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The construction of the Green functions for GMR structures of complex geometry

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Abstract

We constructed the one-particle Green functions for two systems exhibiting giant magnetoresistance. The first one is a multilayer with arbitrary magnetization directions of the ferromagnetic layers, exchange splitting of the conducting electron band and intrinsic potential. The second one is a segmented nanowire with spin-dependent electron scattering at the lateral interfaces.

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1. Introduction

Giant magnetoresistance (GMR) is one of the transport phenomena in solid state physics which has attracted considerable attention in the last decade due to its fundamental interest as well as its application potential [1]. The basic mechanism of the effect is the spin-dependent electron scattering in the bulk and on the interfaces. Common objects exhibiting GMR are multilayers; most of the theoretical work on such systems has been devoted to laterally infinite multilayers with collinear (parallel or antiparallel) magnetization of the ferromagnetic layers, but more complicated systems demonstrate more interesting behaviour and invite further investigation.

Besides an *ab initio* treatment on the basis of realistic band structure (cf e.g. [2]), model calculations are widely applied [3, 4] which are able to give a transparent description of the physical phenomena through several parameters such as spin-dependent mean free path, Fermi momentum, etc. In quantum statistical theories the transport characteristics are calculated within the Kubo linear response formalism. This approach requires us to know the Green function (GF) of the system under consideration. If one is dealing with a complex geometrical structure, the calculation of the GF is a cumbersome but important task. As a serious part of the problem the matching of the GF at the interfaces arises. A review of some matching methods

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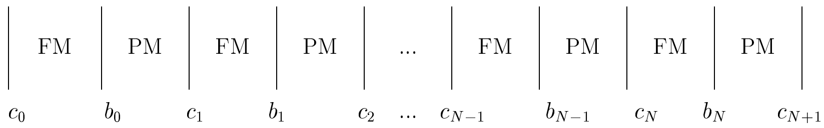

Figure 1. b_i, c_i are the boundaries of the layers.

for the GFs was presented in [5]; in particular, the GF matching for an arbitrary number of interfaces was considered in [6]. Among the investigations of the GMR effect, [7] should be mentioned where the problem of GF matching was considered for collinear magnetization of ferromagnetic layers in the basis of a tight-binding Hamiltonian.

In this paper we consider the construction of the GF for two special systems in the framework of quantum statistical theory [4] proposed for the description of the GMR. The first one is a multilayer with an arbitrary number of layers and arbitrary directions of the magnetization vectors of the ferromagnetic layers in the plane of the layers. We construct an exact GF for this system. The second one is a cylindrical magnetic nanowire consisting of three parts, namely two long ferromagnetic segments separated by a paramagnetic spacer. Spin-dependent electron scattering at the lateral interfaces is taken into account. For this system we construct approximate GF for weak surface scattering.

Following the treatment presented in [4], the free-electron model is used for the conducting s-electrons whose mass is supposed to be much smaller than the mass of the almost localized d-electrons. The mean free path of the conducting s-electrons depends on their spin due to s–d hybridization and the different density of d-states at the Fermi level as a consequence of the exchange splitting of the d-band.

2. GF for multilayers with arbitrary angles between the magnetization vectors

Generalizing the treatment of a trilayer [8], we consider a system consisting of several alternating ferromagnetic and paramagnetic layers, figure 1. The interfaces are considered to be different because of the different direction of the magnetization vector in the ferromagnetic layers. Our aim is to construct a continuous GF with continuous derivatives at the interfaces, but our scheme differs from the method presented in [6] because we use the variation-of-constants method [9] to obtain the GF.

The magnetization of the nth ferromagnetic layer is allowed to subtend an angle γ_n with the quantization axis, and the GF of the conducting electrons is a 2×2 matrix. In the mixed κ, z representation [4] the GF G_n in the nth layer obeys the following equation [8]:

$$\left[\left(\frac{\partial^2}{\partial z^2} + (k^0_{n\mathrm{F}})^2 - \kappa^2 - E_n^{(0)}\right)\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - E_n^{(1)}\begin{pmatrix}\cos\gamma_n & \sin\gamma_n\\ \sin\gamma_n & -\cos\gamma_n\end{pmatrix}\right] \times \begin{bmatrix} G_n^{\uparrow\uparrow}(z,z') & G_n^{\uparrow\downarrow}(z,z') \\ G_n^{\downarrow\uparrow}(z,z') & G_n^{\downarrow\downarrow}(z,z')\end{bmatrix} = \frac{2Ma_0}{\hbar^2}\delta(z-z')\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \tag{1}$$

