Quantitative Simulation of the Superconducting Proximity Effect

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Abstract

A numerical method is developed to calculate the transition temperature of double or multi-layers consisting of films of super- 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 $\lambda$ in the vicinity of the interface. The numerical results show that the normalized initial slope of an SN double layer is independent of almost all film parameters except the ratio of the density of states, $(d_s/T_s)|d\Gamma_s/dd_n| = \Gamma_{sn} (N_n/N_s)$. 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 $\Gamma_{sn}$ 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 author suggests that it is due to strong coupling behavior of Pb in the double layers. The strong coupling gap equation is evaluated in the thin film limit and yields the value of 1.6 for $\Gamma_{sn}$. This agrees much better with the few experimental results that are available.

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1 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 multi layer (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 1960’s by the Hilsch group in Goettingen [1], [2] and stimulated a number of further experimental investigations [3], [4], [5], [6]. For the dirty case (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 Wertheimer theory described the experimental results for double layers of two superconductors quite well (see for example [5], [8], [9]). The Wertheimer theory is restricted to 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 $\xi_{BCS}$ are more difficult and the case where $l, \xi_{BCS}$ 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], [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21], [22], [23] and experimentally [24], [25], [26], [27], [17], [28], [20], [29], [30], [31], [32] particularly during the last 10 years. The studies have been extended to double layers of a superconductor and a ferromagnet (SF) [33], [34], [35].

Recently our group revisited the superconducting proximity effect using it as an experimental tool [31], [30]. One interesting 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 S and 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 [14], [11], [36]. These papers considered the extreme cases, either the clean limit for infinitely large mean free path [14] or the dirty limit [36] where the mean free path is much shorter than the BCS coherence length. Reference [36] 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 multi-mode 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 Wertheimer'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 deGennes work [8]. Below I will sketch the (simple) numerical procedure. In chapter II the theoretical background is reviewed and the numerical procedure discussed in detail. In chapter III some of the numerical results are presented. In the discussion of chapter 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 initial slope $\frac{d_s}{T_s} \frac{dT_c}{dd_n}$, where $d_s$ and $T_s$ are the thickness and transition temperature of the superconductor and $\frac{dT_c}{dd_n}$ is the initial slope of the $T_c$-reduction for zero thickness $d_n$ of the normal conductor.
2 Theoretical Background

2.1 The 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 $\Delta (r)$, 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 [37] was rewritten by deGennes [8] as

$$\Delta (r) = V (r) \int d^3r' \sum_{|\omega_n|<\Omega_D} H_{\omega_n} (r, r') \Delta (r') \quad (1)$$

Here $\Delta (r)$ is the gap function at the position $r$, $\omega_n = (2n+1)\pi k_B T / \hbar$ are the Matsubara frequencies, $V (r)$ is the effective electron-electron interaction at the position $r$. The sum is limited to the range $|\omega_n| < \Omega_D$ where $\Omega_D$ is the Debye temperature. 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 $\Theta_D$ and $\Omega_D$ are the Debye temperature and frequency and $\tau_T = \hbar / (2\pi k_B T)$. The function $H_{\omega_n} (r, r')$ is the product of two Green functions $G_{\omega_n} (r, r')$ and $G^*_{\omega_n} (r, r')$ which represent a Cooperon. Since the Green function $G_{\omega_n} (r, r')$ represents the amplitude of an electron traveling (at finite temperature) from $r'$ to $r$ the product $G_{\omega_n} (r, r') G^*_{\omega_n} (r, r')$ describes the amplitude of a Cooperon traveling from $r'$ to $r$. 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 $r'$ to $r$. If one interprets in equation (1) $G_{\omega_n} (r, r') G^*_{\omega_n} (r, r')$ 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 persued.

From the properties of the Green functions $G_{\omega_n} (r, r')$ (see appendix 6.1) it follows that $H_{\omega_n} (r, r')$ is the electron density if one injects continuously electrons with a rate $N/\tau_T$ at the point $r'$, 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 $r'$) and $N$ is the BCS density of states.

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

For further treatment we define the propagation density $\rho (v_F; r, 0; r', t' < 0)$.

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

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

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

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

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

($\Omega_D =$Debye frequency). Then one can express the gap equation as

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

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

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

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

From this equation one can derive a time dependent Ginsburg-Landau equation [3].

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

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

which yields

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

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 $n_c = \Omega_D \tau_T$. 

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2.2 The gap equation for double and multi-layers

Now we can apply the gap equation \( \mathcal{M} \) to the proximity effect. The direction \( z \) is chosen perpendicular to the multi-layer 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 \( \int dx'dy' \rho (v_F; r, 0; r', t') = \overline{\rho} (z; 0; z', t') \).

