Quantitative simulation of the superconducting proximity effect

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A numerical method is developed to calculate the transition temperature of double or multilayers consisting of films of superconductors and normal conductors. The approach is based on a dynamic interpretation of Gorkov's linear gap equation and is very flexible. The mean free path l of the different metals, transmission through the interface, ratio of specular reflection to diffusive scattering at the surfaces, and fraction of diffusive scattering at the interface can be included. Furthermore, it is possible to vary the mean free path and the BCS interaction NV in the vicinity of the interface. The numerical results show that the normalized initial slope of a superconductor–normal metal (SN) double layer is independent of almost all film parameters except the ratio of the density of states, $(d_s/T_s)|dT_c/dd_n|=\Gamma_{sn}(N_n/N_s)$. There are only very few experimental investigations of this initial slope and they consist of Pb/Nn double layers (Nn stands for a normal metal). Surprisingly the coefficient Γ_{sn} in these experiments is of the order or less than 2 while the (weak coupling) theory predicts a value of about 4.5. This discrepancy has not been recognized in the past. The origin of this discrepancy is not understood.

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I. INTRODUCTION

The transition temperature of a thin superconducting film in contact with a normal metal is reduced. This is known as the superconducting proximity effect (SPE). The double layer SN or a multilayer $(SN)_n$ can consist (i) of a superconductor S and normal conductor N or (ii) of two superconductors with different transition temperatures (the one with the lower T_c is generally denoted as N). Its systematic experimental investigation started in the 1960s by the Hilsch group in Goettingen[1,2] and stimulated a number of further experimental investigations.[3–6] For the dirty case (the mean free path of the conduction electrons is much smaller than the coherence length) Werthamer[7] derived a set of implicit equations for the transition temperature of double layers consisting of two superconductors. After some modification according to de Gennes' boundary condition[8] between the superconductors, the Werthamer theory described the experimental results for double layers of two superconductors quite well (see, for example, Refs. 5, 8, and 9). The Werthamer theory is restricted to a short mean free path (using the diffusion approximation) and uses what is now called the single mode approximation [the gap function is approximated by a $\cos(k_s z)$ dependence]. Theoretical results for the clean case where the mean free path l is larger than the BCS coherence length ξ_{BCS} are more difficult and the case where l, ξ_{BCS} and the film thicknesses are of the same order of magnitude are much more challenging.

In recent years the superconducting proximity effect has experienced a renewed interest. A large number of papers studied the SPE theoretically[10–22] and experimentally[23–30] particularly during the last ten years. The studies have been extended to double layers of a superconductor and a ferromagnet (SF).[31–33]

Recently our group revisited the superconducting proximity effect using it as an experimental tool.[29,28] One interesting piece of information the SPE provides is the transparency of the interface between the two metal films for the conduction electrons. The reduction of T_c in the superconducting component of the SN double layer depends on the rate at which electrons can cross the interface between the superconductor S and the normal metal N. This interface transparency is of interest in a number of other disciplines and applications in solid-state physics.

When our group tried to compare the experimental results for the transition temperature with theoretical predictions we found that only a few recent theoretical investigations calculated the transition temperature of SN double layers.[13,11,34] These papers considered the extreme cases, either the clean limit for an infinitely large mean free path[13] or the dirty limit[34] where the mean free path is much shorter than the BCS coherence length. Reference 34 considered superconductor-ferromagnet double layers in the "dirty limit." It includes the case of an SN double layer by setting the exchange energy in the ferromagnet equal to zero. A multimode expansion of the order parameter is used in the superconductor. This yields a complex set of equations which contain the transition temperature implicitly. Their single mode approximation is similar to Werthamer's result.

Since our experiments used films with short and large mean free paths the author preferred to develop a numerical procedure which is capable of calculating the transition temperature of arbitrary sequences of superconductors and normal conductors in a wide range of the mean free path. This calculation uses a simple interpretation of the gap equation which was stimulated by de Gennes' work.[8] Below I will sketch the (simple) numerical procedure. In Sec. II the theoretical background is reviewed and the numerical procedure is discussed in detail. In Sec. III some of the numerical results are presented. In the discussion of Sec. IV I will point out a discrepancy between all experiments I am aware of which study the change of T_c of a superconducting film when covered with a thin normal conducting film, i.e., the normalized intial slope $(d_s/T_s)(dT_c/dd_n)$, where d_s and T_s are the thickness and transition temperature of the superconductor

and dT_c/dd_n is the initial slope of the T_c reduction for zero thickness d_n of the normal conductor.

II. THEORETICAL BACKGROUND

A. Linear gap equation

The superconducting phase transition in zero magnetic field is generally of second order. Therefore, close to transition temperature T_c of the double layer, the gap function $\Delta(\mathbf{r})$, which is the order parameter of the phase transition, is small and only terms linear in the gap function contribute. This linear gap equation, first formulated by Gorkov,[35] was rewritten by de Gennes[8] as

$$\Delta(\mathbf{r}) = V(\mathbf{r}) \int d^3\mathbf{r}' \sum_{|\omega_n|<\Omega_D} H_{\omega_n}(\mathbf{r},\mathbf{r}')\Delta(\mathbf{r}')$$

$$H_{\omega_n}(\mathbf{r},\mathbf{r}') = k_B T G_{\omega_n}(\mathbf{r},\mathbf{r}')G^*_{\omega_n}(\mathbf{r},\mathbf{r}') \tag{1}$$

Here $\Delta(\mathbf{r})$ is the gap function at the position $\mathbf{r}$, $\omega_n=(2n+1)\pi k_B T/\hbar$ are the Matsubara frequencies, $V(\mathbf{r})$ is the effective electron-electron interaction at the position $\mathbf{r}$. The sum is limited to the range $|\omega_n|<\Omega_D$ where Ω_D is the Debye frequency. This corresponds to a sum over n from $-n_c$ to $+n_c$ where $n_c=\Theta_D/(2\pi T)=\Omega_D\tau_T$, where Θ_D and Ω_D are the Debye temperature and frequency and $\tau_T=\hbar/(2\pi k_B T)$. The function $H_{\omega_n}(\mathbf{r},\mathbf{r}')$ is the product of two Green functions $G_{\omega_n}(\mathbf{r},\mathbf{r}')$ and $G^*_{\omega_n}(\mathbf{r},\mathbf{r}')$ which represent a cooperon. Since the Green function $G_{\omega_n}(\mathbf{r},\mathbf{r}')$ represents the amplitude of an electron traveling (at finite temperature) from $\mathbf{r}'$ to $\mathbf{r}$ the product $G_{\omega_n}(\mathbf{r},\mathbf{r}')G^*_{\omega_n}(\mathbf{r},\mathbf{r}')$ describes the amplitude of a cooperon traveling from $\mathbf{r}'$ to $\mathbf{r}$. Since the two single-particle Green functions are conjugate complex to each other, the product of their amplitudes is proportional to the probability of a single electron to travel from $\mathbf{r}'$ to $\mathbf{r}$. If one interprets in Eq. (1) $G_{\omega_n}(\mathbf{r},\mathbf{r}')G^*_{\omega_n}(\mathbf{r},\mathbf{r}')$ as the propagation of single electrons then one has an equivalent problem and its solution is also the solution of the gap equation. In the following the solution of the equivalent problem will be pursued.

From the properties of the Green functions $G_{\omega_n}(\mathbf{r},\mathbf{r}')$ (see the Appendix, Sec. I) it follows that $H_{\omega_n}(\mathbf{r},\mathbf{r}')$ is the electron density if one injects electrons continuously with a rate N/τ_T at the point $\mathbf{r}'$, while their density decays along the path as $\exp(-2|\omega_n|s/v_F)$ where s is the distance traveled (not the distance from $\mathbf{r}'$) and N is the BCS density of states.

