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Effect of a Barrier at the Superconducting–Normal Metal Interface*

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A superconducting–normal metal sandwich, in which there is a potential barrier at the interface, is considered. The Tomasch effect amplitude is shown to be reduced by a factor related to the barrier transmission coefficient. We then derive from first principles the boundary conditions obeyed by the kernel in the Gor'kov gap equation at the interface, within the diffusion approximation. This represents the first ab initio calculation of the "second" de Gennes boundary condition.

1. INTRODUCTION

In two recent articles,[1,2] we have examined the effect of a potential barrier between the superconducting (S) and normal (N) metal layers of a proximity effect sandwich on the transition temperature. The treatment was based on certain boundary conditions (BC) at the interface, discussed by de Gennes,[3] using the diffusion approximation. In this approximation, the BCs at the barrier are not determined completely; there remains an unknown parameter related to the barrier strength. The purpose of this paper is to find these BCs from elementary quantum mechanical considerations. We use a simple model: identical metals, except for the interaction that leads to superconductivity in S. It is assumed that the pair potential Δ changes abruptly at the interface, i.e., has the form of a step function. With this model, the Green's functions can be constructed exactly, taking into account the potential barrier.

The assumption of a step-function variation of Δ restricts the validity of the model. At zero temperature, the length scale of Δ is the coherence length

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ξ_0. Therefore, our calculations of the local electronic density of states will be meaningful only at points x far from the interface, $x \gg \xi_0$. We find the local density of states in the S side and show that the amplitude of the Tomasch oscillations is reduced compared to that found for a transparent barrier.[4] The reduction factor, for energies $E \gg \Delta$, is the barrier transmission coefficient in the normal state.[5]

In the vicinity of T_c, a step function form for Δ is not a good starting function for a self-consistent calculation of Δ. However, in this region we can use the Gor'kov gap equation for Δ, in which there enter the normal state Green's functions.[3] As these are calculated exactly in our model, we find the kernel of the gap equation. We then examine the BC obeyed at the interface and obtain explicitly the parameter related to the barrier strength. This is a new result and verifies the BC ansatz of de Gennes. The BC is then used to reexamine some previous expressions for the transition temperature.

2. THE POTENTIAL BARRIER EFFECT AT A SUPERCONDUCTING–NORMAL INTERFACE

We consider a S–N geometry in which the S side occupies the region $x>0$, the N side occupies $x<0$, and a potential barrier $u\,\delta(x)$ is at the interface $x=0$. In order to find the BC obeyed by the kernal in the Gor'kov gap equation at the interface, we need the Green's functions of the system. These obey the following equation of motion:

$$\left[E\sigma_3+\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+k_F^2-k_\perp^2\right)-i\,\Delta\theta(x)\sigma_1-u\,\delta(x)\right]G(xx'E)=\delta(x)\sigma_3 \tag{1}$$

Here σ_i are the Pauli spin matrices, $k_\perp$ is the momentum component parallel to the interface, and k_F is the Fermi momentum. The pair potential Δ has a step-function variation, where

$$\theta(x)=\begin{cases}1, & x>0\\ 0, & x<0\end{cases} \tag{2}$$

The Green's functions of (1) are found by the following procedure[4]: The solutions of the homogeneous equation

$$\left[E\sigma_3+\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+k_F^2-k_\perp^2\right)-i\,\Delta\sigma_1\theta(x)-u\,\delta(x)\right]\psi(x)=0 \tag{3}$$

that satisfy the appropriate BC at the interface are found. The Green's functions are given by the product $\psi_{in}^{\dagger}(x)\psi_{out}(x')$ (for $x>x'$), where ψ_{in} (ψ_{out}) denotes incoming (outgoing) waves. A detailed analysis of the solutions of

(3) is given in Ref. 5. We briefly repeat it and construct the Green's functions in the appendix.