Now the function \( \overline{\rho} (z; 0; z', t') \) 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 \((0, \infty)\).

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

The multi-layer will be divided into small sheets parallel to the film surfaces. The layers are indexed by \( \nu \) and possess a thickness \( \lambda_\nu \).

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.

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

- The BCS interaction $V_s$ for the superconductor(s) is fitted, using the density of states $N_s$ and the Debye temperature $\Theta_D$ (appendix 6.2.1).

- 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 6.3).

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

- An initial gap function $\Delta_{\nu} = \Delta (z_{\nu})$ is introduced. Each cell is occupied at the time $t' = 0$ with $O_{\nu}(0) = N (z_{\nu}) \lambda_n \Delta (z_{\nu})$ electrons. ($N (z_{\nu})$ is the local density of states, i.e. equal to $N_s$ in the superconductor) (appendix 6.2.2).

- A procedure for diffusive and ballistic propagation of electrons in the different films is derived (appendix 6.3).

- 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 6.4).

- The density $O_{\nu}(m)$ is calculated in discrete steps for the time $t' = m\tau_d$. (appendix 6.3).
• Due to thermal dephasing this density is, at each step, multiplied with the time factor $\eta_T (m\tau_d)$.

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

• The resulting function $\tilde{\Delta}_\nu$ is the input $\Delta_\nu$ for the next iteration.

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

• The iteration process is completed when initial and final $\Delta_\nu$ agree with a relative accuracy of $10^{-5}$. This is generally achieved after a few iterations.

All the step of the numerical procedure are described in details in the appendix.
3 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 $\xi_{BCS}$ if one uses the transition temperature in $\tau_T = h/(2\pi k_B T)$), 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 included if they are known or used as fit parameters.

3.1 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 ($N_{s,n}, v_{Fs,n}$) 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.3a. The parameter $\alpha$ 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.3b $T_c$ is plotted versus the reduced thickness $d_s/d_{cr}$. The points lie almost on an universal
curve, particularly those for smaller $l_s$. 

Fig. 3: 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 $d_s/\xi$ ($\xi =$ BCS coherence of S) a) For different mean free paths $l_n$ of S, the parameter $\alpha = l_s/\xi$. 

3.2 Pair amplitude

In the next step the actual dependence of the gap function on position is of interest. In Fig. 4a-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 $T_c/T_s \approx 0.3$. Fig. 4a shows $\Delta (z')/\Delta_0$ for the superconductor with $l_s/\xi_0 = 0.01$. (Since the amplitude of $\Delta (z')$ approaches zero at the transition temperature the value $\Delta_0$ 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 Fig. 4a-d. Fig. 4a 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. [36] where a series consisting of $\cos (\Omega_0 (d_s - z)/\xi d))$ and $\cosh (\Omega_m (z - d_s)/\xi d))$ is used, $\xi_d = \sqrt{\xi \xi}$ is the superconducting diffusion length and $\Omega_0, \Omega_m$ are coefficients defined in that work).
Fig. 4a-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. 3a. $d_s$ is close to the critical thickness $d_{cr}$. The ratio $l_s/\xi_0$ is noted in the figures.

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. 5a 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.

Fig. 5a,b: 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 0.9 $T_s$.) a) dirty limit $l_s/\xi=0.01$. b) clean limit $l_s = \infty$.

3.3 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 worth to check the situation when both metals are dirty. This is the case which most
superconducting diffusion lengths \( \xi \) paths are chosen in both films to be \( \xi \) the superconducting coherence lengths \( \xi \) temperature) is larger by a factor of 1.5 than for superconductor S. Therefore the density of states for superconductor N (with the lower transition temperature) 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 \( T_{N \rightarrow S}/T_{S \rightarrow N} = .444 \).

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

\[
\cosh (k_n (d_n + z)) \quad \text{in the superconductor with } T_n \text{ in the range } -d_n < z < 0 \\
\cos (k_s (d_s - z)) \quad \text{in the superconductor with } T_s \text{ in the range } 0 < z < d_s
\]

Fig.6a shows for \( z < 0 \) a fit 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 $k_s = 0.0506 \, nm^{-1}$, $k_n = 0.0468 \, nm^{-1}$ 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: $4.29 \times 10^{-2}$ and $1.77 \times 10^{-2}$. 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 only from $T_c = 7.6K$ by just $0.1K$ to $7.7K$. In Fig.6b 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 numerical points).

3.4 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 how the initial 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 Fig.7a,b. In both figures the thickness of the superconductor is equal to the BCS coherence length $\xi_0$. The transition temperature $T_c/T_s$ is plotted versus the thickness of the normal conductor. In Fig.7a the mean free paths in both films are equal and vary between $l_s = l_n = \xi_0/10$, $\xi_0$ and $10^3\xi_0$. In Fig.7b 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 density of states are assumed equal $N_s = N_n$.)
Fig. 7a, b: $T_c$ for an SN double layers as a function of $d_n/\xi$. The thickness of the superconductor is equal to the BCS coherence length $\xi$. ($N_s = N_n$).