The right side of Eq. (1), $d^3\mathbf{r}'H_{\omega_n}(\mathbf{r},\mathbf{r}')\Delta(\mathbf{r}')$ (excluding $\Sigma_{n=-n_c}^{n_c}$, yields the density of electrons at the position $\mathbf{r}$ when one injects constantly $N\Delta(\mathbf{r}')d^3\mathbf{r}'dt'/\tau_T$ electrons in the incremental volume volume $d^3\mathbf{r}'$ at the position $\mathbf{r}'$ per time interval dt', which decay during their propagation with the decay rate of $2|\omega_n|$ $[\tau_T=\hbar/(2\pi k_B T)]$. $[N\Delta(\mathbf{r}')d^3\mathbf{r}'$ represents a (dimensionless) number of electrons and the rate of injected electrons per volume is $N\Delta(\mathbf{r}')/\tau_T]$. These electrons propagate with their Fermi velocity from $\mathbf{r}'$ to $\mathbf{r}$, either directly or diffusively. Their density decays along the path as $\exp(-|\omega_n|t'_\Delta)$ where t'_Δ is the time since the departure from $\mathbf{r}'$. At the position $\mathbf{r}$ the surviving density of all arriving electrons is integrated over $\int d^3\mathbf{r}'\int_{-\infty}^0 dt'$. When summed over ω_n and multiplied with the attractive electron interaction $V(\mathbf{r})$ one has to recover the original $\Delta(\mathbf{r})$.

For further treatment we define the propagation density $\rho(v_F;\mathbf{r},0;\mathbf{r}',t'<0)$. If an electron with Fermi velocity v_F is introduced at the time $t'<0$ at the position $\mathbf{r}'$ then $\rho(v_F;\mathbf{r},0;\mathbf{r}',t')$ describes the probability to find the electron at the time 0 at the position $\mathbf{r}$. With this definition we can express $H_{\omega_n}(\mathbf{r},\mathbf{r}')$,

$$H_{\omega_n}(\mathbf{r},\mathbf{r}') = N(\mathbf{r}')\int_{-\infty}^0 \rho(v_F;\mathbf{r},0;\mathbf{r}',t')\exp(-2|\omega_n||t'|)\frac{dt'}{\tau_T},$$

where $1/\tau_T=2\pi k_B T/\hbar$.

The sum over ω_n in Eq. (1) applies only to the exponential decay functions $\exp(-2|\omega_n||t'|)$ and yields the time function $\eta_T(t')$,

$$\eta_T(t') = \sum_{|\omega_n|<\Omega_D} \exp(-|\omega_n||t'|) = \frac{1-\exp[-2(\Omega_D\tau_T+1)|t'|/\tau_T]}{\sinh(|t'|/\tau_T)} \tag{2}$$

(Ω_D=Debye frequency). Then one can express the gap equation as

$$\Delta(\mathbf{r}) = V(\mathbf{r})\int d^3\mathbf{r}'N(\mathbf{r}')\int_{-\infty}^0 \frac{dt'}{\tau_T}\eta_T(t')\rho(v_F;\mathbf{r},0;\mathbf{r}',t')\Delta(\mathbf{r}'). \tag{3}$$

It is obvious that the superconducting properties of the system occur only in the effective interaction $V(\mathbf{r}')$ and the decay function $\eta_T(t')$. Of course, $\Delta(\mathbf{r})$ is the superconducting pair amplitude but in Eq. (3) it is just the eigenvector of the integral kernel. The self-consistency condition requires that this eigenvalue is equal to 1.

This interpretation of the gap equation yields a natural extension to a time-dependent pair amplitude or gap function. One obtains

$$\Delta(\mathbf{r},t) = V(\mathbf{r})\int d^3\mathbf{r}'N(\mathbf{r}') \times \int_{-\infty}^t \frac{dt'}{\tau_T}\eta_T(t')\rho(v_F;\mathbf{r},0;\mathbf{r}',t')\Delta(\mathbf{r}',t'). \tag{4}$$

From this equation one can derive a time-dependent Ginsburg-Landau equation.[36]

For a homogeneous superconductor one has a constant energy gap. In this case one can perform the integral over $d^3\mathbf{r}'$, using $\int d^3\mathbf{r}\rho(v_F;\mathbf{r},0;\mathbf{r}',t')=1$ and dividing by Δ,

$$1 = (VN)_s\int_{-\infty}^0 \frac{dt'}{\tau_T}\eta_T(t'), \tag{5}$$

which yields

$$\frac{1}{NV} = \sum_{n=0}^{n_c}\frac{1}{n+\frac{1}{2}}.$$

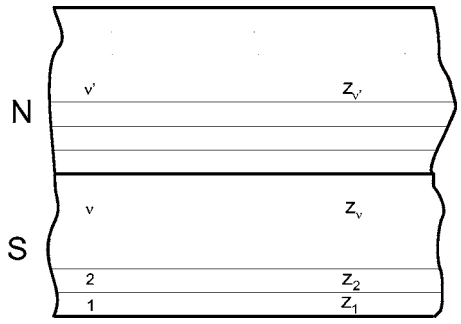

FIG. 1. A double layer of a superconductor S and a normal conductor N. The two films are split in thin parallel layers ν with the z position z_ν.

The condition (5) is used to determine the BCS coupling strength $(NV)_s$. It has the advantage that it is not restricted to integer values of $n_c=\Omega_D\tau_T$.

B. Gap equation for double and multilayers

Now we can apply the gap equation (3) to the proximity effect. The direction z is chosen perpendicular to the multilayer and the films are treated as homogeneous in the x-y plane. If there is no magnetic field then the gap depends only on the z direction. Therefore one can perform the integration over $\int dx'dy'\rho(v_F;\mathbf{r},0;\mathbf{r}',t')=\bar{\rho}(z,0;z',t')$.

Now the function $\bar{\rho}(z,0;z',t')$ describes the density at the time $t=0$ and the position z integrated over the x and y directions. For the numerical procedure it is more convenient to shift the time integration from the range $(-\infty,0)$ to the range $(0,\infty)$,

$$\Delta(z)=V(z)\int dz'N(z')\int_0^\infty \frac{dt}{\tau_T}\eta_T(t)\bar{\rho}(z,t;z',0)\Delta(z').$$

The multilayer will be divided into small sheets parallel to the film surfaces. The layers are indexed by ν and possess a thickness λ_ν (see Fig. 1).

In the present paper we determine the gap function $\Delta(z)$ at the transition temperature of an SN (superconductor–normal metal) double layer. We proceed with the following steps which are demonstrated by Fig. 2.

(a) The superconductor is divided into Z_s layers of thickness λ_s where $\lambda_s=d_s/Z_s$ (d_s is the thickness of the superconducting film).

(b) The BCS interaction V_s for the superconductor(s) is fitted, using the density of states N_s and the Debye temperature Θ_D (Appendix Sec. 2 a).

(c) The time interval $\tau_d=2\lambda_s/v_{F,s}$ is the time step of the numerical calculation ($v_{F,s}$ is the Fermi velocity of the superconductor) (Appendix Sec. 3).

(d) For the normal conductor (superconductor with lower T_c) the same time step is used by dividing its thickness in layers of thickness $\lambda_n=v_{F,n}\tau_d/2$.

(e) An initial gap function $\Delta_\nu=\Delta(z_\nu)$ is introduced. Each cell is occupied at the time $t'=0$ with $O_\nu(0)=N(z_\nu)\lambda_\nu\Delta(z_\nu)$ electrons. [$N(z_\nu)$ is the local density of states, i.e., equal to N_s in the superconductor] (Appendix Sec. 2 b).

