
\text{Im} \left[ \gamma_e D_{m,\sigma}^{(e)}(E,\hbar) D_{m,\sigma}^{(h)}(E,\hbar) \right] = 0,
\] (3a)

where \(\text{Im} \{ \cdot \} \) stands for the imaginary part and
\[
D_{m,\sigma}^{(e)}(E,\hbar) = \left( Z - i \frac{m_F}{m_S} q_{m,\sigma}^{(e)} \right) \sin k_{m,\sigma}^{(e)} d + k_m^{(e)} \cos k_{m,\sigma}^{(e)},
\] (3b)
\[
D_{m,\sigma}^{(h)}(E,\hbar) = \left( Z + i \frac{m_F}{m_S} q_{m,\sigma}^{(h)} \right) \sin k_{m,\sigma}^{(h)} d + k_m^{(h)} \cos k_{m,\sigma}^{(h)},
\] (3c)

and \(Z = 2 m_F U_0/\hbar^2\) is the normalized barrier strength. The number of propagating modes for the electron/hole are the maximum of \(m\) for which \(k_{m,\sigma}^{(e,h)}\) is a real number, i.e., \(M_{m,\sigma}^{(e,h)} = \lfloor \sqrt{1 \pm (E + \sigma \hbar)/k_F^{(F)}} \rfloor\), where \(M = k_F^{(F)} W/\pi\) and \(\lfloor \cdot \rfloor\) stands for the integer part. For nonpropagating modes \(k_{m,\sigma}^{(e,h)}\) have to be replaced with their imaginary part and the functions \(\sin\) and \(\cos\) with the functions \(\sinh\) and \(\cosh\), respectively. For fixed \(m\) and \(\sigma\) the solutions of Eq. (3a) for \(E\) give the discrete subgap energy spectrum \((E < \Delta)\). These levels are numerically exact.

We now calculate density of states below the gap. In what follows, we assume that there is no mismatch and tunnel barrier at the FS interface \((m_F = m_S, E_F^{(F)} = E_F^{(S)}),\) and \(Z = 0\). For simplicity, we shall omit the superscript \(F\) and \(S\) in the wave numbers and the Fermi energies. In Andreev’s approximation, i.e., for \(|E + \sigma \hbar| \ll E_F\) we have \(k_{m,\sigma}^{(e,h)} \approx q_{m,\sigma}^{(e,h)}\) and \(D_{m,\sigma}^{(e)}(E,\hbar) = k_m^{(e)} e^{-i q_{m,\sigma}^{(e)} d}\). Therefore, the quantization condition (3a) can be simplified as
\[
I_{m,\sigma}(E) = \frac{(k_m^{(e)} - q_{m,\sigma}^{(h)}) - \arccos(E/\Delta)}{\pi} = n.
\] (4)

The density of states for energies below the gap \((|E| < \Delta)\) is
\[
\varrho(E) = \sum_{\sigma = \pm 1} \sum_{n = -\infty}^{\infty} \delta(E - E_{m,\sigma}),
\] (5)

where \(E_{m,\sigma}\) are the solutions of Eq. (4). Using Eq. (4) the DOS becomes
\[
\varrho(E) = \sum_{\sigma = \pm 1} \sum_{n = -\infty}^{\infty} \left| \frac{d I_{m,\sigma}(E)}{d E} \right| \delta(I_{m,\sigma}(E) - n),
\] (6)

where \(M_0 = M_{m,\sigma}^{(e,h)} + 1\), the number of propagating modes for spin-up hole. Applying the Poisson summation formula10 to the summation over \(m\) and keeping only the nonoscillating term one finds
\[
\varrho(E) = \sum_{n = -\infty}^{\infty} \left| \frac{d I_{m,\sigma}(E)}{d E} \right| \delta(I_{m,\sigma}(E) - n) \frac{\Theta(M_0 - m^*) \Theta(m^* - 1)}{\left| \frac{\partial I_{m,\sigma}}{\partial m} \right|_{m = m^*}},
\] (7)

where the \(E\)-dependent \(m^*\) satisfies Eq. (4) for a given \(n\) and \(\sigma\). To simplify \(I_{m,\sigma}\) we Taylor expand \(k_{m,\sigma}^{(e,h)}\) in terms of \(E + \sigma \hbar\) in first order (which is consistent with the Andreev’s approximation) and find
\[
I_{m,\sigma}(E) = (E + \sigma \hbar) \frac{2d}{\sqrt{1 - (m/M)^2} - \arccos(E/\Delta) / \pi},
\] (8)