- a) The mean free paths $l_s = l_n$ are parameters.
- b) Different combinations of the mean free paths are used as parameters.

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.
Fig. 8: $T_c$ for SN double layers as a function of $d_n/\xi$.

The parameter $d_s$ is the thickness of the superconductor. ($N_s = N_n$, $l_s = l_n = \xi/10$).

In table I the normalized initial slope is collected. (The numerical points had to 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.

| $d_s/\xi$ | $d_s$ | $dT_c/dd_n$ |
|----------|-------|-------------|
| 0.25     | 4.35  |
| 0.5      | 4.34  |
| 0.75     | 4.31  |
| 1.0      | 4.26  |
| 1.5      | 4.13  |
| 2.0      | 4.02  |

Table I: Normalized initial slope for different thicknesses $d_s$ of the superconductor.

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. 9: $T_c$ for an SN double layers as a function of $d_n/\xi$. The parameter $t$ is the transparency of the interface. ($N_s = N_n$, $d_s = \xi$, $l_s = l_n = \xi/10$).
4 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 \( \Gamma_{sn} \) 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 \( \Gamma_{sn} \) in equation (6) numerically. Using \( T_s = 7.2K \) for Pb then the
prefactor is about 4.5. (This is actually the value for a wide range of the Debye
temperature between 100K and 300K).

Recently our group investigated the proximity effect between the supercon-
ductor Pb and several alkali metals [31]. It was a great surprise that the exper-
imental 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 two. 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.)

| metals   | \( d_s \) (nm) | \( d_n \) (nm) | \( S_{sn} |_{exp} \) | \( N_n/N_s \) ratio |
|----------|----------------|----------------|-----------------|-------------------|
| Pb/K     | 12.9           | 2.04           | 0.423           | 0.223             |
| Pb/Na    | 13.9           | 2.18           | 0.546           | 0.300             |
| Pb/Ag    | 17.9           | 2.10           | 0.625           | 0.335             |

Table II: The normalized initial slope of SN double layers with Pb as
superconductor and different normal metals. The 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 \( S_{sn}|_{exp}/(N_n/N_s) \).

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 et al. [11, 12]
who investigated quench condensed PbCu layers. The second work was by Min-
gerode [3] 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 of the experimental (normalized) slope to the density of states ratio. Again the experimental normalized slopes are much smaller than the theory predicts.

| metals | d_s (nm) | d_n (nm) | S_{sn|exp} | N_n/N_s | ratio |
|--------|----------|----------|------------|---------|-------|
| Pb/Cu$^1$ | 10.0 | 10.0 | 0.542 | 0.448 | 1.21 |
| Pb/Cu$^2$ | 15.0 | 10.0 | 0.500 | 0.448 | 1.12 |
| Pb/Cu$^2$ | 22.9 | 3.30 | 1.110 | 0.448 | 2.48 |
| Pb/Cu$^2$ | 24.3 | 3.90 | 0.935 | 0.448 | 2.08 |
| Pb/Cu$^2$ | 32.9 | 4.10 | 0.883 | 0.448 | 1.97 |
| Pb/Cu$^2$ | 27.2 | 13.10 | 0.683 | 0.448 | 1.52 |
| Pb/Cu$^2$ | 28.0 | 26.40 | 0.842 | 0.448 | 1.88 |
| Pb/Cu$^2$ | 33.4 | 17.70 | 0.608 | 0.448 | 1.36 |

Table III: The normalized initial slope of PbCu double layers, data$^1$ from ref. [1] are quench condensed and data$^2$ from ref. [6] are condensed at room temperature. The 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 $S_{sn|exp}/(N_n/N_s)$.