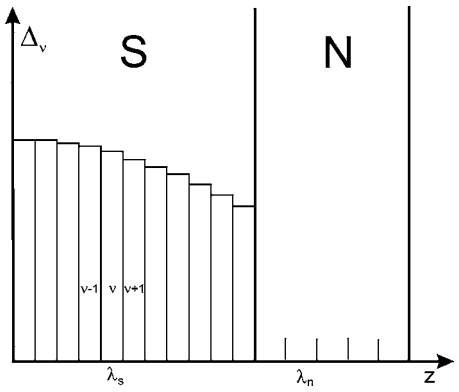

FIG. 2. The double layer is sliced into sheets of thickness λ_s,λ_n parallel to the film planes.

(f) A procedure for diffusive and ballistic propagation of electrons in the different films is derived (Appendix Sec. 3).

(g) The maximal transmission of an electron through the interface in each direction is calculated. It can be scaled down to include a barrier at the interface (Appendix Sec. 4).

(h) The density $O_\nu(m)$ is calculated in discrete steps for the time $t'=m\tau_d$ (Appendix Sec. 3).

(i) Due to thermal dephasing this density is, at each step, multiplied with the time factor $\eta_T(m\tau_d)$.

(j) The sum $\Sigma_m O_\nu(m)\eta_T(m\tau_d)$ is formed, multiplied with $(\tau_d/\tau_T)/\lambda_\nu$ and, in the superconductor(s), multiplied with V_s, the attractive electron-electron interaction.

(k) The resulting function $\tilde{\Delta}_\nu$ is the input Δ_ν for the next iteration.

(l) Since the eigenvalue has to be 1 the ratio $r=\Sigma_\nu\tilde{\Delta}(z_\nu)/\Sigma_\nu\Delta(z_\nu)$ is calculated. If $r>1(r<1)$ one increases (lowers) the temperature.

(m) The interation process is completed when initial and final Δ_ν agree with a relative accuracy of 10^{-5}. This is generally achieved after a few iterations.

All the steps of the numerical procedure are described in detail in the Appendix.

III. RESULTS

There are numerous parameters in the superconducting proximity effect: the coherence lengths $\xi_{s,n}=v_F\tau_T$ (for the superconductor this is the BCS ξ_{BCS} if one uses the transition temperature in $\tau_T=\hbar/(2\pi k_BT)$, the mean free path $l_{s,n}$, and the film thickness $d_{s,n}$ for each film. In addition one has the interface and the boundaries. Any barrier between the two metals will reduce the transfer through the interface. Furthermore, one can have additional scattering at the interface between the two films due to a mismatch of the two lattices. The two surfaces with the vacuum can reflect or scatter the incident electrons or anything in between. All these scattering parameters influence the propagation of the electrons and therefore the transition temperature of the double layer. In the numerical calculation all these parameters can be in-

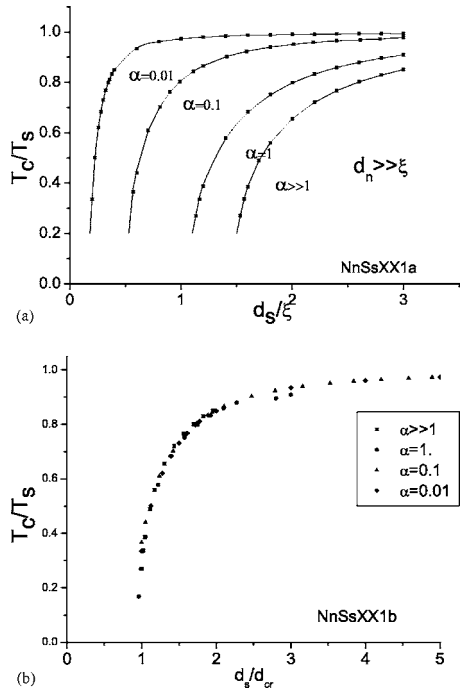

FIG. 3. (a) The reduced transition temperature T_c/T_s for an NS double layer where $d_n=\infty$, $l_n=\infty$ as a function of thickness d_s/ξ (ξ=BCS coherence of S). (a) For different mean free paths l_n of S, the parameter $\alpha=l_s/\xi$. (b) The same plot as (a) with the S thickness scaled with the critical thickness d_{cr}.

cluded if they are known or used as fit parameters.

A. Transition temperature

In the majority of experiments the onset of superconductivity is measured for a double layer of a thick normal conducting film which is covered with a superconducting film of increasing thickness. Therefore the first plotted numerical result represents a double layer of an infinitely thick normal conductor which is covered with a superconductor of increasing thickness. Among the large number of possible parameters the following choice is made: (i) the electronic properties $(N_{s,n}, v_{F,n})$ of the normal metal and the superconductor are identical, (ii) the mean free path of the normal conductor is infinite, (iii) the thickness of the normal conductor is infinite, (iv) the interface is perfectly transparent, (v) for the mean free path of the superconductor the following values are chosen: $l_s=\infty, \xi_0, \xi_0/10, \xi_0/100$. The results are shown in Fig. 3(a). The parameter α is defined as $\alpha=l_s/\xi_0$. The curves of the transition temperature versus thickness of the superconductor show the typical behavior; they approach T_s for large d_s and show a steep decline at a critical thickness d_{cr}. The value of the critical thickness decreases strongly with decreasing mean free path l_s of the superconductor. It might be surprising that even a mean free path $l_s=\xi_0$ shifts the T_c-d_s curve considerably to smaller thicknesses. For the smallest mean free path of $l_s=\xi/100$ the critical thickness is about $d_{cr}\approx 0.19\xi_0$. In Fig. 3(b) T_c is plotted versus the reduced thickness d_s/d_{cr}. The points lie almost on a universal curve, particularly those for smaller l_s.

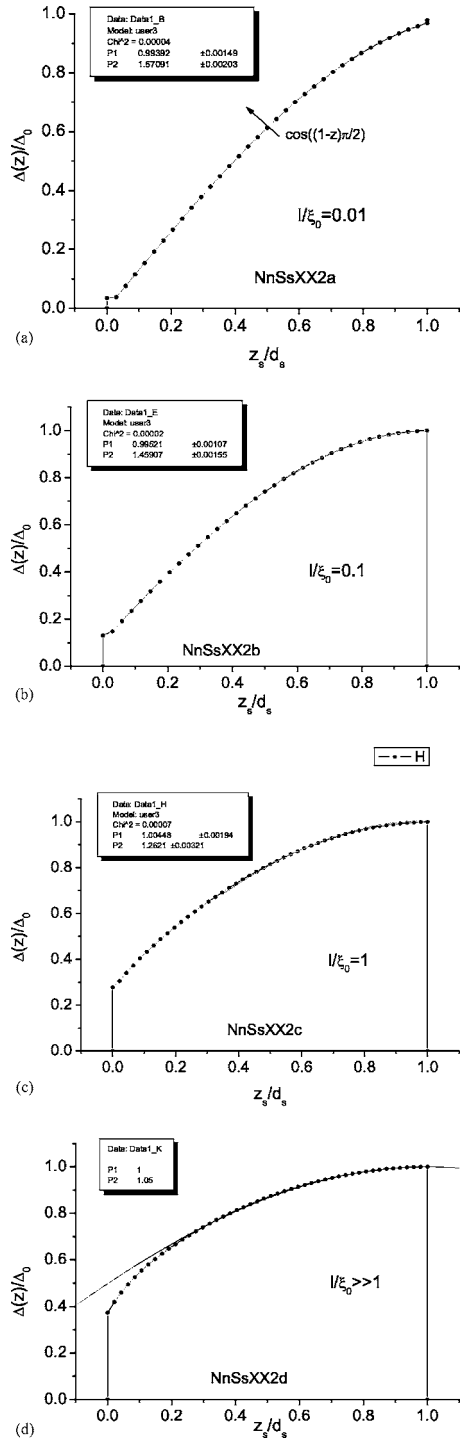

FIG. 4. (a)–(d) The gap function $\Delta(z)$ is plotted versus the position z/d_s in the superconductor for NS double layers. Each drawing corresponds to one of the curves in Fig. 3(a). d_s is close to the critical thickness d_{cr}. The ratio l_s/ξ_0 is noted in the figures.