where a_0 is the lattice constant, M is the electron mass, $(k^0_{n\mathrm{F}})^2 = 2ME_{n\mathrm{F}}/\hbar^2$, $E_{n\mathrm{F}}$ is the Fermi energy in the nth layer, and κ is the in-plane momentum;

$$E_n^{(0)} = \tfrac{1}{2}\left(\Sigma^\uparrow + \Sigma^\downarrow\right) \qquad E_n^{(1)} = \tfrac{1}{2}\left(\Sigma^\uparrow - \Sigma^\downarrow\right) \tag{2}$$

and the real parts of the electron self-energy Σ^σ determine the exchange splitting of the s-electrons with spin σ, whereas the imaginary parts are proportional to the inverse lifetime of the electrons. We impose zero boundary conditions[5] on the GF at the outer interfaces:

$$G(z=0,z') = G(z=c_N,z') = G(z,z'=0) = G(z,z'=c_N) = 0. \quad (3)$$

Therefore the quantization in the direction perpendicular to the layers is taken into account.

The first and second columns of the GF are independent and we can solve the differential equation (1) separately for the pairs $G_n^{\uparrow\uparrow}(z,z')$, $G_n^{\downarrow\uparrow}(z,z')$ and $G_n^{\uparrow\downarrow}(z,z')$, $G_n^{\downarrow\downarrow}(z,z')$.

We now consider a solution for the first column of the matrix equation (1). There are two types of alternating layers: ferromagnetic layers with $E_n^{(1)} \neq 0$ and arbitrary angles γ_n, and paramagnetic layers for which $E_n^{(1)} = 0$. We assume that the first layer is ferromagnetic and the last one is paramagnetic (figure 1).

First of all we will rewrite the initial differential equation:

$$\begin{aligned}
&\left(\frac{\partial^2}{\partial z^2} + (k_{n\mathrm{F}}^0)^2 - \kappa^2 - E_n^{(0)} - E_n^{(1)}\cos\gamma_n\right) G_n^{\uparrow\uparrow}(z,z') - E_n^{(1)}\sin\gamma_n G_n^{\downarrow\uparrow}(z,z') \\
&\qquad = (2Ma_0/\hbar^2)\delta(z-z') \\
&\left(\frac{\partial^2}{\partial z^2} + (k_{n\mathrm{F}}^0)^2 - \kappa^2 - E_n^{(0)} + E_n^{(1)}\cos\gamma_n\right) G_n^{\downarrow\uparrow}(z,z') - E_n^{(1)}\sin\gamma_n G_n^{\uparrow\uparrow}(z,z') = 0.
\end{aligned} \quad (4)$$

In order to assure the continuity of the first derivatives as well as the continuity of the functions themself, it is convenient at this stage to pass to 4×4 notations, adding the derivatives as unknown functions.

Introducing the notation

$$\begin{aligned}
W_n^{\uparrow\uparrow}(z,z') &= \frac{\partial}{\partial z} G_n^{\uparrow\uparrow}(z,z') \\
W_n^{\downarrow\uparrow}(z,z') &= \frac{\partial}{\partial z} G_n^{\downarrow\uparrow}(z,z')
\end{aligned} \quad (5)$$

one can rewrite (4) as a system of first order:

$$\left(\hat{I} \times \frac{\partial}{\partial z} + \hat{L}_n\right) G_n(z,z') = f(z,z') \quad (6)$$

where

$$G_n(z,z') = \begin{pmatrix} G_n^{\uparrow\uparrow}(z,z') \\ W_n^{\uparrow\uparrow}(z,z') \\ G_n^{\downarrow\uparrow}(z,z') \\ W_n^{\downarrow\uparrow}(z,z') \end{pmatrix} \qquad f(z,z') = (2Ma_0/\hbar^2)\begin{pmatrix} 0 \\ \delta(z-z') \\ 0 \\ 0 \end{pmatrix} \quad (7)$$

and the matrix $\hat{L}_n$ (for instance for the nth ferromagnetic layer) is given by

$$\hat{L}_n = \begin{pmatrix} 0 & -1 & 0 & 0 \\ ((k_{n\mathrm{F}}^0)^2 - \kappa^2 - E_n^{(0)} - E_n^{(1)}\cos\gamma_n) & 0 & -E_n^{(1)}\sin\gamma_n & 0 \\ 0 & 0 & 0 & -1 \\ -E_n^{(1)}\sin\gamma_n & 0 & ((k_{n\mathrm{F}}^0)^2 - \kappa^2 - E_n^{(0)} + E_n^{(1)}\cos\gamma_n) & 0 \end{pmatrix}. \quad (8)$$