The local electronic density of states in the S side is given by

$$N(E, x) = (1/\pi)\,\mathrm{Im}\, G_{11}(xxE) \tag{4}$$

where G_{11} is the 11 matrix element. From (A16) we obtain

$$N(E,x) = \frac{1}{\pi\hbar v_F}\,\mathrm{Re}\,\frac{1}{2\Omega}\left\{(E+\Omega)\left[1-\frac{\alpha+i\sqrt{\alpha}}{1+\alpha(1-B^2)}(1-B^2)e^{2ik_+x}\right]\right.$$

$$+(E-\Omega)\left[1-\frac{\alpha-i\sqrt{\alpha}}{1+\alpha(1-B^2)}(1-B^2)\,e^{-2ik_-x}\right]$$

$$\left.-2(E-\Omega)\frac{1}{1+\alpha(1-B^2)}\,e^{i(k_+-k_-)x}\right\} \tag{5}$$

where

$$B^2 = (E-\Omega)/(E+\Omega), \qquad \Omega^2 = E^2-\Delta^2 \tag{6}$$

$$(k^{\pm})^2 = k_F^2 - k_\perp^2 \pm (2m/\hbar^2)\Omega \tag{7}$$

and α is related to the barrier strength*

$$\alpha = (2m/\hbar^2)u^2/4k_F^2 \tag{8}$$

In the normal state, the transmission coefficient of the barrier is[5] $1/(1+\alpha)$. There are two types of oscillations in (5). The first one is $\exp(\pm 2ik^{\pm}x) \sim \exp(\pm 2ik_{Fx}x)$, from (7). These terms arise from reflections of excitations from the potential barrier and are similar to Friedel oscillations in the normal state. The second type of oscillations is $\exp[i(k^+-k^-)x] \sim \exp[i(2\Omega/\hbar v_F)x]$ and appears only in the superconducting state. These are the Tomasch oscillations.[4] We find that their amplitude is modified by the potential barrier, through the factor $[1+\alpha(1-B^2)]^{-1}$. In the limit $\Delta \ll E$, this factor tends to the transmission coefficient of the barrier.

The transition temperature of a proximity effect sandwich can be calculated from the Gor'kov gap equation, valid in the vicinity of T_c (see, for example, Ref. 3)

$$\Delta(x) = V(x)\int dx'\,\Delta(x')k_B T\sum_n H(xx'\omega_n) \tag{9}$$

*For a barrier of width a and height U_0, it can be verified that $\alpha = \{[(\kappa^2+k^2)/2\kappa k]\}^2 \sinh^2 \kappa a$, where $\kappa^2 \approx k^2 + (2m/\hbar^2)U_0$ (see Ref. 5). We treat the case $U_0 \to \infty$, $a \to 0$ such that $U_0 a$ remains finite, and neglect over-the-barrier transmission.

where $V(x)$ is the BCS attractive potential. The kernel of (9) is a product of two Green's functions of the normal state[3]

$$H(xx'\omega_n)=\sum_{k_\perp} G_n^*(x'x\omega_n)G_n(x'x\omega_n) \tag{10}$$

where

$$\hbar\omega_n=\pi k_B T(2n+1) \tag{11}$$

and the sum in (9) runs over all integers. In (10), G_n is the 11 matrix element of G, in the normal state,[3] and the product is summed over $k_\perp$, on which G_n depends [from (1)].

The usual procedure to proceed from (9) is to write down a diffusion equation for the kernel.[3] This diffusion equation is valid for each metal, in the dirty limit, when it is in a homogeneous bulk form. The kernel is found from the diffusion equation, with two BCs satisfied by it and its derivative at the interface. When there is a potential barrier at the interface, it affects the BCs.[1,2] However, within the diffusion approximation, the BCs cannot be determined completely, and the barrier strength enters through an unknown parameter.[1,2] In the model presented here, we can calculate the kernel of (9) exactly and then construct the BCs it obeys at the interface.