B. Pair amplitude

In the next step the actual dependence of the gap function on position is of interest. In Figs. 4(a)–4(d) this gap function $\Delta(z')$ is plotted as a function of $z'=z/d_s$. We choose double layers where T_c lies in the steep decline of the T_c curves in Fig. 3 at about $T_c/T_s\approx 0.3$. Figure 4(a) shows $\Delta(z')/\Delta_0$ for

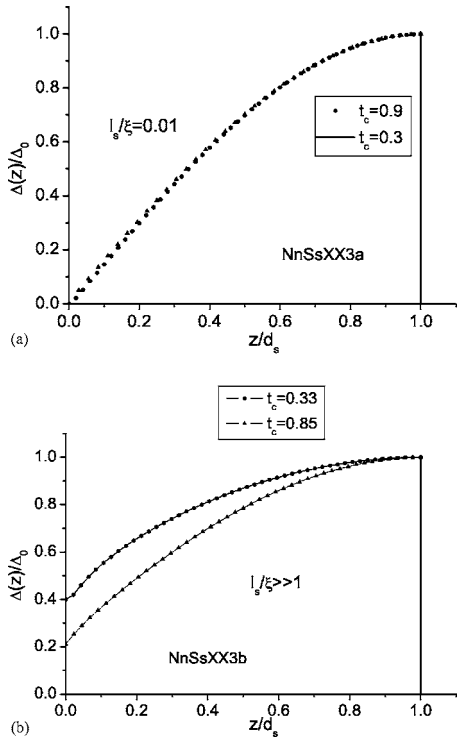

FIG. 5. (a) The gap function $\Delta(z)$ is plotted versus the position z/d_s for two NS double layers, each at two different d_s (resulting in different T_c of about 0.3 and $0.9T_s$). (a) Dirty limit $l_s/\xi=0.01$. (b) Clean limit $l_s=\infty$.

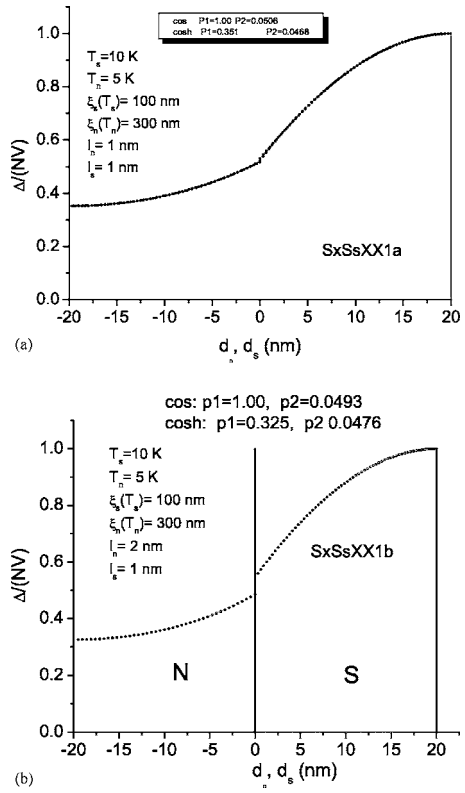

FIG. 6. (a),(b) The function $\Delta/(NV)$ for an S_1S_2 double layer, $T_{c1}=T_{s2}/2$ (details in text and figures). Both films are in the dirty limit. In (a) the transmission coefficient from S_2 to S_1 is $t=1.0$ while in (b) $t=0.8$.

the superconductor with $l_s/\xi_0=0.01$. [Since the amplitude of $\Delta(z')$ approaches zero at the transition temperature the value Δ_0 at the maximum is of no physical significance]. Since the gap function has a horizontal slope at the free surface a comparison with a cosine function $\cos[p(1-z')]$ is useful. The resulting fits are shown in Figs. 4(a)–4(d). Figure 4(a) for $l_s/\xi_0=0.01$ shows an almost perfect quarter of a cosine function with $p=1.57$ which is as close to $\pi/2$ as it can be. For $l_s/\xi_0=0.1$ the shape of the gap curve is still quite close to a cosine function but the factor has the value $p=1.46$. For $l_s/\xi_0=1$ the shape of the gap curve shows already clear deviations from a cosine curve and the coefficient is $p\approx 1.25$. Finally in the clean limit the gap function curves stronger for small z' than the cosine curve and the coefficient is $p\approx 1.05$ for the shown fit. This behavior is interesting because in a number of theoretical papers the gap function is expanded into a series (see, for example, Ref. 34 where a series consisting of $\cos[\Omega_0(d_s-z)/\xi_d]$ and $\cosh[(\Omega_m(z-d_s)/\xi_d)]$ is used, $\xi_d=\sqrt{l_s\xi}$ is the superconducting diffusion length, and Ω_0, Ω_m are coefficients defined in that work).

The simple form of the gap function in the case of $l_s/\xi_0=0.01$ makes it very obvious why the very disordered superconductors (often discriminatingly called dirty superconductors) are much easier to describe. This becomes still more obvious if one compares the shape of the gap function at different T_c/T_s values (which means, of course, using different thicknesses of the superconductor). In Fig. 5(a) the (normalized) gap functions for T_c/T_s values of about 0.3 and 0.9 are shown as a function of z/d_s. They lie perfectly on the same quarter of a cosine function. This is very different for the clean limit where the shape depends strongly on the temperature.

C. Dirty limit

Since in the dirty limit the gap function approached such a simple form for a superconductor in contact with an infinite clean normal metal it is worthwhile to check the situation when both metals are dirty. This is the case which most theoretical papers investigate.

In Fig. 6(a) $\Delta/(NV)$ is plotted for a double layer of two superconductors with different transition temperatures of $T_n=5$ K and $T_s=10$ K. In addition the density of states for superconductor N (with the lower transition temperature) is larger by a factor of 1.5 than for superconductor S. Therefore the superconducting coherence lengths $\xi_{0s}=\hbar v_{Fs}/(2\pi k_B T_s)=100$ nm and $\xi_{0n}=\hbar v_{Fn}/(2\pi k_B T_n)=300$ nm are different (the additional factor of 2 stems from the ratio of the transition temperatures). The difference in the density of states and the Fermi velocity of the two metals yields a ratio of the two transmission coefficients at the interface $T_{N\to S}/T_{S\to N}=0.444$.