The method of the variation of constants is usually applied to a system of differential equations with a continuous (or piecewise continuous) right-hand side. We formally apply it to the inhomogeneous system of differential equations (6) whose right-hand side contains a δ function, and verify that our approach is able to give the solution. According to the general

[5] Specific boundary conditions depend on the geometry of the problem. So, for the current in plane problem the zero boundary conditions on the outer interfaces can be used, whereas for the current perpendicular to the plane geometry, the zero boundary conditions at $z = \pm\infty$ for infinitely thick outer layers can be applied.

scheme we first need to construct the fundamental 4×4 matrix whose columns are the linear independent solutions of the homogeneous equation (6):

$$\left(\hat{I} \times \frac{\partial}{\partial z} - \hat{L}_n\right)\phi_n(z) = 0 \tag{9}$$

where ϕ_n is a column.

In the nth ferromagnetic layer equation (9) has four linear independent solutions which can be combined into a 4×4 matrix:

$$\Phi_n^{(0)}(z) = \begin{pmatrix} (1+\cos\gamma_n)\mathrm{e}^{\mathrm{i}k_{n1}z} & (1+\cos\gamma_n)\mathrm{e}^{-\mathrm{i}k_{n1}z} & -\sin\gamma_n\,\mathrm{e}^{\mathrm{i}k_{n2}z} & -\sin\gamma_n\,\mathrm{e}^{-\mathrm{i}k_{n2}z} \\ \mathrm{i}k_{n1}(1+\cos\gamma_n)\mathrm{e}^{\mathrm{i}k_{n1}z} & -\mathrm{i}k_{n1}(1+\cos\gamma_n)\mathrm{e}^{-\mathrm{i}k_{n1}z} & -\mathrm{i}k_{n2}\sin\gamma_n\,\mathrm{e}^{\mathrm{i}k_{n2}z} & \mathrm{i}k_{n2}\sin\gamma_n\,\mathrm{e}^{-\mathrm{i}k_{n2}z} \\ \sin\gamma_n\,\mathrm{e}^{\mathrm{i}k_{n1}z} & \sin\gamma_n\,\mathrm{e}^{-\mathrm{i}k_{n1}z} & (1+\cos\gamma_n)\mathrm{e}^{\mathrm{i}k_{n2}z} & (1+\cos\gamma_n)\mathrm{e}^{-\mathrm{i}k_{n2}z} \\ \mathrm{i}k_{n1}\sin\gamma_n\,\mathrm{e}^{\mathrm{i}k_{n1}z} & -\mathrm{i}k_{n1}\sin\gamma_n\,\mathrm{e}^{-\mathrm{i}k_{n1}z} & \mathrm{i}k_{n2}(1+\cos\gamma_n)\mathrm{e}^{\mathrm{i}k_{n2}z} & -\mathrm{i}k_{n2}(1+\cos\gamma_n)\mathrm{e}^{-\mathrm{i}k_{n2}z} \end{pmatrix} \tag{10}$$

where

$$\begin{aligned} k_{n1} &= \sqrt{(k_{n\mathrm{F}}^{(0)})^2 - \kappa^2 - \Sigma_n^{\uparrow}} = \sqrt{(k_{n\mathrm{F}}^{(\uparrow)})^2 - \kappa^2 + (2\mathrm{i}k_{n\mathrm{F}}^{(\uparrow)}/l_n^{(\uparrow)})} \\ k_{n2} &= \sqrt{(k_{n\mathrm{F}}^{(0)})^2 - \kappa^2 - \Sigma_n^{\downarrow}} = \sqrt{(k_{n\mathrm{F}}^{(\downarrow)})^2 - \kappa^2 + (2\mathrm{i}k_{n\mathrm{F}}^{(\downarrow)}/l_n^{(\downarrow)})}. \end{aligned} \tag{11}$$

Similarly, the basis of the solution of the differential equation for a paramagnetic layer ($E_n^{(1)} = 0$) can be chosen as

$$\Psi_n^{(0)}(z) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k_n z} & \mathrm{e}^{-\mathrm{i}k_n z} & 0 & 0 \\ \mathrm{i}k_n\mathrm{e}^{\mathrm{i}k_n z} & -\mathrm{i}k_n\mathrm{e}^{-\mathrm{i}k_n z} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}k_n z} & \mathrm{e}^{-\mathrm{i}k_n z} \\ 0 & 0 & \mathrm{i}k_n\mathrm{e}^{\mathrm{i}k_n z} & -\mathrm{i}k_n\mathrm{e}^{-\mathrm{i}k_n z} \end{pmatrix} \tag{12}$$

and

$$k_n = \sqrt{(k_{n\mathrm{F}}^{(\mathrm{para})})^2 - \kappa^2 + (2\mathrm{i}k_{n\mathrm{F}}^{(\mathrm{para})}/l_n^{(\mathrm{para})})}. \tag{13}$$