We shall first calculate (10) at zero temperature and then transform to the finite-temperature expression. In the normal state $\Delta=0$, hence $B=0$ [from (6)], and $\Omega=E$. From (A16) we find that the 11 matrix element in the normal state is

$$G_n(xx'E)=\frac{i}{\hbar v_F}\left\{\exp[ik_+(x-x')]-\frac{i\sqrt{\alpha}}{1+i\sqrt{\alpha}}\exp[ik_+(x+x')]\right\},$$
$$x>x'>0 \tag{12}$$

and similarly

$$G_n(xx'E)=\frac{i}{\hbar v_F}\left\{\exp[ik_+(x-x')]-\frac{i\sqrt{\alpha}}{1+i\sqrt{\alpha}}\exp[-ik_+(x+x')]\right\},$$
$$x'<x<0 \tag{13}$$

$$G_n(xx'E)=\frac{i}{\hbar v_F}\times\frac{1}{1+i\sqrt{\alpha}}\exp[ik_+(x-x')],$$
$$x'<0<x \tag{14}$$

where

$$k_+^2=k_F^2-k_\perp^2-(2m/\hbar^2)E \tag{15}$$

The Green's functions for $x<x'$ are obtained by interchanging x and x' in (12)–(14).

To find the kernel of (9), we have to transform (12)–(14) into the finite-temperature form. This is simply done by changing $E \to i\omega_n$, since the kernel is a sum over all frequencies. Then, constructing the products $G_n^*(x'x, i\omega_n)G_n(x'x, i\omega_n)$, we encounter two types of terms: oscillatory terms, of the form $\exp[\pm i(k_+ + k_+^*)x] \sim \exp(\pm 2ik_{Fx}x)$, and exponential terms $\exp[\pm i(k_+ - k_+^*)] \sim \exp(2\omega_n x/\hbar v_F)$. The oscillatory terms are neglected, since in the gap equation we are interested in the variation of Δ, which is described by only the exponential terms.[3] Thus, inserting (12)–(14) into (10), we obtain

$$H(xx'\omega_n) = N(0)\frac{\pi}{\hbar v_F}\begin{cases}\left\{\exp[i(k_+ - k_+^*)(x'-x)] + \dfrac{\alpha}{1+\alpha}\exp[-i(k_+ - k_+^*)(x'+x)]\right\}, & x<x'<0 \\ \left\{\dfrac{1}{1+\alpha}\exp[i(k_+ - k_+^*)(x'-x)],\right\} & x<0<x' \\ \left\{\exp[i(k_+ - k_+^*)(x'-x)] + \dfrac{\alpha}{1+\alpha}\exp[i(k_+ - k_+^*)(x'+x)]\right\}, & 0<x<x'\end{cases} \tag{16}$$

where $N(0)$ is the density of states at the Fermi level. It can be easily checked that the kernel obeys the sum rule[3]

$$\int_{-\infty}^{\infty} dx'\, H(xx'\omega_n) = N(0)\frac{\pi}{\hbar v_F}\frac{-2}{i(k_+ - k_+^*)} = \frac{\pi N(0)}{|\omega_n|} \tag{17}$$

The BCs at the interface obeyed by our construct for $H(xx'\omega_n)$ are

$$\frac{d}{dx'}H(xx'\omega_n)\Big|_{x'=0^-}^{x'=0+} = 0 \tag{18}$$

$$H(xx'\omega_n)\Big|_{x'=0^-}^{x'=0+} = \frac{-2\alpha}{i(k_+ - k_+^*)}\frac{d}{dx'}H(xx', \omega_n)\Big|_{x'=0}$$

$$= 2\alpha\frac{\hbar v_F}{2|\omega_n|}\frac{d}{dx'}H(xx'\omega_n)\Big|_{x'=0} \tag{19}$$

The first BC, Eq. (18), describes the fact that the particle current through the interface in one direction is equal to the current in the reverse direction. This BC was derived by de Gennes[3] from the sum rule (17). [When comparing (17) and (18) with the BCs of the diffusion approximation, it must be

remembered that in our model the two metals are identical, except for the interaction leading to superconductivity in S.] The second BC, Eq. (19), was postulated by de Gennes. Within the diffusion approximation, one cannot determine the factor of the derivative in (19), although it can be argued that it is inversely proportional to the barrier penetration probability.[1,2] Here, however, we are able to evaluate this factor explicitly. Denoting it by L, we obtain

$$L = 2\alpha(\hbar v_F/(2|\omega_n|)) = 2\alpha\xi(\omega_n) \tag{20}$$

where $\xi(\omega_n)$ is the energy-dependent coherence length. It is interesting to note that by the neglect of the oscillating terms $\exp(\pm 2ik_{Fx}x)$ in the kernel, it acquires BCs of the diffusion type. If those terms are kept, the kernel being a product of two Green's functions, would obey the BCs of the solutions, i.e., it would be continuous at $x = 0$, but its first derivative would jump according to (A5).