It is rather amazing that this fundamental discrepancy between experiment and theory has not been realized. What is the reason for this disagreement? The authors best guess at the present time 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 electron $\mathbf{k}$ which lies below the Fermi energy within the Debye energy $k_B\Theta_D$ can emit a virtual phonon and perform a transition into a state $\mathbf{k}'$ above the Fermi energy. As a consequence the states below $k_F$ have an occupation less than 1 and the states above $k_F$ have an occupation larger than 0, even at zero temperature. At $k_F$ the occupation does not jump from one to zero, but has a smaller step of $1/(1 + \lambda)$, where $(1 + \lambda)$ is the electron-phonon enhancement factor. The parameter $\lambda$ can be calculated with the Eliashberg function $\alpha^2 F(\Omega)$ which describes the probability of an electron to emit or absorb a phonon of energy $\hbar\Omega$. (A nice treatment of the electron-phonon physics can be found in the book by Grimvall [39]). If one moves now an electron from the Fermi energy to a $\mathbf{k}$-value above the Fermi energy then it changes the occupation of the $\mathbf{k}$-state only by $(1 + \lambda)^{-1}$. The change in kinetic energy is therefore reduced by the same factor; the energy states lie closer together by the factor $(1 + \lambda)$. As a consequence the density of states is enhanced by $(1 + \lambda)$ and the Fermi velocity reduced by $1/(1 + \lambda)$. This enhancement is restricted to a small region in the vicinity of the Fermi energy. The new density of states $N^* = N(1 + \lambda) = N = m(1 + \lambda)k_F/(2\pi^2\hbar^2)$ and Fermi velocity $v^*_F = v_F/(1 + \lambda) = \hbar k_F/m(1 + \lambda)$ are called the renormalized
density of states and Fermi velocity and marked with a star. The Fermi wave number \( k_F \) does not change and both changes in \( N \) and \( v_F \) can be expressed by a change of the mass \( m^* = m (1 + \lambda) \) (therefore the name mass enhancement).

Many properties of the electron gas and the strong coupling superconductor can be reasonably well calculated in a renormalized strong coupling description. For the superconductivity this means that one applies the weak coupling BCS theory using renormalized density of states and Fermi velocity. The error for Pb is generally less than 20% as the ratio of \( 2\Delta_0/k_BT_c = 4.2 \) instead of 3.5 demonstrates. (For other parameters see [40]).

In strong coupling superconductors the effective interaction \( (NV)_s \) is replaced by \( (\lambda - \mu^*) \) where \( \lambda \) describes the strength of the electron-phonon interaction and \( \mu^* \) is the Coulomb pseudo-potential. In the literature one find \( \lambda \)-values for Pb which vary between 0.8 and 1.6 [39]. Depending how much the strong coupling theory modifies the expression for the initial slope it could alter dramatically the theoretical prediction for the initial slope. In the appendix we show that a renormalized strong coupling theory would yield an initial slope of \( \Gamma_{sn} = (\lambda - \mu^*) / (1 + \lambda) \). This appears to alter the theoretical value for the initial slope. The difficulty is that the weak coupling treatment just a replaces \( (NV)_s \) by \( (\lambda - \mu^*) / (1 + \lambda) \). This means that for the transition temperature one obtains the equivalent condition

\[
\Delta = \frac{2\pi k_B T}{\hbar} \sum_{|\omega| \leq \Omega_D} \frac{\lambda - \mu^*}{1 + \lambda} \frac{1}{2|\omega|} \Delta
\]

This does not alter the situation and yields, as observed by Morel and Anderson [41], a too small value of 0.4 for \( \lambda \).

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 \( \Delta (r, \omega_l) \) which has the equations (4) and (7) as limiting cases. This is a very demanding job which goes beyond the scope of the present paper and has to be left for future investigations. However, we can check whether this extension is a promising one. For this purpose we consider the analogy to the Cooper limit for strong superconductors.

Let us consider a double layer composed of (very) thin films of a strong coupling superconductor and a normal metal. The super- and normal conductor have \( \lambda \) values \( \lambda_s \) and \( \lambda_n \). Both have the same value for the renormalized Coulomb repulsion \( \mu^* \). For sufficiently thin films the electrons in the double layer travel so quickly from the superconductor to the normal metal and vice versa that they average over the properties of the two metals. We have essentially a new superconductor with a new averaged electron-phonon interaction \( \overline{\lambda} \) (in complete analogy to Cooper’s argument)

\[
\overline{\lambda} = \frac{d_s N_s \lambda_s + d_n N_n \lambda_n}{d_s N_s + d_n N_n}
\]

Now we apply the strong coupling gap equation (7) to this artificial strong coupling superconductor.
For the superconductor we chose Pb, but somewhat simplify its properties slightly. For the Eliashberg function we use a simple square law for $\Omega < \Omega_D$ and express the prefactor in terms of the electron-phonon parameter $\lambda$:

$$\alpha^2 F(\Omega) = \lambda \left( \frac{\Omega}{\Omega_D} \right)^2$$

We use for the Debye temperature $\Theta_D = 80K$ and for the Coulomb parameter $\mu^* = 0.1$. Next we calculate $\lambda(\Omega_l)$ for $\Omega_l = l \ast 2\pi k_B T / h = \omega_{j+l} - \omega_j$:

$$\lambda(\Omega_l) = 2 \int_0^{\Omega_D} \lambda \left( \frac{\Omega}{\Omega_D} \right)^2 \frac{\Omega}{\Omega^2 + \Omega_l^2} d\Omega$$

$$= \lambda \left( 1 + \frac{\Omega_l^2}{\Omega_D^2} \ln \left( \frac{\Omega_l^2}{(\Omega_l^2 + \Omega_D^2)} \right) \right)$$