The thickness of each film is $d_n=d_s=20$ nm. In Fig. 6(a) the mean free paths are chosen in both films to be $l_s=l_n=1$ nm. For the corresponding superconducting diffusion lengths ξ_{ds}, ξ_{dn} one finds $\xi_{ds}=\sqrt{\xi_{0s}l_s}=10$ nm and $\xi_{dn}=\sqrt{\xi_{0n}l_n}=17.3$ nm. According to de Gennes the function $\Delta/(NV)$ should be continuous at the interface. As can be easily recognized from the plot in Fig. 6(a) this condition is well ful-

filled. Werthamer[7] expressed the z dependence of the gap function $\Delta(z)$ in the two superconductors as

$$\cosh[k_n(d_n+z)] \quad \text{for } -d_n < z < 0,$$
$$\cos[k_s(d_s-z)] \quad \text{for } 0 < z < d_s.$$

Figure 6(a) shows a fit for $z<0$ to the function $a\cosh[k_n(d_n+z)]$ and for $z>0$ to the function $\cos[k_s(d_s-z)]$. The fitted curves lie within the trace of the points. The fitted values for the parameters are $k_s=0.0506\ \text{nm}^{-1}$, $k_n=0.0468\ \text{nm}^{-1}$, and $a=0.351$. This yields for the value of $\Delta/(NV)$ on the left and the right side of the interface: 0.516 and 0.530. The corresponding slopes on the left and right side of the interface are 4.29×10^{-2} and 1.77×10^{-2}. According to de Gennes the derivative $(D/V)d\Delta/dz$ should be continuous at the interface for the dirty limit. Using the input data of the two superconductors $D_{s,n}$ and $V_{s,n}$ one obtains for the ratio of the slopes 2.61. The simulated $\Delta(z)$ yields a slope ratio at the interface of 2.42. So the de Gennes condition is verified with an accuracy of about 10%.

In a second simulation the transmission through the interface is reduced by a factor 2. It is quite remarkable that this changes the transition temperature by just 0.1 K from $T_c=7.6$ K to 7.7 K. In Fig. 6(b) the function $\Delta/(NV)$ is plotted for the double layer as a function of z. One recognizes that now $\Delta/(NV)$ is no longer continuous at the interface. The functional form in N and S can still be well fitted by a hyperbolic cosine and a cosine function. (The fitted curves lie within the width of the numercal points.)

D. Initial slope

When one condenses the normal metal on top of the superconductor then the transition temperature of the double layer decreases. Here the focus is on the question of how the intial slope at $d_n=0$ depends on various parameters, such as the mean free path in the superconductor and the normal conductor and the transparency of the interface.

The dependence of the initial slope on the mean free path is shown in Figs. 7(a) and 7(b). In both figures the thickness of the superconductor is equal to the BCS coherence length ξ_0. The transition temperature T_c/T_s is plotted versus the thickness of the normal conductor. In Fig. 7(a) the mean free paths in both films are equal and vary between $l_s=l_n=\xi_0/10$, ξ_0, and $10^3\xi_0$. In Fig. 7(b) four different combinations of (l_s,l_n) are chosen. From the top to the bottom (l_s,l_n) is equal to $(\xi_0/100,\xi_0/100)$, $(\xi_0/100,10^3\xi_0)$, $(10^3\xi_0,\xi_0/100)$, and $(10^3\xi_0,10^3\xi_0)$. For all curves the initial slope is identical. (In all the numerical calculations which were discussed so far the two densities of states are assumed equal, $N_s=N_n$.)

In Fig. 8 the dependence of the initial slope on the thickness of the superconducting first layer is tested. The graph shows the dependence of T_c/T_s for a small range of the thickness d_n of the normal conductor to emphasize the initial range.

In Table I the normalized initial slope is collected. (The numerical points had to be fitted with a polynomial to extract the slope from the numerical results.) Up to a thickness of $d_s=\xi$ the S_{sn} is constant within about ±1%. For larger d_s it decreases slightly. But since the value of dT_c/dd_n becomes quite small this thickness range is not well suited for the experimental determination of the slope. The main result is that the normalized initial slope is essentially independent of the thickness of the superconductor.

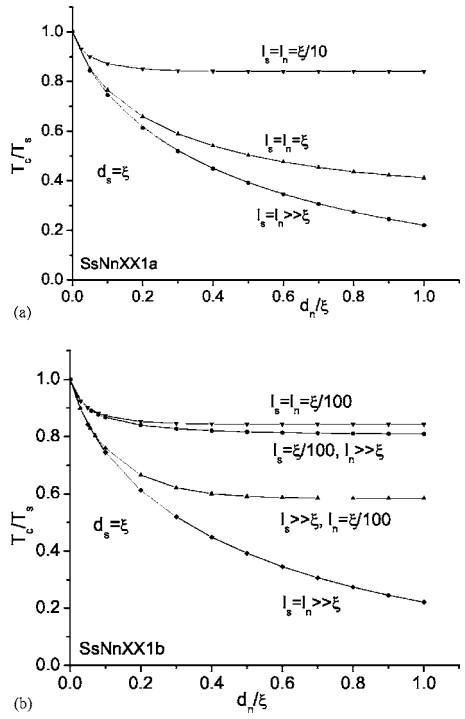

FIG. 7. (a),(b) T_c for an SN double layers as a function of d_n/ξ. The thickness of the superconductor is equal to the BCS coherence length ξ ($N_s=N_n$). (a) The mean free paths $l_s=l_n$ are parameters. (b) Different combinations of the mean free paths are used as parameters.

Finally, Fig. 9 shows that the initial slope does not depend on the transmission through the interface. In this calculation the density of states in both metals is chosen to be equal, $N_s=N_n$, and the mean free paths are $l_s=l_n=\xi/10$. The transmission coefficient is varied between 0.2 and 1.0. The resulting T_c-d_n curves show the same initial slope.

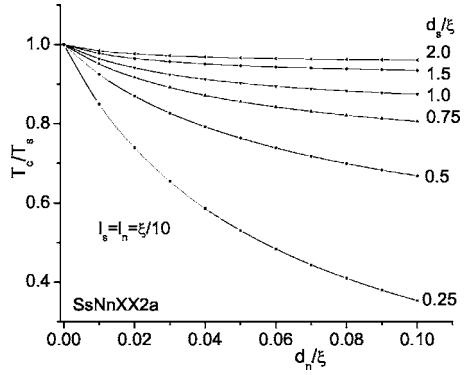

FIG. 8. T_c for an SN double layers as a function of d_n/ξ. The parameter d_s is the thickness of the superconductor ($N_s=N_n$, $l_s=l_n=\xi/10$).

TABLE I. Normalized initial slope for different thicknesses d_s of the superconductor.

$\mathbf{d}_s$ / ξ	$\frac{d_s}{T_s}\frac{dT_c}{dd_n}$
0.25	4.35
0.5	4.34
0.75	4.31
1.0	4.26
1.5	4.13
2.0	4.02

IV. DISCUSSION

The intention of this paper was to develop a convenient numerical procedure for the superconducting proximity effect so that graduate students could instantly compare their experimental results with the theory. One important result of this investigation is the fact that the (normalized) initial slope of an SN double layer is independent of most film parameters except the density of states ratio and the effective BCS interaction,

$$S_{sn} = \frac{d_s}{T_{c0}} \left| \frac{dT_c}{dd_n} \right| = \Gamma_{sn} \frac{N_n}{N_s}. \tag{6}$$

In the case of a weak-coupling superconductor Γ_{sn} is given by the Cooper limit, i.e., $\Gamma_{sn}=1/(NV)_s$, the inverse of the BCS interaction. If the Debye temperature is not several orders of magnitude larger than T_s then one has to determine Γ_{sn} in Eq. (6) numerically. Using $T_s=7.2$ K for Pb then the prefactor is about 4.5. (This is actually the value for a wide range of the Debye temperature between 100 and 300 K.)

Recently our group investigated the proximity effect between the superconductor Pb and several alkali metals.[29] It was a great surprise that the experimental initial slope of these SN double layers could not be explained with the density of states from the literature. Instead the experimental $(d_s/T_s)(dT_c/dT)$ was too small by more than a factor of 2. Table II gives some of the data of the SN double layers. (The thickness of the normal metal was the smallest thickness in a full curve.)