3. DISCUSSION

A superconducting–normal geometry with a potential barrier at the interface has been considered. Assuming that Δ varies abruptly at the interface, we have found that the amplitude of the Tomasch oscillations is reduced by a factor related to the barrier transmission coefficient.

The interesting result is expression (20) for L, which yields the effect of the barrier on the BCs at $x = 0$ obeyed by the kernel of the Gor'kov gap equation. We found that diffusion-type BCs are obtained when the oscillatory terms $\exp(\pm ik_{Fx}x)$, caused by the barrier, are neglected. The parameter L has not been determined previously within the diffusion approximation, but expressions for T_c including it have been derived.[1,2] We now review them, in view of the result (20). In Eq. (37) of Ref. 1, we found that the extrapolation length[3] b is given by

$$b \equiv \frac{\Delta_S(x)}{d\Delta_S(x)/dx}\bigg|_{x=0} = \frac{N_S D_S}{N_N D_N}(q^{-1}\coth qd_N + L) \tag{21}$$

Here N_S and D_S are the density of states and the diffusion coefficient of the S side, respectively, and similarly for the N side. The thickness of the N side is d_N, and q^{-1} is the depth of penetration of Cooper pairs into N. (Note that in Ref. 1, L is denoted L_0/σ.) As b becomes larger, T_c is increased. We see that the effect of the barrier on T_c is negligible for

$$Lq \ll 1 \tag{22}$$

This means that when α is smaller than the ratio of the depth of penetration to $\xi(\omega_n)$, T_c is almost unchanged by the barrier. When the thickness of the

two metals is much smaller than the respective coherence lengths, the sandwich is in the Cooper limit. In that case the equation for the transition temperature turns out to be of the same functional form as the one obtained from McMillan's tunneling model for the proximity effect.[2] Comparing the two results (see Ref. 2), we find (σ is the penetration probability)

$$L = 2lB(l/d_N)/\sigma = 2\alpha\xi(\omega_n) \tag{23}$$

Here l is the mean free path in N, of the order of the thickness d_N in the Cooper limit, and B is of order unity. McMillan[6] introduced the penetration probability σ to describe the barrier. This causes some trouble, since $0 \leq \sigma \leq 1$ and therefore for $\sigma = 1$ should get the same result as in the absence of a potential barrier. This is not the case, as can be seen from Refs. 2 and 3. However, with the result for L, (20), the expression for T_c is appropriately normalized. For small α (for which the penetration probability is ~ 1), the effect of the barrier is negligible, whereas for $\alpha \to \infty$ (small σ), we get an appreciable effect. This is in accordance with the remark by de Gennes[3] about the importance of the L term. From Ref. 2, Eq. (11), we find that the effect of the barrier is negligible for

$$Ld_N/\xi^2(\omega_n) \ll 1, \qquad \text{i.e.,} \quad 2\alpha \ll \xi(\omega_n)/d_N \tag{24}$$

i.e., when the strength of the barrier (inversely proportional to its transmission coefficient) is much smaller than the ratio of the coherence length to the thickness (of the order of the mean free path in the Cooper limit).

