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Surface Green function approach to the calculation of tunnelling currents in normal metal–superconductor junctions

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Abstract. A formalism which combines Gorkov's Green function description of the superconducting state and a surface Green function method is proposed to calculate tunnelling currents in normal metal–superconductor junctions. The method allows a straightforward calculation of the reflection and transmission matrices, among other physical magnitudes of interest. A simple example (at $T = 0$), based upon elementary BCS theory, is carried out in detail. The results are in full agreement with previous analyses on this system, which used the matching of wavefunctions at the interface. The formalism is compared with other Green function approaches to the present problem.

1. Introduction

In the last 15 years, tunnelling has been widely used to investigate the properties of superconducting materials [1]. In particular, a great deal of experimental and theoretical work has been devoted to the understanding and utilisation of the properties of normal metal–superconductor (N–S) junctions [1, 2]. This interest has recently grown with the invention of the scanning tunnelling microscope [3] and its applications to the study of global and local properties of superconducting materials [4]. Lately, the discovery of high-temperature superconductors [5] has prompted a strong revival of the research in the whole field of superconductivity.

Despite these developments, a full calculation of the tunnelling currents in N–S junctions has only been carried out rather recently [2, 6]. Previous analyses of the problem used the simplest semiconductor description of the superconducting ground state [7], which, as discussed in [2], does not account for the temperature-independent currents, at energies in the superconducting gap. Although this is the most important failure of the semiconductor model [6], it also masks most of the physics which characterise the junction [2].

The exact solution of tunnelling at the N–S interface was achieved through matching at the interface of the superconductor wavefunctions (as given by the Bogoliubov

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equations [8]) to the normal metal wavefunctions. Although this procedure is in principle straightforward, it already reveals the intriguing characteristics of the system, and its extension to more complicated problems is rather intricate. The purpose of the present paper is to show how the Green function formulation of the microscopic theory of superconductivity proposed by Gorkov [9] can be extended to treat the present problem. Gorkov's [9] approach has been recognised as one of the most useful in the investigation of the bulk properties of superconductors in the presence of magnetic fields or at finite temperatures [10, 11]. To generalise Gorkov's formalism to problems without translational invariance, such as surfaces or interfaces, we use the surface Green function (SGF) method developed in [12, 13]. Combining both formalisms, we are able to solve the matching of Green functions at the interface and, therefore, to obtain the full Green function of the system [12]. The SGF method proposed by Garcia-Moliner and Rubio [12] has already been used to investigate the properties of metal [14] and semiconductor [15] surfaces, and their interfaces; in the present paper we shall show that it can also handle junctions in which a superconductor material is involved. Although the resultant formalism is rather similar to that proposed by Arnold [16], it is formally more simple. We shall describe the general procedure and illustrate its use by means of a calculation of the reflection and transmission coefficients for the N–S junction, a system which has been thoroughly investigated by means of the matching of wavefunctions at the interface [2, 6].

2. Green function formalism

2.1. Microscopic theory of superconductivity

Gorkov [9] reformulated the microscopic theory of superconductivity, introduced by Bardeen, Cooper and Schrieffer [17], in terms of Green functions. This formalism naturally includes finite temperatures, in terms of temperature Green functions, and can be easily extended to investigate the properties of superconductors in the presence of magnetic fields. In summarising the main features of the formalism, we follow the approach suggested in [18, 19] and restrict ourselves to the case of zero temperatures. We define a 2×2 matrix Green function in terms of the following two-component field operator:

$$\Psi_k(\boldsymbol{r}, t) \equiv \begin{bmatrix} \psi_{k\uparrow}(\boldsymbol{r}, t) \\ \psi_{k\downarrow}(\boldsymbol{r}, t) \end{bmatrix} \tag{1}$$

where $\psi_{k\sigma}(\boldsymbol{r}, t)$ are the standard field operators for particles with a given z component of the spin and wavenumber $\boldsymbol{k}$. Then the matrix Green function is written as

$$\mathbb{G}(\boldsymbol{r}, t; \boldsymbol{r}', t') \equiv -\langle T_t[\Psi_k(\boldsymbol{r}, t)\Psi_k(\boldsymbol{r}', t')]\rangle$$

$$= \begin{bmatrix} G(\boldsymbol{r}t; \boldsymbol{r}'t') & F(\boldsymbol{r}t; \boldsymbol{r}'t') \\ F^+(\boldsymbol{r}t; \boldsymbol{r}'t') & -G(\boldsymbol{r}'t'; \boldsymbol{r}t) \end{bmatrix} \tag{2}$$

where T_t is the time ordering operator. The diagonal elements of the above matrix are the standard single-particle Green functions, whereas the off-diagonal elements are usually referred to as anomalous Green functions [11] and are related to the density of