We searched the literature for other measurements of SN double layers and their initial slope. It turned out that there are very few measurements of SN layers. (At this stage we excluded transition metals because they show two-band superconductivity and it is not obvious how the different superconducting bands couple to the normal conductor.) There were essentially two groups of publications which had measured SN double layers which contained information about the initial slope. The first group of papers was by Hilsch and co-workers[1,2] who investigated quench condensed PbCu layers. The second work was by Minnigerode[6] who also investigated PbCu layers but prepared the layers at room temperature. Particularly, the second paper gives detailed tables of thicknesses of the two components and transition temperatures. The results of these papers are collected in Table III. The first column gives the components of the SN double layer, the second and third columns the thicknesses of the superconductor and normal metal. The fourth column contains the experimental normalized slope and the fifth gives the ratio N_n/N_s. The last column contains the ratio of the experimental (normalized) slope to the density-of-states ratio. Again the experimental normalized slopes are much smaller than the theory predicts.

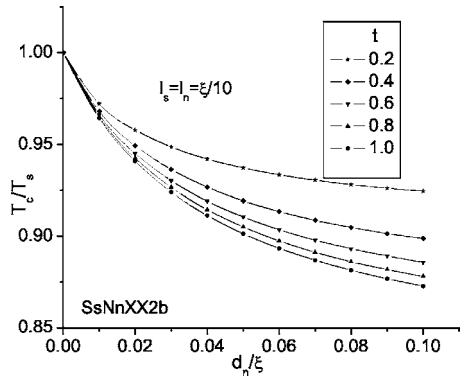

FIG. 9. T_c for SN double layer as a function of d_n/ξ. The parameter t is the transparency of the interface ($N_s=N_n$, $d_s=\xi$, $l_s=l_n=\xi/10$).

Ashida *et al.*[13] have calculated the transition temperature of SN double and multilayers in the clean limit. Propagation through the interface is described by the coefficient of reflection R from the normal conductor side. For thin normal conductor thickness dn they found some analytic expressions for T_c. In the thin-film limit they obtained a divergence of the initial slope $dT_c/d(d_n)$, and their thin-film limit differs from the Cooper result. Ashida *et al.* do not interpret or explain their result. The underlying equations are complex and interwoven, and it is difficult to uncover the underlying physics and the influence of the simplifications. One has to be very careful with the limiting cases; this can be seen from Ashida *et al.*'s expression for T_c in the limit of R close to 1. Ashida *et al.* obtained in this limit that T_c does not depend on d_n,

TABLE II. The normalized initial slope of SN double layers with Pb as superconductor and different normal metals. Columns 2–6 give the thickness of the superconductor, the normal conductor, the experimental initial slope, the ratio of the density of states, and the ratio $\mathbf{S}_{sn}|_{\mathrm{exp}}/(N_n/N_s)=\Gamma_{sn}$.

Metals	$\mathbf{d}_s$ (nm)	$\mathbf{d}_n$ (nm)	$\mathbf{S}_{sn}\|_{\mathrm{expt.}}$	$\mathbf{N_n/N_s}$	Ratio Γ_{sn}
Pb/K	12.9	2.04	0.423	0.223	1.90
Pb/Na	13.9	2.18	0.546	0.300	1.82
Pb/Ag	17.9	2.10	0.625	0.335	1.86

TABLE III. The normalized initial slope of PbCu double layers. Columns 2–6 give the thickness of the superconductor, the normal conductor, the experimental initial slope, the ratio of the density of states, and the ratio $\mathbf{S}_{sn}|_{\mathrm{exp}}/(N_n/N_s)$.

Metals	$\mathbf{d}_s$ (nm)	$\mathbf{d}_n$ (nm)	$\mathbf{S}_{sn}\|_{\mathrm{expt.}}$	$\mathbf{N_n/N_s}$	Ratio
Pb/Cu[a]	10.0	10.0	0.542	0.448	1.21
Pb/Cu[a]	15.0	10.0	0.500	0.448	1.12
Pb/Cu[b]	22.9	3.30	1.110	0.448	2.48
Pb/Cu[b]	24.3	3.90	0.935	0.448	2.08
Pb/Cu[b]	32.9	4.10	0.883	0.448	1.97
Pb/Cu[b]	27.2	13.10	0.683	0.448	(1.52)
Pb/Cu[b]	28,0	26.40	0.842	0.448	(1.88)
Pb/Cu[b]	33.4	17.70	0.608	0.448	(1.36)

[a]Data from Ref. 1 are quench condensed.

[b]Data from Ref. 6 are condensed at room temperature.

corresponding to a vanishing initial slope $dT_c/d(d_n)$. We pointed out in a recent paper that even for R close to 1 one obtains for sufficiently small dn a large interface crossing from the normal metal because the attempt rate is roughly $v_F/4d_n$, yielding again the Cooper limit.

It is rather amazing that this fundamental discrepancy between experiment and theory has not been realized. What is the reason for this disagreement? One possibility is that the use of the weak-coupling theory of superconductivity is not adequate for the double layers containing the superconductor Pb. The superconductor Pb is a convenient component of an SN double layer because it has a rather large T_c and is easy to condense. However, Pb is a strong-coupling superconductor. The Fermi sphere of free electrons is modified by the electron-phonon interaction.

An obvious proposal would be to solve the superconducting proximity effect for strong-coupling superconductors. This means to develop and solve a series of equations for the energy and position dependent gap function $\Delta(\mathbf{r},\omega_l)$ which has Eq. (4) as limiting case. This is a very demanding job which goes beyond the scope of the present paper and has to be left for future investigations. Instead I considered the analogy to the Cooper limit for strong superconductors. This thin-film limit, strong-coupling treatment yields for the initial slope

$$\frac{d_s}{T_s}\left|\frac{dT_c}{dd_n}\right| \approx 1.7\frac{N_n}{N_s}.$$

The prefactor of 1.7 appears to be a very satisfactory result. However, in the strong-coupling treatment one uses the bare density of states and treats the enhancement separately while in the comparison with the experiment one uses the dressed density of states. This introduces an additional factor of $(1+\lambda)\approx 1.8$ so that the initial slope becomes about $3N_n^*/N_s^*$, which is similar to the weak-coupling calculation. This is in one way rather satisfying, because it means that a renormalized treatment yields in first approximation the same as the strong-coupling treatment. However, it does not solve the puzzling difference between experiment and theory.

V. CONCLUSION

This paper derives the transition temperature of a double or multilayer of a superconductor and a normal conductor numerically. The equivalence in the propagation of the superconducting pair amplitude and a single electron in Gorkov's linear gap equation is used. The single electrons act as messengers who carry the information about the superconducting gap $[N_s\Delta(\mathbf{r}')/\tau_T]$ from one position-time $(\mathbf{r}',t'<0)$ to another position-time $(\mathbf{r},t=0)$. This message which decays thermally with time as $\eta_T(t)=\Sigma_{|\omega_n|<\Omega_D}\exp(-2|\omega_n||t'|)$ is integrated at $(\mathbf{r},t=0)$ over all start position times $(\mathbf{r}',t')$ and, after multiplication with the BCS interaction V_s, yields the new gap function $\Delta(\mathbf{r})$. At the transition temperature the procedure has to be self-consistent, i.e., the initial and final gap function have to be identical. The propagation of the single electrons is then quasi-classically simulated. The framework of the calculation is the weak-coupling theory of superconductivity.

This numerical procedure to calculate the transition temperature of double or multilayers consisting of thin films of superconductors and normal conductors is very flexible. The following parameters can be taken from the experiment or fitted during the calculation:

(a) mean free path of the different metals

(b) transmission through the interface

(c) ratio of specular reflection to diffusive scattering at the surfaces

(d) fraction of diffusive scattering at the interface.