Using equations (10) and (12) we construct four linear independent solutions continuous in the interval $0 \leqslant z \leqslant c_{N+1}$. For our purpose it is convenient to choose solutions of the homogeneous system so that two of them obey the boundary conditions on the left ($F^{(l)}(z)$) and two on the right ($F^{(r)}(z)$) interfaces:

$$F^{(l)}(z) = \begin{cases} c_n \leqslant z \leqslant b_n & \Phi_n^{(0)}(z)\cdot A_n^{(l)} \\ b_n \leqslant z \leqslant c_{n+1} & \Psi_n^{(0)}(z)\cdot R_n^{(l)} \end{cases} \tag{14}$$

and

$$F^{(r)}(z) = \begin{cases} c_n \leqslant z \leqslant b_n & \Phi_n^{(0)}(z)\cdot A_n^{(r)} \\ b_n \leqslant z \leqslant c_{n+1} & \Psi_n^{(0)}(z)\cdot R_n^{(r)} \end{cases} \tag{15}$$

where $A_n^{(l,r)}$, $R_n^{(l,r)}$ are the columns of numbers which provide the corresponding boundary conditions (left or right) and continuity of the functions $F^{(l)}(z)$ and $F^{(r)}(z)$. The thicknesses of the ferromagnetic ($c_n \leqslant z \leqslant b_n$) and paramagnetic ($b_n \leqslant z \leqslant c_{n+1}$) layers can be arbitrary. We impose zero boundary conditions on the 'right' and 'left' solutions at the corresponding end points:

$$\Phi_0^{(0)}(z=0)\cdot A_0^{(l)} = \begin{pmatrix} 0 \\ \cdots \\ 0 \\ \cdots \end{pmatrix} \tag{16}$$

and

$$\Psi^{(0)}(z=c_{N+1})\cdot R_N^{(r)} = \begin{pmatrix} 0 \\ \cdots \\ 0 \\ \cdots \end{pmatrix} \tag{17}$$

where the second and fourth elements of the columns can take arbitrary values since the boundary conditions were imposed only on the functions $G^{\uparrow\uparrow}$, $G^{\downarrow\uparrow}$, not on its derivatives.

The conditions of continuity at the interfaces require

$$\begin{aligned}
&\Phi_n^{(0)}(b_n)A_n^{(l)} = \Psi_n^{(0)}(b_n)R_n^{(l)}\\
&\Phi_{n-1}^{(0)}(b_{n-1})A_{n-1}^{(l)} = \Psi_{n-1}^{(0)}(b_{n-1})R_{n-1}^{(l)}\\
&\Phi_{n-2}^{(0)}(b_{n-2})A_{n-2}^{(l)} = \Psi_{n-2}^{(0)}(b_{n-2})R_{n-2}^{(l)}\\
&\Psi_n^{(0)}(c_{n+1})R_n^{(l)} = \Phi_{n+1}^{(0)}(c_{n+1})A_{n+1}^{(l)}\\
&\Psi_{n-1}^{(0)}(c_n)R_{n-1}^{(l)} = \Phi_n^{(0)}(c_n)A_n^{(l)}\\
&\Psi_{n-2}^{(0)}(c_{n-1})R_{n-2}^{(l)} = \Phi_{n-1}^{(0)}(c_{n-1})A_{n-1}^{(l)}.
\end{aligned} \tag{18}$$

Therefore we get

$$\begin{aligned}
A_n^{(l)} &= \Phi_n^{(0)^{-1}}(c_n)\Psi_{n-1}^{(0)}(c_n)R_{n-1}^{(l)}\\
&= \Phi_n^{(0)^{-1}}(c_n)\Psi_{n-1}^{(0)}(c_n){\Psi_{n-1}^{(0)}}^{-1}(b_{n-1})\Phi_{n-1}^{(0)}(b_{n-1})A_{n-1}^{(l)}\\
&= \Phi_n^{(0)^{-1}}(c_n)\Psi_{n-1}^{(0)}(c_n){\Psi_{n-1}^{(0)}}^{-1}(b_{n-1})\Phi_{n-1}^{(0)}(b_{n-1}){\Phi_{n-1}^{(0)}}^{-1}(c_{n-1})\\
&\quad\times\Psi_{n-2}^{(0)}(c_{n-1}){\Psi_{n-2}^{(0)}}^{-1}(b_{n-2})\\
&\quad\times\Phi_{n-2}^{(0)}(b_{n-2})\ldots\Phi_1^{(0)^{-1}}(c_1)\Psi_0^{(0)}(c_1)\Psi_0^{(0)^{-1}}(b_0)\Phi_0^{(0)}(b_0)A_0^{(l)}.
\end{aligned} \tag{19}$$