These parameters are inserted into equation (7) in the appendix and yield the dependence of $T_c$ on $\lambda$. In Fig.10 this dependence is plotted, $T_c$ as a function of $\lambda$ for $\mu^* = 0.1$, $\Theta_D = 80K$ and $\alpha^2 F(\Omega) = \lambda (\Omega/\Omega_D)^2$. The transition temperature of Pb, $T_c = 7.2K$, corresponds to value of $\lambda_{Pb} = 0.75$.

\[\text{Fig.10: The dependence of } T_c \text{ on the electron-phonon parameter } \lambda \text{ using the (linear) strong coupling gap equation.}\]

From Fig.10 one obtains $dT_c/d\lambda$. At $T_s = 7.2K$ this slope has the value $dT_c/d\lambda = 18.8K$. Within the thin film approximation for $\lambda$ one finds for the initial slope of $T_c$ in a thin double layer:
\[
\frac{dT_c}{dd_n} = \frac{dT_c}{d\lambda} \frac{d\lambda}{dd_n} = 18.8 \left(\circ K\right) \frac{d}{dd_n} \left(\frac{d_s N_s \lambda_s + d_n N_n \lambda_n}{d_s N_s + d_n N_n}\right)
\]

or

\[
\frac{d_s}{T_s} \left| \frac{dT_c}{dd_n} \right| = 2.6 \left(\lambda_s - \lambda_n\right) \frac{N_n}{N_s}
\]

If we take \(\lambda_n = 0.1\) and use \(\lambda_s = 0.75\) then we find

\[
\frac{d_s}{T_s} \left| \frac{dT_c}{dd_n} \right| \approx 1.7 \frac{N_n}{N_s}
\]

The strong coupling treatment (in the thin film limit) reduces the prefactor in the initial slope to 1.7. This is a very satisfactory result. The strong coupling theory yields the correct initial slope. On the other hand it is also disappointing. It means that the superconducting proximity effect with superconductors such as Pb one can not be solved with the weak coupling theory. Furthermore it means that the simulation developed here (as all other theoretical treatments the author is aware of) can only be applied to weak coupling superconductors such as Al. But I believe that this disappointment is more than compensated by the knowledge that the use of strong coupling superconductors gives an additional window to the study of strong coupling effects.
5 Conclusion

This paper derives the transition temperature of a double or multi layer 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 \( N_s \Delta (r') / \tau_F \) from one position-time \( (r', t' < 0) \) to another position-time \( (r, t = 0) \). This message which decays thermally with time as \( \eta_T (t) = \sum_{|\omega_n| < \Omega_D} \exp (-2 |\omega_n| |t'|) \), is integrated at \( (r, t = 0) \) over all start position-times \( (r', t') \) and, after multiplication with the BCS interaction \( V_s \), yields the new gap function \( \Delta (r) \). 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 multi-layers 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:

- mean free path of the different metals
- transmission through the interface
- ratio of specular reflection to diffusive scattering at the surfaces
- fraction of diffusive scattering at the interface.

Furthermore it is possible

- to vary the mean free path along the thickness of the films
- to vary the BCS interaction \( NV \) at the interface.

The few examples which were presented in chapter III demonstrate why the dirty case is so much simpler than the clean one. They also show that even for small thickness 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 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

- the mean free path of the two metal
- the thickness of the superconductor
- a (not to large) barrier between the two metal.
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 \( \Gamma_{sn} \) 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 \( \Gamma_{sn} \) lie in the range of 1.5 – 2.0. The author believes that the discrepancy is due to the strong coupling properties of the Pb. An analysis of the strong coupling gap equation in the thin-film limit confirms this supposition. It yields the value of about \( \Gamma_{sn} = 1.6 \) for a (simplified) Pb film in contact with a normal metal which is characterized by \( \lambda = 0.1 \) and \( \mu^* = 0.1 \).
6 Appendix

6.1 The kernel in the clean limit

In the clean limit the thermal Green function has the form

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

That yields

\[ H_\omega (r, r') = k_B T G_\omega (r, r') G^*_\omega (r, r') \]

or

\[ H_\omega (R) = \frac{2\pi k_B T}{\hbar v_F} N \frac{1}{4\pi R^2} \exp \left( -\frac{2|\omega| R}{v_F} \right) \]