Cooper pairs. The matrix Green function of equation (2) obeys the following equation of motion:

$$\mathbb{D}_{rt}\mathbb{G}(rt; r't') = \delta(r - r')\delta(t - t')\mathbb{1} \tag{3}$$

where $\mathbb{1}$ is the unit matrix and the differential operator $\mathbb{D}_{rt}$ is given by

$$\mathbb{D}_{rt} = \begin{bmatrix} i\,\partial/\partial t - \frac{1}{2}\nabla^2 + \mu & \Delta(r) \\ \Delta^*(r) & i\,\partial/\partial t + \frac{1}{2}\nabla^2 - \mu \end{bmatrix} \tag{4}$$

where atomic units ($e = \hbar = m = 1$) are used here and subsequently. In equation (4), μ is the chemical potential which is used as the independent variable instead of the number of particles [10], and $\Delta(r)$ the gap function.

In cases where the Hamiltonian is time independent and translationally invariant and, consequently, the corresponding Green functions depend only on $t - t'$ and $r - r'$, it is useful to Fourier transform the equation of motion and to solve it for the energy (or frequency) and momentum p. This is the simple model considered in section 3.

2.2. *Surface Green function*

In combining the previous formalism with the SGF method of Garcia-Moliner and Rubio [12], we note that the key point is the matrix differential operator in the equation of motion (3). In fact we have to carry out the matching procedure for the Green function related to that operator instead of the standard Green function appearing in the Schrödinger equation [12]. In doing so, we remark on the following points.

(i) The diagonal elements of the matrix Green function behave as standard Green functions and their spatial derivatives are, therefore, discontinuous at the interface [12].

(ii) Instead the anomalous Green functions (off-diagonal terms in (2)) have derivatives which are continuous at the interface; both features are a consequence of the structure of the equation of motion.

(iii) The discontinuities of the derivatives of the two diagonal elements of the matrix Green functions at the interface have opposite signs; this is a consequence of the plus sign in front of the Laplacian operator in the lower diagonal element of equation (3), which is due to its relation to hole states.

When these remarks have been taken into account, the SGF method can be straightforwardly generalised to handle Gorkov's Green functions. We shall mention here only how the physical magnitudes pertinent to the present study can be derived from this formalism.

Consider a system formed by two media with the bulk matrix Green function $\mathbb{G}_\nu(r, r'; \omega)$, $\nu = 1, 2$; we shall discuss only problems described by Hamiltonians independent of time and, therefore, the arguments of the matrix Green function will be r and r' and the frequency ω.

The matrix Green function of the whole systems $\mathbb{G}_s$ is obtained by carrying out a full matching of the Green functions of the two media, at the interface; the result is [12, 13]

$$\mathbb{G}_s = \mathbb{G}_\nu + \mathbb{G}_\nu \mathbf{G}_\nu^{-1}(\mathbf{G}_s - \mathbf{G}_\nu)\mathbf{G}_\nu^{-1}\mathbb{G}_\nu \tag{5}$$

where the arguments r, ω have been dropped here and subsequently for clarity. This result holds for $\nu = 1, 2$ and for the two spatial arguments r and r' lying on the same side of the interface; expressions for the two arguments on different sides of the interface

can be found in [13]. The objects denoted by $\mathbf{G}_1$ are the surface projections of the corresponding three dimensional matrix Green functions $\mathbb{G}_\nu$. The surface projection of the Green function of the whole system is

$$\mathbf{G}_s = (\mathbf{G}_2^{-1(-)}\mathbf{G}_2' - {}'\mathbf{G}_1^{(+)}\mathbf{G}_1^{-1})^{-1}. \tag{6a}$$