Furthermore, it is possible

(a) to vary the mean free path along the thickness of the films

(b) to vary the BCS interaction NV at the interface.

The few examples which were presented in Sec. III demonstrate why the dirty case is so much simpler than the clean one. They also show that even for small thicknesses of the normal metal the gap parameter in the superconductor is not quite constant. Still the initial slope for an SN double layer follows the prediction of the Cooper limit.

An important outcome of the numerical simulation is the result that the normalized initial slope of an SN double layer

as a function of d_n at $d_n=0$ does not depend on

(a) the mean free path of the two metals
(b) the thickness of the superconductor
(c) a (not too large) barrier between the two metals.

This slope is essentially given by

$$\frac{d_s}{T_{c0}}\left|\frac{dT_c}{dd_n}\right| = \Gamma_{sn}\frac{N_n}{N_s}.$$

For the extreme weak-coupling superconductor the value of Γ_{sn} is $1/(NV)_s$. If one applies the numeric procedure to double layers with Pb as the superconducting component then one obtains $\Gamma_{sn}\approx 4.6$. This is in strong disagreement with the results of the few experiments which allow the evaluation of the initial slope. Their values for Γ_{sn} lie in the range of 1.5–2.0.

APPENDIX

1. Kernel in the clean limit

In the clean limit the thermal Green function has the form

$$G_\omega(\mathbf{r},\mathbf{r}') = -\frac{m}{2\pi\hbar^2|\mathbf{r}-\mathbf{r}'|}\exp\left(ik_F|\mathbf{r}-\mathbf{r}'|\frac{\omega}{|\omega|}-\frac{|\omega|}{v_F}|\mathbf{r}-\mathbf{r}'|\right)$$

that yields

$$H_\omega(\mathbf{r},\mathbf{r}') = k_BTG_\omega(\mathbf{r},\mathbf{r}')G^*_\omega(\mathbf{r},\mathbf{r}')$$

or

$$H_\omega(R) = \frac{2\pi k_BT}{\hbar v_F}N\frac{1}{4\pi R^2}\exp\left(-\frac{2|\omega|}{v_F}R\right)$$

since $H_\omega(\mathbf{r},\mathbf{r}')$ depends only $R=|\mathbf{r}-\mathbf{r}'|$ [using the BCS-density of state $N=m^2v_F/(2\pi^2\hbar^3)$].

Without the damping the number of electrons between the radius R and $R+dR$ is

$$\frac{2\pi k_BT}{\hbar v_F}NdR = \frac{2\pi k_BT}{\hbar}Ndt$$

using $dR=v_Fdt'$. This means that $H_\omega(\mathbf{r},\mathbf{r}')\Delta(\mathbf{r}')d^3\mathbf{r}'$ corresponds to an injection of

$$dZ = \frac{2\pi k_BT}{\hbar}N\Delta(\mathbf{r}')d^3\mathbf{r}'dt$$

electrons in the volume $d^3\mathbf{r}'$ during the time dt' at the position $\mathbf{r}'$. dZ is indeed a (dimensionless) number. The exponential decay $\exp(-2|\omega|R/v_F)$ corresponds to a decay with time since $R=v_Ft$:

$$\exp(-2|\omega|R/v_F) = \exp(-2|\omega|t).$$

The density of an electron at the position $\mathbf{r}$ and the time $t=0$ that was injected at $(\mathbf{r}',t'<0)$ and propagates with Fermi velocity v_F can be described by the propagation density $\rho(v_F;\mathbf{r},0;\mathbf{r}',t')$. Therefore $H_\omega(\mathbf{r},\mathbf{r}')$ can be written as

$$H_\omega(\mathbf{r},\mathbf{r}') = \frac{2\pi k_BT}{\hbar}N(\mathbf{r}')\int_{-\infty}^{0}dt'\rho(v_F;\mathbf{r},0;\mathbf{r}',t')\times\exp(-2|\omega||t'|).$$

This yields the gap equation using $\eta_T(t')$ from Eq. (2),

$$\Delta(\mathbf{r}) = V(\mathbf{r})\int d^3\mathbf{r}'N(\mathbf{r}')\int_{-\infty}^{0}\frac{dt'}{\tau_T}\rho(v_F;\mathbf{r},0;\mathbf{r}',t')\eta_T(t')\Delta(\mathbf{r}').$$

This result is not restricted to the clean case but applies to the arbitrary mean free path.

2. Numerical procedure

As shown in Fig. 2 the metal films are divided in sheets of thickness λ_ν. Furthermore, the time development is performed in diffusion steps of $\tau_d=2\lambda_s/v_{Fs}$, $t'=m\tau_d$. Then the self-consistent gap equation takes the form

$$\Delta(z_\nu) = \frac{V(z_\nu)}{\lambda_\nu}\sum_{\nu'}\lambda_{\nu'}N(z_{\nu'})\times\sum_{m=0}^{\infty}\frac{\tau_d}{\tau_T}\eta_T(m\tau_d)\bar{\rho}(z_\nu,m\tau_d;z_{\nu'},0)\Delta(z_{\nu'}).$$

(For the zero term in the time summation only half the value is taken.) In the following we denote $\Delta(z_\nu),V(z_\nu),N(z_\nu)$ as Δ_ν,V_ν,N_ν.

a. Value of the BCS interaction $(NV)_s$

For the superconductor with the transition temperature T_s, the density of states N_s, and the Debye temperature Θ_s the implicit equation

$$\frac{1}{(NV)_s} = \int_0^\infty\frac{dt}{\tau_T}\eta_{T_s}(t/\tau_{T_s})$$

is used.

b. Initial conditions

At the time $t=0$ a simple gap function Δ_ν in the superconducting film(s) is chosen, for example, $\Delta_{\nu'}=k_BT_s$ for the superconducting film(s). At the time $t=0$ or $m=0$ we define an occupation $O_{\nu'}(m=0)$ of the different cells,

$$O_\nu(0) = \Delta_\nu\lambda_\nu N_\nu.$$

This occupation is equally divided in left and right moving electrons $\overleftarrow{O}_\nu(0)$ and $\overrightarrow{O}_\nu(0)$ with $\overleftarrow{O}_\nu(0)=\overrightarrow{O}_\nu(0)=O_\nu(0)/2$. In the following subsections the recipe is given for how to calculate from the occupation $\overleftarrow{O}_\nu(m),\overrightarrow{O}_\nu(m)$ at the time $t=m\tau_d$ the occupation $\overleftarrow{O}_\nu(m+1),\overrightarrow{O}_\nu(m+1)$. The total occupation is $O_\nu(m)=\overleftarrow{O}_\nu(m)+\overrightarrow{O}_\nu(m)$. With this time developing occupation the new gap function becomes

$$\tilde{\Delta_\nu} = \frac{V_\nu}{\lambda_\nu}\frac{\tau_d}{\tau_T}\sum_{m=0}^{\infty}\eta_T(m\tau_d)O_\nu(m).$$

This iterated gap function has two defects: (i) its shape generally does not agree with the original gap function Δ_ν, and

(ii) the ratio of the average amplitudes $r=\langle\tilde{\Delta}_\nu\rangle/\langle\Delta_\nu\rangle$ will not be 1. By determining numerically dr/dT from two iterations with the same initial gap function and two temperatures T and $T+T_\Delta$ the temperature is adjusted, using Newton's extrapolation method. After a few iterations $\langle\tilde{\Delta}_\nu\rangle$ becomes sufficiently close to $\langle\Delta_\nu\rangle$ and the adjusted temperature is the transition temperature of the multilayer. The iteration is completed when

$$\frac{\sqrt{\frac{1}{Z_s}\sum_\nu(\tilde{\Delta}_\nu-\Delta_\nu)^2}}{\frac{1}{Z_s}\sum_\nu\Delta_\nu}<10^{-5}.$$

3. Diffusive and ballistic propagation

The important task is to devise a simple fast procedure that describes the ballistic propagation of the electrons for distances shorter than the mean free path l and the diffusive propagation for distances larger than l. It helps considerably that only the propagation in the z direction has to be modeled properly (as long as no magnetic field perpendicular to the film is applied). We consider the electrons in a thin layer of thickness dz in the interval $(z,z+dz)$. Half of the electrons have a positive z component $v_z=v_F\cos\theta$ of the velocity. As long as they are not scattered their average velocity in the z direction is

$$\langle v_z\rangle=\frac{\int_0^{\pi/2}2\pi\sin\theta v_F\cos\theta d\theta}{\int_0^{\pi/2}2\pi\sin\theta d\theta}=\frac{1}{2}v_F.$$

We take this as the minimum requirement for the ballistic simulation.