APPENDIX. THE GREEN'S FUNCTIONS IN THE SUPERCONDUCTING SIDE

Here we give the solutions to the homogeneous equation (3) and the construction of the Green's functions. Consider first a solution describing an electron incoming from the left

$$\psi^e_{\text{in}}(x) = \begin{cases} b_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(ik_+x) + \tilde{b}_2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(-ik_+x) + b_3 \begin{pmatrix} 0 \\ -i \end{pmatrix} \exp(ik_-x), & x < 0 \\ a_1\phi_1 \exp(ik^+x) + \tilde{a}_4\phi_2 \exp(-ik^-x), & x < 0 \end{cases} \tag{A1}$$

The various terms are as follows: In the N side ($x < 0$), we have an electron (the b_1 term) incident on the surface. There it is partly reflected as an electron going in the reverse direction (the $\tilde{b}_2$ term) and partly as a hole (the b_3 term). The b_3 term is due to Andereev reflection,[7] caused by the change in Δ at the interface, and the $\tilde{b}_2$ term is due to the usual reflection from a

potential barrier. The wave vectors in the N side are

$$k_{\pm}^2 = k_F^2 - k_\perp^2 \pm \frac{2m}{\hbar^2}E \tag{A2}$$

Here E is the excitation energy. The transmitted wave into the S side is partly an electronlike excitation (the a_1 term), and partly a holelike excitation (the $\tilde{a}_4$ term), with

$$(k^{\pm})^2 = k_F^2 - k_\perp^2 \pm (2m/\hbar^2)\Omega, \qquad \Omega^2 = E^2 - \Delta^2 \tag{A3}$$

The two component vectors in S are

$$\phi_1 = \left(\frac{E+\Omega}{2E}\right)^{1/2}\begin{pmatrix}1\\ -iB\end{pmatrix}, \qquad \phi_2 = \left(\frac{E+\Omega}{2E}\right)^{1/2}\begin{pmatrix}B\\ -i\end{pmatrix}, \qquad B^2 = \frac{E-\Omega}{E+\Omega} \tag{A4}$$

We now have to determine the constants in (A1). This is done as follows: The wave functions are continuous at $x=0$, but because of the potential barrier, there is a jump in the first derivative[5]

$$\left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{d\psi}{dx}\right|_{x=0^-} = q\psi(0), \qquad q = \frac{2m}{\hbar^2}u \tag{A5}$$

as can be seen from (3). Thus we obtain

$$a_1 = b_1\left(\frac{2E}{E+\Omega}\right)^{1/2}\frac{-2ik(q+2ik)}{D}, \qquad \tilde{a}_4 = b_1\left(\frac{2E}{E+\Omega}\right)^{1/2}\frac{2ikqB}{D}$$

$$b_3 = b_1\frac{4k^2B}{D}, \qquad \tilde{b}_2 = b_1\frac{-q(2ik+q)(1-B^2)}{D} \tag{A6}$$

where we have defined

$$D = 4k^2 + q^2(1-B^2) \tag{A7}$$

Here we have approximated[5] $k_{\pm} \sim k^{\pm} \sim k$. The incoming hole solution is

$$\psi_{\text{in}}^h(x) = \begin{cases} b_4\begin{pmatrix}0\\ -i\end{pmatrix}\exp(-ik_-x) + \tilde{b}_3\begin{pmatrix}0\\ -i\end{pmatrix}\exp(ik_-x) \\ \quad + b_2\begin{pmatrix}1\\ 0\end{pmatrix}\exp(-ik_+x), & x<0 \\ a_4\phi_2\exp(-ik^-x) + \tilde{a}_1\phi_1\exp(ik^+x), & x>0 \end{cases} \tag{A8}$$

From the continuity of the wave functions at $x=0$ and (A5) we find

$$a_4 = b_4\left(\frac{2E}{E+\Omega}\right)^{1/2}\frac{2ik(-2ik+q)}{D}, \qquad \tilde{a}_1 = b_4\left(\frac{2E}{E+\Omega}\right)^{1/2}\frac{-2ikqB}{D}$$

$$b_2 = b_4\frac{4k^2B}{D}, \qquad \tilde{b}_3 = b_4\frac{q(2ik-q)(1-B^2)}{D} \tag{A9}$$