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

Without the damping the number of electrons between the radius \( R \) and \( R + dR \)

\[ \frac{2\pi k_B T}{\hbar v_F} N dR = \frac{2\pi k_B T}{\hbar} N dt \]

using \( dR = v_F dt' \). This means that \( H_\omega (r, r') \Delta (r') d^3r' \) corresponds to an injection of

\[ dZ = \frac{2\pi k_B T}{\hbar} N \Delta (r') d^3r' dt \]

electrons in the volume \( d^3r' \) during the time \( dt' \) at the position \( r' \). \( dZ \) is indeed a (dimensionless) number. The exponential decay \( \exp (-2|\omega| R/v_F) \) corresponds to a decay with time since \( R = v_F t \):

\[ \exp (-2|\omega| R/v_F) = \exp (-2|\omega| t) \]

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

\[ H_\omega (r, r') = \frac{2\pi k_B T}{\hbar} N (r') \int_{-\infty}^{0} dt' \rho (v_F; r, 0; r', t') \exp (-2|\omega||t'|) \]

This yields the gap equation using \( \eta_T (t') \) from equation 2

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

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

As shown in Fig. 2 the metal films are divided in sheets of thickness \( \lambda \). Furthermore the time development is performed in diffusion steps of \( \tau_d = 2 \lambda s / v F_s \), \( t' = m \tau_d \). Then the self-consistent gap equation takes the form

\[
\Delta (z_\nu) = \frac{V(z_\nu)}{\lambda_\nu} \sum_{\nu'} \lambda_\nu' N (z_\nu') \sum_{m=0}^{\infty} \frac{\tau_d}{\tau T} \eta_T (m \tau_d) \overline{p} (z_\nu, m \tau_d; z_\nu', 0) \Delta (z_\nu')
\]

(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 \( \Delta_\nu, V_\nu, N_\nu \).

6.2.1 The 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 \( \Theta_s \) the implicit equation

\[
\frac{1}{(NV)_s} = \int_0^\infty \frac{dt}{\tau T} \eta_T (t / \tau T_s)
\]

is used.

6.2.2 Initial conditions

At the time \( t = 0 \) a simple gap function \( \Delta_\nu \) in the superconducting film(s) is chosen, for example \( \Delta_\nu = k_B T_s \) 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 \( \overrightarrow{O}_\nu (0) \) and \( \overleftarrow{O}_\nu (0) \) with \( \overrightarrow{O}_\nu (0) = \overleftarrow{O}_\nu (0) = O_\nu (0) / 2 \). In the following sub-sections the recipe is given how to calculate from the occupation \( \overrightarrow{O}_\nu (m), \overleftarrow{O}_\nu (m) \) at the time \( t = m \tau_d \) the occupation \( \overrightarrow{O}_\nu (m + 1), \overleftarrow{O}_\nu (m + 1) \). The total occupation is \( O_\nu (m) = \overrightarrow{O}_\nu (m) + \overleftarrow{O}_\nu (m) \). With this time developing occupation the new gap function becomes

\[
\widetilde{\Delta}_\nu = \frac{V_\nu \tau_d}{\lambda_\nu \tau T} \sum_{m=0}^{\infty} \eta_T (m \tau_d) O_\nu (m)
\]

This iterated gap function has two defects: (i) its shape generally does not agree with the original gap function \( \Delta_\nu \), and (ii) the ratio of the average amplitudes \( r = \langle \widetilde{\Delta}_\nu \rangle / \langle \Delta_\nu \rangle \) will not be one. 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 \( \langle \widetilde{\Delta}_\nu \rangle \) becomes sufficiently close to \( \langle \Delta_\nu \rangle \) and the adjusted
temperature is the transition temperature of the multi-layer. The iteration is completed when

\[
\frac{1}{Z_s} \sum_{\nu} \left( \tilde{\Delta}_\nu - \Delta_\nu \right)^2 < 10^{-5}
\]
6.3 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 $\lambda$ and an electron needs the time $\epsilon_0 = \lambda / v_F$ to cross a cell. We divide the initial occupation $O_{\nu}(0)$ into $O_{\nu}^+ (0) = O_{\nu}^- (0) = O_{\nu}(0) / 2$ 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 how one obtains from the occupations at the time $t = m\epsilon_0$ the occupation at the next time step $t = (m + 1)\epsilon_0$

$$O_{\nu}^+ (m + 1) = pO_{\nu-1}^+ (m) + (1 - p)O_{\nu}^- (m)$$
$$O_{\nu}^- (m + 1) = pO_{\nu+1}^- (m) + (1 - p)O_{\nu}^+ (m)$$

This yields a one-dimensional diffusion with the diffusion constant $D = \frac{1}{2} \frac{p - 1}{p} \frac{\lambda^2}{\epsilon_0}$.