The determinant of $\mathbf{G}_s^{-1}$ is the secular determinant for the interface problem [12]. The surface projections of the derivatives of the Green matrices are given by [12, 13]

$${}'\mathbb{G}_\nu^{(\pm)} = \lim_{z' \to \pm 0} [(\partial \langle z | \hat{\mathbb{G}}_\nu | z' \rangle / \partial z)|_{z=0}] \tag{6b}$$

$${}^{(\pm)}\mathbb{G}_\nu' = \lim_{z \to \pm 0} [(\partial \langle z | \hat{\mathbb{G}}_\nu | z' \rangle / \partial z')|_{z'=0}] \tag{6c}$$

for the first diagonal element of the Green matrix. The derivates of the second diagonal element have opposite signs to those given in equations (6*b*) and (6*c*); this is a consequence of the structure of the differential operator in equation (4).

Note that this formalism takes full account of the non-locality of the Green function, in contrast with the well known quasi-classical approximation [20]. On the other hand, the method introduced by Arnold [16], although it also accounts for all the properties of the Green functions, shows some technical differences with respect to that presented here.

(i) It is based on the integrodifferential equation which gives the Green function for interacting particles in terms of a self-energy [10], whereas here we obtain the Green function from a differential operator [21]; the latter procedure has definite computational advantages.

(ii) The first spatial derivatives of the Green function are assumed to be continuous at the interface, a procedure not usually followed in standard treatments of Green functions [21].

The most interesting information in the present study is contained in the transmission and reflection matrices. The way in which the transmission and reflection operators can be obtained from the SGF method is discussed in [13]; for an incoming state in medium ν (= 1, 2) the reflection matrix is

$$\mathbb{R} = \mathbf{G}_\nu^{-1}(\mathbf{G}_s - \mathbf{G}_\nu) \tag{7}$$

and the transmission matrix is given by

$$\mathbb{T} = \mathbf{G}_\nu^{-1}\mathbf{G}_s. \tag{8}$$

The SGF method allows calculation of all the physical properties of the system, both local and total densities of states, interface states and reflection and transmission matrices. In the next section we shall illustrate how the combined formalism proposed here works.

3. The N–S junction

3.1. Superconductor model and bulk Green functions

In the simplest version of the microscopic theory of superconductivity, the gap function $\Delta(r)$ is assumed to be a real and positive constant; moreover the crystal potential and

the chemical potential are both constants. We shall solve this model in the small-gap approximation; this assumption is not far from reality [2] and allows an analytical calculation of Green functions. Although the formalism is completely general, we shall consider only a one-dimensional model.

In this model the Fourier transform of the matrix differential operator given in equation (4) takes the form

$$\mathbb{D}^{-1}(p,\omega)=\frac{1}{\omega^2-\varepsilon^2(p)}\begin{bmatrix}\omega+\eta_p & -\Delta\\ -\Delta & \omega-\eta_p\end{bmatrix} \tag{9}$$

where

$$\varepsilon(p)=(\Delta^2+\eta_p^2)^{1/2} \tag{10}$$

the frequency ω is referred to the superconductor midgap (or the chemical potential μ), and $\eta_p=\frac{1}{2}p^2-\mu$. The solutions of $\det\mathbb{D}=0$ are the dispersion relations in the superconducting phase ($\pm\varepsilon(p)$ in equation (9)). The small-gap approximation allows one to write η_p as

$$\eta_p=\tfrac{1}{2}p^2-\mu\simeq p_F(p-p_F) \tag{11}$$

where p_F is the Fermi momentum.

The matrix Green function is directly given by the spatial Fourier transform of $\mathbb{D}^{-1}$ in equation (9); hereafter only retarded Green functions will be considered. Before proceeding to give the actual expressions for the Green function we note that, in the case of a non-constant Bloch potential, it might be essential to describe hole and electron states by means of rather large sets of plane waves. In such a case, the elements in the matrix of equation (9) will, in their turn, be matrixes of order equal to the number of plane waves included in the calculation [15].