where \(v_F\) is the Fermi velocity. In our approximation, \(M_0 = M\). From Eq. (4) and using Eq. (8) we obtain
\[
m^* = M \sqrt{1 - \frac{2d}{s_{n,\sigma}(E)}}
\] (8c)

where
\[
s_{n,\sigma}(E) = \frac{n \pi + \arccos(E/\Delta)}{(E + \sigma \hbar)/\Delta - \xi_0},
\] (9)

and \(\xi_0 = \hbar v_F/\Delta\) is proportional (up to a factor of \(\pi\)) to the coherence length in the bulk superconductor.

Using Eq. (8) and performing the derivatives in Eq. (7) we find
\[
\varrho(E) = \sum_{\sigma = \pm 1} M |E + \sigma \hbar|^{1/2} \sum_{n = -\infty}^{\infty} \left[ s_{n,\sigma}(E) + \xi_c(E) \right] P[s_{n,\sigma}(E)],
\] (10a)

where
is a purely geometry-dependent function, $\xi_s(E) = \xi_0/\sqrt{1 - E^2/\Delta^2}$ and $s_{n,\sigma}(E)$ is given by Eq. (9). It can be shown that $P(s)$ is the classical probability that an electron entering the billiard at the FS interface returns to the interface after a path length $s$. Thus, the density of states are expressed through a classical quantity which can be regarded as a semiclassical result. The distribution $P(s)$ is normalized to one, i.e., $\int_0^1 P(s) ds = 1$. Note that the result for the DOS, given in Eq. (10), differs from that obtained in Ref. 10 by a factor multiplying $P(s)$ in the summation.

To compare the exact DOS obtained from the quantization condition (3a) with that calculated from the semiclassical expression (10), we introduce the integrated DOS: $N(E) = \int_0^E dE \varrho(E')$. From Eq. (10) we have

$$N(E) = M \sum_{n=\infty}^{+\infty} \left[ F_n^{(a)}(E) + F_n^{(b)}(E) \right],$$

where

$$F_n^{(a)}(E) = F[s_{n+1}(0)] - F[s_{n+1}(E)].$$
FIG. 6. Counting function $N(E)$ as a function of $E/\Delta$ obtained from the exact (solid line) and the semiclassical calculation (dashed line) for $h\Delta = 40.0$ ($h/E_F = 1.0$). The other parameters are the same as in Fig. 2.

$$F_n^{(b)}(E) = \begin{cases} 1 - F[s_{n,-1}(0)] - F[s_{n,-1}(E)] & \text{if } E > h \\ -F[s_{n,-1}(0)] + F[s_{n,-1}(E)] & \text{otherwise,} \end{cases}$$

and $F(s) = \int_0^s P(s') ds' = \Theta(s - 2d) \sqrt{1 - 4d^2 s^2}$ is the integrated length distribution. Note that $F(\infty) = 1$ since $P(s)$ is normalized to 1.

The small parameter used in reaching the semiclassical result is $h/E_F$. Figures 2 and 3 show a comparison between the semiclassical result, Eq. (11), and the exact result, Eq. (3), when $h/E_F = 0.0025$ and 0.25, respectively. For better resolution, in the insets enlarged parts of the main frames are shown. Figures 4 and 5 show the corresponding densities of states [in units of $2\pi^{N/2}$, where $\rho_N = m_F A/(\pi\hbar^2)$ is the DOS of the ferromagnetic region including spin up/down states and $A = WD$ is the area of this region] with singularities given by the semiclassical formula $s_{n,\sigma}(E_{\text{sing}}) = 2d$, where $\sigma = \pm 1$ and $n$ is such that $E_{\text{sing}} < \Delta$. These figures show that the semiclassical formula given by Eqs. (10) and (11) yield good agreement with the exact result, even for large values of $h/\Delta$, provided $h/E_F$ is small. Figure 6 shows a comparison with the exact result when the latter condition is violated. Clearly the agreement is poor in this limit.

In summary we have shown that a semiclassical treatment of the clean limit yields an expression for the DOS in terms of the classical return probability $P(s)$, which in turn is known analytically. This formula is analogous to the quasiclassical result of Ref. 10, where $P(s)$ is not known exactly and must be determined via a numerical simulation. We have also shown that the semiclassical formula agrees very well with the exact result for small exchange field compared with the Fermi energy.

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