Ballistic propagation requires setting $p$ almost equal to 1. In this case almost all the $O_{\nu}^+ (m)$ electrons move from cell $\nu$ to cell $(\nu + 1)$ during the time $\epsilon_0$. This means that they propagate the average distance $\lambda = v_F \epsilon_0$ during the time $\epsilon_0$. Therefore this model does not fulfill the basic requirement for ballistic propagation in three dimension that $\langle v_z \rangle = \frac{1}{2} v_F$.

A three-dimensional diffusion can be obtained by a sequential propagation in $x$, $y$ and $z$ direction, each for a time of $\epsilon_0$ with the velocity $v_F$. This yields a diffusion constant $D = \frac{1}{2} \frac{p - 1}{p} \frac{\lambda^2}{\epsilon_0}$ and triples the average time for the diffusion in the $z$ direction. Since the electrons propagate only during every third of the interval $3\epsilon_0$ in the $z$ direction they propagate the distance $\lambda$ during the time $3\epsilon_0$, 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 $\epsilon_0$ in the $z$ direction. Then the time step is $\tau_d = 2\epsilon_0$. In this case the diffusion constant is $D = \frac{1}{2} \frac{p - 1}{p} \frac{\lambda^2}{\tau_d}$ 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
-z direction. A single density component with hopping to neighbor places
yields only small diffusion constants of $D = \frac{\varepsilon}{2\varepsilon_0}$ and can’t describe the ballistic
propagation at all.

For the normal conductor the same time element $\tau_d$ 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 form the experimental con-
ductivity $\sigma$ of the films, where

$$D_m = \frac{\sigma_m}{2e^2N_m}, \quad p_m = \frac{D_m}{\frac{1}{2}\frac{\lambda^2}{2\varepsilon_0} + D_m}$$

where $m$ stands for $s$ or $n$. 

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6.4 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 then \( k_{F,n} \) then any electron in S whose component \( k_\rho \) parallel to the surface is larger than \( k_{F,n} \) cannot cross the interface because afterwards it would have an energy of a 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

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

\[
f(x) = \frac{4}{15} \left( \sqrt{x+1} \right)^3 (x+6) - (\sqrt{x})^5 - 10x - 6
\]

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

The detailed balance requires that in equilibrium the number of electrons which cross from S to N is equal to the number of electron 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

\[
\begin{align*}
\vec{O}_s(m+1) &= T_{ns} \vec{O}_n(m) + (1 - T_{sn}) \vec{O}_s(m) \\
\vec{O}_n(m+1) &= T_{sn} \vec{O}_s(m) + (1 - T_{ns}) \vec{O}_n(m)
\end{align*}
\]

In equilibrium one has \( \vec{O}_{s,n} = \vec{O}_{s,n} = \frac{1}{2} O_{s,n} \) 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 superconductor have, in particular the strong coupling ones). We return to the mass enhancement below. However, independent how complicated the individual transmission probabilities are, the detailed balance will always apply. In our simulation we use \( T_{ns} \leq 1 \) as a fit parameter and calculate \( T_{sn} \) using the detailed balance.
6.5 Strong coupling effects

In appendix (6.1) the kernel $H_\omega (r, r')$ was derived for free electrons

$$H_\omega (r, r') = k_B T G_\omega (r, r') G_\omega^* (r, r')$$

where

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

$G_\omega (r, r')$ is a Fourier transform of $G_\omega (k)$

$$G_\omega (k) = \frac{1}{i\omega - \epsilon_k}$$

In the renormalized strong coupling case one has

$$G_\omega (k) = \frac{1}{1 + \lambda \frac{1}{i\omega - \epsilon_k}}$$

where $(1 + \lambda)$ is the ”mass enhancement” of the electrons at the Fermi surface due to the electron-phonon interaction. Here $\lambda$ is defined as

$$\lambda = 2 \int_0^{\Omega_D} \alpha^2 F (\omega) \frac{d\omega}{\omega}$$

and $\alpha^2 F (\omega)$ is the Eliashberg function of the electron-phonon interaction. In performing the Fourier transform one obtains

$$G_\omega (R) = \frac{m}{2\pi \hbar^2 R} \exp \left[ ik_F R \frac{\omega}{|\omega|} - \frac{|\omega|}{\hbar v_F^*} R \right]$$

(using $|r - r'| = R$). Compared with the free electron Green function the Fermi velocity is now renormalized.

This yields for the function $H_\omega (R)$

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

using the bare BCS-density of state $N = m^2 v_F / 2\pi^2 \hbar^3$ and the bare Fermi velocity $v_F$.