In writing the expressions for the Green function we differentiate two energy regions: within or outside the superconductor gap. For energies within the gap ($\omega<\Delta$) the retarded Green function is given by

$$G(z,z';\omega)=-[\exp(-\alpha p_F|z-z'|)/p_F][(\omega/\alpha)\times\cos(p_F|z-z'|)\pm\sin(p_F|z-z'|)] \tag{12}$$

where

$$\alpha=|\Delta^2-\omega^2|^{1/2}. \tag{13}$$

The two signs in equation (12) correspond to the two diagonal elements in the matrix Green function. On the other hand, the anomalous Green function is

$$F(z,z';\omega)=[\Delta\exp(-\alpha p_F|z-z'|)/\alpha p_F]\cos(p_F|z-z'|). \tag{14}$$

For energies outside the gap ($|\omega|>\Delta$), we find that

$$G(z,z';\omega)=-[\mathrm{i}\exp(+\mathrm{i}\alpha p_F\,\mathrm{sgn}(\omega)|z-z'|)/p_F][(|\omega|/\alpha)\cos(p_F|z-z'|)\pm\mathrm{i}\sin(p_F|z-z'|)]. \tag{15}$$

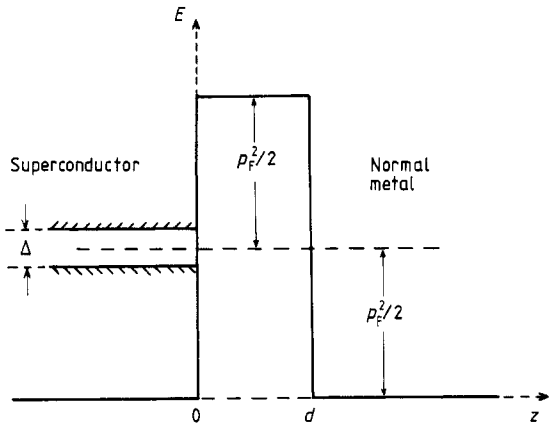

Figure 1. Sketch of the model of the N–S junction investigated in this work.

Again the two signs correspond to the two diagonal elements. The off-diagonal elements are in this case

$$F(z, z'; \omega) = (\mathrm{i}\Delta/\alpha p_F^2) \exp(\mathrm{i}\alpha|z - z'|) \cos(p_F|z - z'|). \tag{16}$$

In the case of $\Delta = 0$ (normal metal) the non-diagonal elements vanish and the Green functions are given by

$$G_0(z, z'; \omega) = -(\mathrm{i}/p_F) \exp(\pm \mathrm{i}p_F|z - z'|). \tag{17}$$

In deriving equation (17), and as we are interested in energies around the gap, we have let $p_F^2 \pm \omega \simeq p_F^2$; this substitution does not lead to any qualitative change and is consistent with the small-gap approximation.

Equations (15)–(17) are the ingredients which combined with our choice for the interface potential will allow us to solve the matching problem and to calculate the reflection and transmission matrices. This is considered in the next section.

3.2. Matching at the interface

We describe the potential at the interface by means of a constant potential barrier (figure 1) of width d and height $p_F^2/2$; choosing this value for the barrier height strongly simplifies the expressions derived here. The constant barrier may adequately simulate an insulator layer. In the appendix the Green functions and transmission coefficient for the case $\Delta = 0$ are derived. As there, we call medium 2 the system formed by the normal metal and the potential barrier extended to $z = +\infty$ (figure 1); medium 1 will be the superconductor (at $z < 0$). For energies outside the gap the surface projection ($z = 0$) of the inverse of the superconductor matrix Green function is

$$\mathbf{G}_1^{-1}(\omega) = \frac{\mathrm{i}p_F}{(\omega^2 - \Delta^2)^{1/2}} \begin{bmatrix} \omega & \Delta \\ \Delta & \omega \end{bmatrix}. \tag{18}$$