The simulation of the diffusion in the z direction is rather straightforward. At the time $t=0$ we have the initial occupation $O_\nu(0)$.

Let us first consider the diffusion in one dimension. Here the electrons have either the velocity $+v_F$ or $-v_F$. The size of the cells is λ and an electron needs the time $\varepsilon_0=\lambda/v_F$ to cross a cell. We divide the initial occupation $O_\nu(0)$ into $\overleftarrow{O_\nu}(0)=\overrightarrow{O_\nu}(0)=O_\nu(0)/2$ for the left- and right-moving electrons. When the electrons reach the boundary of the cell they will be partially transmitted through the boundary with the probability p and partially reflected with the probability $(1-p)$. This yields the rule of how one obtains from the occupations at the time $t=m\varepsilon_0$ the occupation at the next time step $t=(m+1)\varepsilon_0$,

$$\overrightarrow{O_\nu}(m+1)=p\overrightarrow{O_{\nu-1}}(m)+(1-p)\overleftarrow{O_\nu}(m),$$

$$\overleftarrow{O_\nu}(m+1)=p\overleftarrow{O_{\nu+1}}(m)+(1-p)\overrightarrow{O_\nu}(m).$$

This yields a one-dimensional diffusion with the diffusion constant $D=\frac{1}{2}[p/(1-p)](\lambda^2/\varepsilon_0)$.

Ballistic propagation requires setting p almost equal to 1. In this case almost all the $\overrightarrow{O_\nu}(m)$ electrons move from cell ν to cell $(\nu+1)$ during the time ε_0. This means that they propagate the average distance $\lambda=v_F\varepsilon_0$ during the time ε_0. Therefore this model does not fulfill the basic requirement for ballistic propagation in three dimensions that $\langle v_z\rangle=\frac{1}{2}v_F$.

A three-dimensional diffusion can be obtained by a sequential propagation in the x, y, and z directions, each for a time of ε_0 with the velocity v_F. This yields a diffusion constant $D=\frac{1}{2}[p/(1-p)](\lambda^2/3\varepsilon_0)$ and triples the average time for the diffusion in the z direction. Since the electrons propagate only during every third of the interval $3\varepsilon_0$ in the z direction they propagate the distance λ during the time $3\varepsilon_0$, i.e., their average velocity in the z direction is only $\langle v_z\rangle=v_F/3$.

We can simulate the average diffusive and ballistic propagation of the electrons in the z direction by propagating every other time interval ε_0 in the z direction. Then the time step is $\tau_d=2\varepsilon_0$. In this case the diffusion constant is $D=\frac{1}{2}[p/(1-p)](\lambda^2/\tau_d)$ and the ballistic propagation yields $\langle v_z\rangle=v_F/2$ as required.

It should be mentioned that it is essential that the electron density is divided into (at least) two components, one for motion in the $+z$ and the other for the $-z$ direction. A single density component with hopping to neighbor places yields only small diffusion constants of $D=(p/2)(\lambda^2/\varepsilon_0)$ and cannot describe the ballistic propagation at all.

For the normal conductor the same time element τ_d is used to simulate the propagation. The thickness d_n is divided in cells (or layers) of thickness $\lambda_n=v_{F,n}\varepsilon_0=v_{F,n}\tau_d/2$. This synchronizes the diffusion in the whole double layer.

The transparency p of the cell walls is obtained from the experimental conductivity σ of the films, where $\sigma_m=2e^2N_mD_m$ or

$$D_m=\frac{\sigma_m}{2e^2N_m},\quad p_m=\frac{D_m}{\left(\frac{1}{2}\frac{\lambda_m^2}{2\varepsilon_0}+D_m\right)},$$

where m stands for s or n.

4. Interface between two films

The transmission of electrons through an interface between two metals (which we denote with S and N) is only in exceptional cases equal to 1. If, for example, the Fermi wave number $k_{F,s}$ is larger than $k_{F,n}$ then any electron in S whose component k_ρ parallel to the surface is larger than $k_{F,n}$ cannot cross the interface because afterwards it would have an energy of at least $(\hbar k_\rho)^2/2m$ which is larger than the Fermi energy $E_{F,n}=(\hbar k_{F,n})^2/2m$ in the normal conductor. An electron in N with Fermi energy would not violate the conservation of energy when crossing the interface. However, a plane wave which crosses a step in the potential energy is partially reflected. Therefore the transition probability is less than 1 for any electron. If one averages the transition probability of all these electrons (to cross the interface from N to S) one finds

$$T_{N\to S} = f\left(\frac{E_{F,n}}{E_{F,s}} - 1\right), \quad \text{where}$$

$$f(x) = \frac{4}{15}\frac{(\sqrt{(x+1)})^3(x+6) - (\sqrt{x})^5 - 10x - 6}{x^2}.$$

For small x the asymptotic expansion is $f(x) \simeq \left(1 - \frac{4}{15}\sqrt{x}\right)$.

The detailed balance requires that in equilibrium the number of electrons which cross from S to N is equal to the number of electrons which cross from N to S. Let us assume that the electron distribution is in equilibrium and we consider an interface S/N. $O_s(m)$ and $O_n(m)$ are the occupations in the cells on the left and right side of the interface. The transmission coefficients are by T_{sn} and T_{ns}. Then the occupation at the time $(m+1)\tau_d$ is

$$\overleftarrow{O_s}(m+1) = T_{ns}\overleftarrow{O_n}(m) + (1 - T_{sn})\overrightarrow{O_s}(m),$$

$$\overrightarrow{O_n}(m+1) = T_{sn}\overrightarrow{O_s}(m) + (1 - T_{ns})\overleftarrow{O_n}(m).$$

In equilibrium one has $\overleftarrow{O_{s,n}} = \overrightarrow{O_{s,n}} = \frac{1}{2}O_{s,n}$ and $O_{s,n}(m+1) = O_{s,n}(m)$. This yields

$$T_{ns}O_n(m) = T_{sn}O_s(m).$$

Since $O_{s,n} = \lambda_{s,n}N_{s,n}$ one obtains finally

$$\frac{T_{sn}}{T_{ns}} = \frac{\lambda_n N_n}{\lambda_s N_s}.$$

If one considers real metals a considerably more difficult situation arises when the superconductor has a mass enhancement of the density of states (as most superconductors have, in particular the strong-coupling ones). However, independent of how complicated the individual transmission probabilities are, the detailed balance will always apply. In our simulation we use $T_{ns} \leqslant 1$ as a fit parameter and calculate T_{sn} using the detailed balance.

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