Now we use the same argument as before: The term $H_\omega (r, r') \Delta (r') d^3 r'$ corresponds to an injection of

$$dZ = \frac{1}{(1 + \lambda)} \frac{2\pi k_BT}{\hbar} N \Delta (r') d^3 r' dt$$

electrons in the volume $d^3 r'$ during the time $dt$ at the position $r'$ which propagate with $v_F^*$. The factor $1/(1 + \lambda)$ arrives from the ratio of $v_F^*/v_F$. The exponential
decay \exp\left(-2|\omega|R/v_F^2\right) \text{ corresponds to a decay with time as } \exp\left(-2|\omega|R/v_F^2\right) = \exp\left(-2|\omega|t'\right) \text{ since } R = v_F^2t'. \text{ Now we replace the BCS interaction } V \text{ by an effective interaction strength } (\lambda - \mu^*)/N. \text{ (}\alpha^2F(\omega)\text{ and therefore } \lambda \text{ contains the bare density of states } N \text{ as a factor)}.

The gap equation is then

\frac{\Delta(r)}{N(r)} = \frac{\lambda(r) - \mu^*}{N(r)} \frac{2\pi k_B T}{\hbar} \int d^3r' \frac{N(r')}{(1 + \lambda(r'))} \int_0^t \rho(v_F^*; r; 0; r', t') \eta_T(t') dt' \Delta(r')

A test for constant \Delta using \int d^3r' \rho(v_F^*; r; 0; r', t') = 1 yields

\Delta = \frac{(\lambda - \mu^*)}{\alpha^2F(\omega)} \frac{2\pi k_B T}{\hbar} \frac{N}{1 + \lambda} \int_{-\infty}^0 \eta_T(t') dt' \Delta(r')

This yields McMillan's first approximation for the \(T_c) \text{ of a strong coupling superconductor}

\frac{(1 + \lambda)}{(\lambda - \mu^*)} = \sum_{n=0}^{\Omega_D/\pi} \frac{1}{n + \frac{1}{2}}\frac{1}{2\omega_i - \omega_j}

\quad T_c \approx \langle \Omega \rangle \exp\left(\frac{(1 + \lambda)}{(\lambda - \mu^*)}\right)

### 6.5.1 Strong coupling gap equations

For the strong coupling superconductor one has to use the Eliashberg theory. It replaces the "one" gap equation by series of gap equations at different Matsubara frequencies. Equation (7) \[ \Delta(\omega_i) = \frac{2\pi k_B T}{\hbar} \sum_j \left\{ \lambda(\omega_i - \omega_j) - \mu^* \right\} \frac{1}{2|\omega_j|} \Delta(\omega_j) \] defines the gap \(\Delta(\omega)\) at \(\omega\) as a function of the gap at all other Matsubara frequencies \(\omega_j\).

\[ \tilde{\omega}_j = \omega_j + \frac{\pi k_B T}{\hbar} \sum_l \frac{\omega_l}{|\omega_l|} \lambda(\omega_j - \omega_l) \]

\[ \lambda(\omega_i - \omega_j) = 2 \int_0^\infty d\omega \frac{\omega \alpha^2F(\omega)}{\omega^2 + (\omega_i - \omega_j)^2} \]

The effective BCS interaction \(NV\) is replaced by \(\{\lambda(\omega_i - \omega_j) - \mu^*\}\). The electron-phonon parameter \(\lambda(\omega_i - \omega_j)\) is determined by the Eliashberg function \(\alpha^2F(\omega)\). The denominator \(1/2|\omega_n|\) is replaced by the dressed Matsubara frequencies \(1/2|\tilde{\omega}_j|\). Here is \(\tilde{\omega}_j = \omega_j (1 + \bar{X})\) where \(\bar{X}\) is an average over \((2j + 1)\) different values of \(\lambda(\Omega_m)\), \(\langle \Omega_m \rangle = \nu 2\pi k_B T/\hbar, 0 \leq \nu \leq j\).

One can derive from the energy dependent gap equation a renormalized gap equation by the following simplifications

- \(\Delta(\omega_i) \Rightarrow \Delta = \text{const} \text{ for } |\omega_i| < \Omega_D\)
• $\Delta(\omega_i) \rightarrow 0$ for $|\omega_i| > \Omega_D$

• one replaces $\lambda(\omega_i - \omega_j) \rightarrow \lambda(0) = \lambda$ for $|\omega_i|, |\omega_j| < \Omega_D$

Then one finds that $\tilde{\omega}_j$ is renormalized as $\tilde{\omega}_j = \omega_j (1 + \lambda)$ where $(1 + \lambda)$ is the electron-phonon renormalization factor. Using these simplifications the renormalized gap equation takes the form

$$\Delta = \frac{2\pi k_B T}{h} \sum_{|\omega_j| \leq \Omega_D} \frac{\lambda - \mu^*}{1 + \lambda} \frac{1}{2|\omega_j|} \Delta$$

as before.
7 Literature

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