On the other hand, the derivatives of the diagonal elements of the matrix Green functions are diagonal and, within the small-gap approximation, ${}'\mathbf{G}_{i,j}^{(+)} = -\frac{1}{2}\delta_{i,j}$ and ${}^{(-)}\mathbf{G}'_{i,j} = \frac{1}{2}\delta_{i,j}$. Then, the surface projection of the matrix Green function of the whole

system, obtained through the matching of the superconductor matrix Green function (equations (12)–(16)) to that of medium 2 (equation (A2)), is given by

$$\mathbf{G}_s(\omega) = \frac{-i(2-t_0)}{2\gamma p_F}\begin{bmatrix} \omega - if & -\Delta \\ -\Delta & \omega + if^* \end{bmatrix} \tag{19}$$

where

$$f = [(\omega^2 - \Delta^2)^{1/2}/(2 - t_0)][2(1 - t_0)^{1/2} + it_0] \tag{19a}$$

$$\gamma = \tfrac{1}{2}[(2 - t_0)(\omega^2 - \Delta^2)^{1/2} + \omega t_0] \tag{19b}$$

where t_0 is the transmissivity for electrons in a junction formed by two normal metals and is given by $|T_0|^2$ (see equation (A5)). Similar expressions are obtained for energies inside the gap.

Then the transmission matrix for an incoming wave in medium 1 (superconductor) incident on the surface ($z = 0$) and being transmitted into medium 2 (at $z = d$) is given by

$$\mathbb{T} = \mathbf{G}_1^{-1}\mathbf{G}_s\mathbf{G}_2^{-1}\mathbb{G}_2(0, d) \tag{20}$$

and the reflection matrix for a wave reflected at $z = 0$ is

$$\mathbb{R} = \mathbf{G}_1^{-1}\mathbf{G}_s - \mathbb{1}. \tag{21}$$

Replacing equations (18) and (19), in combination with (A4), in equations (20) and (21) leads to the analytic expressions for the transmission and reflection matrices presented below.

3.3. Results

In this section we follow the notation used by Blonder *et al* [2]; we define the weights of electron (u_0) and hole (v_0) states at $k = 0$, for $|\omega| > \Delta$, as

$$u_0^2 = 1 - v_0^2 = \tfrac{1}{2}[1 + (1 - \Delta^2/\omega^2)^{1/2}]. \tag{22}$$

For $|\omega| < \Delta$, u_0 and v_0 will be complex conjugates; then γ in equation (19*b*) is rewritten as

$$\gamma = u_0^2 - v_0^2(1 - t_0).$$

Then the elements of the transmission matrix can be written in terms of these magnitudes as

$$T_{11} = (t_0^{1/2}/\gamma)[u_0^2 - iv_0^2(1 - t_0)^{1/2}] \tag{23a}$$

$$T_{12} = (t_0^{1/2}u_0v_0/\gamma)[1 + i(1 - t_0)^{1/2}]. \tag{23b}$$

$$T_{22} = T_{11}^* \qquad T_{21} = T_{12}^* \tag{23c}$$

On the other hand, the elements of the reflection matrix are

$$R_{11} = -i(1 - t_0)^{1/2}/\gamma \tag{24a}$$

$$R_{12} = (u_0v_0/\gamma)[t_0 + 2i(1 - t_0)^{1/2}] \tag{24b}$$

$$R_{22} = R_{11}^* \qquad R_{21} = R_{12}^*. \tag{24c}$$

The reflection coefficients calculated by Blonder *et al* [2] can then be easily obtained from the reflection matrix as follows. Let us consider an incident wave of the form

$$\begin{vmatrix} u_0 \\ v_0 \end{vmatrix} \exp(ip_F z);$$

thus the process of reflection at $z = 0$ is described by

$$\mathbb{R} \begin{vmatrix} u_0 \\ v_0 \end{vmatrix} = \begin{vmatrix} av_0 + bu_0 \\ au_0 + bv_0 \end{vmatrix} \tag{25}$$

where $|a|^2$ gives the probability of Andreev [22] reflection [2] and $|b|^2$ of ordinary reflection; the results for these probabilities are

$$|a|^2 = (u_0^2 v_0^2/\gamma^2) t_0^2 \tag{26a}$$

$$|b|^2 = (u_0^2 - v_0^2)^2 (1 - t_0)/\gamma^2 \tag{26b}$$

in complete agreement with previous results [2, 6]. The probability of transmission through the barrier (between $z = 0$ and $z = d$) for the incoming wave considered above can be calculated through

$$\mathbb{T} \begin{vmatrix} u_0 \\ v_0 \end{vmatrix} = \begin{vmatrix} c \\ d \end{vmatrix} \tag{27}$$