The outgoing electronlike solution is

$$\psi^e_{\text{out}}(x)=\begin{cases} b'_2\begin{pmatrix}1\\0\end{pmatrix}\exp(-ik_+x)+\tilde{b}'_3\begin{pmatrix}0\\-i\end{pmatrix}\exp(ik_-x), & x<0 \\ a'_2\phi_1\exp(-ik^+x)+\tilde{a}'_1\phi_1\exp(ik^+x)+a'_4\phi_2\exp(-ik^-x), & x>0 \end{cases} \tag{A10}$$

with

$$a'_4=a'_2\frac{-4k^2B}{D},\qquad \tilde{a}'_1=a'_2\frac{-q(q+2ik)(1-B^2)}{D}$$

$$b'_2=a'_2\left(\frac{E+\Omega}{2E}\right)^{1/2}\frac{-2ik(q+2ik)(1-B)^2)}{D},$$

$$\tilde{b}'_3=a'_2\left(\frac{E+\Omega}{2E}\right)^{1/2}\frac{-2ikqB(1-B^2)}{D} \tag{A11}$$

The outgoing holelike solution is

$$\psi^h_{\text{out}}(x)=\begin{cases} b'_3\begin{pmatrix}0\\-i\end{pmatrix}\exp(ik_-x)+\tilde{b}'_2\begin{pmatrix}1\\0\end{pmatrix}\exp(-ik_+x), & x<0 \\ a'_3\phi_2\exp(ik^-x)+\tilde{a}'_4\phi_2\exp(-ik^-x) & \\ \quad +a'_1\phi_1\exp(ik^+x), & x>0 \end{cases} \tag{A12}$$

with

$$a'_1=a'_3\frac{-4k^2B}{D},\qquad \tilde{a}'_4=a'_3\frac{-q(q-2ik)(1-B^2)}{D}$$

$$b'_3=a'_3\left(\frac{E+\Omega}{2E}\right)^{1/2}\frac{2ik(q-2ik)(1-B^2)}{D},$$

$$\tilde{b}'_2=a'_3\left(\frac{E+\Omega}{2E}\right)^{1/2}\frac{2ikqB(1-B^2)}{D} \tag{A13}$$

The Green's functions are constructed according to the procedure described in Ref. 4, with

$$\psi_{\text{in}}=\psi^e_{\text{in}}+\psi^h_{\text{in}},\qquad \psi_{\text{out}}=\psi^e_{\text{out}}+\psi^h_{\text{out}} \tag{A14}$$

In the product $\psi_{in}(x)\psi_{out}(x')$ four constants appear: b_1a_2', b_1a_3', b_4a_2', and b_4a_3'. These are determined from

$$G(xx'E)|_{x=x'^+} = G(xx'E)|_{x=x'^-}$$

$$\frac{d}{dx}G(xx'E)\bigg|_{x=x'^+} - \frac{d}{dx}G(xx'E)\bigg|_{x=x'^-} = -\frac{2m}{\hbar^2}\sigma_3 \tag{A15}$$

which should hold in order for (1) to be obeyed. For $x > x' > 0$ we find

$$\begin{aligned} G(xx'E) = \frac{i}{\hbar v_F}\frac{E}{\Omega}\Big(&\phi_1\phi_1^+\Big\{\exp[ik^+(x-x')] - \frac{1}{D}q(q+2ik) \\ &\times(1-B^2)\exp[ik^+(x+x')]\Big\} \\ &-\phi_2\phi_2^+\Big\{\exp[-ik^-(x-x')] - \frac{1}{D}q(q-2ik) \\ &\times(1-B^2)\exp[-ik^-(x+x')]\Big\} \\ &-\frac{4k^2B}{D}[\phi_1\phi_2^+\exp(ik^+x - ik^-x') + \phi_2\phi_1^+\exp(-ik^-x + ik^+x')]\Big) \end{aligned} \tag{A16}$$

Here we used $k = mv_F/\hbar$, and ϕ_1^+ and ϕ_2^+ are the row vectors

$$\phi_1^+ = \left(\frac{E+\Omega}{2E}\right)^{1/2}(1\ iB), \qquad \phi_2^+ = \left(\frac{E+\Omega}{2E}\right)^{1/2}(B\ i) \tag{A17}$$

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