where $|c|^2$ is the probability of ordinary transmission and $|d|^2$ that of transmission with branch crossing [2]; these magnitudes turn out to be

$$|c|^2 = [(u_0^2 - v_0^2)^2 u_0^2/\gamma^2] t_0 \tag{28a}$$

$$|d|^2 = [(u_0^2 - v_0^2) v_0^2/\gamma^2] t_0 (1 - t_0). \tag{28b}$$

Note that equations (26) and (28) actually give probability currents. There is no need to introduce the normalised density of states as required in calculations which use the matching of wavefunctions [2]; the proper normalisation factors are already included in the Green functions.

This simple calculation illustrates how the formalism proposed here works, and it gives support for further applications.

4. Discussion and final remarks

In this paper, the SGF method introduced by Garcia-Moliner and Rubio [12] has been extended to the case of superconductor junctions. This has been accomplished by combining that formalism with the Green function description of the superconducting state proposed by Gorkov [9]. The outcome is a formalism which allows direct calculation of the Green function of the whole system, from which relevant physical information, such as local and total densities of states, localised-state energies, and transmission and reflection matrices, can be obtained. To show how the method works, we have chosen a simple problem already discussed by other workers [2, 6, 16].

In comparing the present method with that developed by Arnold [16], we note that they primarily differ in the way followed to calculate the Green functions. More specifically, whereas Arnold calculates the Green functions in the interacting case by

solving an integrodifferential equation which includes the electron–electron interaction through a self-energy, here we have obtained them from a matrix differential operator in which the non-diagonal elements account for the gap function. We think that, within our framework, the usual description of the superconducting state in terms of normal and anomalous Green functions, related to single particles and Cooper pairs respectively, is more clearly shown; on the other hand it also has definite computational advantages. Other technical differences concern the way in which the matching at the interface is carried out.

This formalism could be applied to many interfacial problems in which, as in the case of bulk superconductors, a Green function approach should work efficiently [10, 11]. We refer for instance to the effects of temperature and magnetic fields or to spatially varying gap functions.

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Appendix

Here we derive the well known expression for the transmission coefficient through a constant barrier by means of the Green function formalism. The aim is to provide the formulae required for solving the matching problem in the N–S junction. The model is obtained by letting $\Delta = 0$ in the model used to describe that junction (see section 3.2); here we summarise its main features.

(i) We consider two jellium metals of identical densities.

(ii) The barrier height is taken to be equal to $p_F^2/2$ (all energies referred to the chemical potential).

(iii) As we are interested in energies around the chemical potential, we shall calculate the transmission coefficient at $\omega = 0$.

The Green functions within the barrier are

$$G(z, z', \omega) = \pm(1/p_F)\exp(-p_F|z, z'|). \tag{A1}$$

Hereafter the two signs correspond to the two diagonal elements of the matrix Green function of equation (2) related to electrons and holes. Then, we refer to the system formed by the barrier height (extended to $z = -\infty$) and the metal on the right of figure 1 ($z > d$), as medium 2; its Green function is given by

$$G_2(z, z'; \omega) = \pm(1/p_F)\{\exp(-p_F|z - z'|) \pm i\exp[-p_F(|z - d| + |d - z'|)]\}. \tag{A2}$$

This Green function should be matched, at the interface $z = 0$, to the Green function of

medium 1 given in equation (17). The surface projection of the Green function of the whole system (1 + 2) then becomes

$$\mathcal{G}_s(\omega) = [-i(1 \pm i)/p_F]\{[1 \pm i \exp(-2dp_F)]/[1 + \exp(-2dp_F)]\}. \quad (A3)$$

On the other hand, the product $\mathcal{G}_2^{-1}G_2(0, d)$ required to calculate the transmission coefficient (see equation (20)) is given by

$$\mathcal{G}_2^{-1}G_2(0, d) = (1 \pm i) \exp(-dp_F)/[1 \pm i \exp(-2dp_F)]. \quad (A4)$$

Finally, the transmission coefficient is

$$T_0 = 2 \exp(-dp_F)/[1 + \exp(-2dp_F)] \quad (A5)$$

which coincides with the expression reported in standard quantum mechanical textbooks [23].

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