Similarly

$$\begin{aligned}
R_n^{(l)} &= \Psi_n^{(0)^{-1}}(b_n)\Phi_n^{(0)}(b_n)A_n^{(l)}\\
&= \Psi_n^{(0)^{-1}}(b_n)\Phi_n^{(0)}(b_n)\Phi_n^{(0)^{-1}}(c_n)\Psi_{n-1}^{(0)}(c_n){\Psi_{n-1}^{(0)}}^{-1}(b_{n-1})\\
&\quad\times\Phi_{n-1}^{(0)}(b_{n-1}){\Phi_{n-1}^{(0)}}^{-1}(c_{n-1})\Psi_{n-2}^{(0)}(c_{n-1}){\Psi_{n-2}^{(0)}}^{-1}(b_{n-2})\\
&\quad\times\Phi_{n-2}^{(0)}(b_{n-2})\ldots\Phi_1^{(0)^{-1}}(c_1)\Psi_0^{(0)}(c_1)\Psi_0^{(0)^{-1}}(b_0)\Phi_0^{(0)}(b_0)A_0^{(l)}.
\end{aligned} \tag{20}$$

$A_n^{(r)}$ and $R_n^{(r)}$ can be determined analogously.

The left and right boundary conditions can be provided by a corresponding choice of the columns $A_0^{(l)}$ and $R_N^{(r)}$. We define four linear independent solutions $F^{(l,1)}$, $F^{(l,2)}$, $F^{(r,1)}$, $F^{(r,2)}$ of the homogeneous equation in the following way: the solutions $F^{(l,1)}(z)$ and $F^{(l,2)}(z)$ are determined by the two columns

$$A_0^{(l,1)} = \begin{pmatrix} 1\\ -1\\ 0\\ 0 \end{pmatrix} \qquad A_0^{(l,2)} = \begin{pmatrix} 0\\ 0\\ 1\\ -1 \end{pmatrix}. \tag{21}$$

Similarly, $F^{(r,1)}(z)$ and $F^{(r,2)}(z)$ are determined by

$$R_N^{(r,1)} = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}kc_{N+1}}\\ -\mathrm{e}^{\mathrm{i}kc_{N+1}}\\ 0\\ 0 \end{pmatrix} \qquad R_N^{(r,2)} = \begin{pmatrix} 0\\ 0\\ \mathrm{e}^{-\mathrm{i}kc_{N+1}}\\ -\mathrm{e}^{\mathrm{i}kc_{N+1}} \end{pmatrix} \tag{22}$$

(note that $F^{(l,1,2)}(0) = F^{(r,1,2)}(c_{N+1}) = 0$). Then we construct the 4×4 fundamental matrix F, whose columns are $F^{(l,1)}$, $F^{(l,2)}$, $F^{(r,1)}$, $F^{(r,2)}$. The elements of the matrix F are the continuous functions of the variable for $0 \leqslant z \leqslant c_{N+1}$. The matrix F is non-singular, so the inverse matrix F^{-1} is defined for all $0 \leqslant z \leqslant c_{N+1}$. We search for the GF, i.e. a solution of the equations (6) and (7) which obeys the zero boundary conditions in the form

$$G(z, z') = F(z)\int_0^z F^{-1}(s)f(s, z')\,\mathrm{d}s + F(z)h(z') \tag{23}$$

where $h(z')$ should be chosen such as to provide the boundary conditions for the GF $G(z, z')$. From equation (23) one can easily get

$$h(z') = -(2Ma_0/\hbar^2)\begin{pmatrix} F_{12}^{-1}(z') \\ F_{22}^{-1}(z') \\ 0 \\ 0 \end{pmatrix}. \tag{24}$$

Then the elements of the GF $G^{\uparrow\uparrow}$, $G^{\downarrow\uparrow}$ are the first and the third elements of the column:

$$G(z > z') = (2Ma_0/\hbar^2)F(z)\begin{pmatrix} 0 \\ 0 \\ F^{-1}(z')_{32} \\ F^{-1}(z')_{42} \end{pmatrix} \tag{25}$$

$$G(z < z') = -(2Ma_0/\hbar^2)F(z)\begin{pmatrix} F^{-1}(z')_{12} \\ F^{-1}(z')_{22} \\ 0 \\ 0 \end{pmatrix}. \tag{26}$$

If the right-hand side of equation (6) is equal to

$$f(z, z') = (2Ma_0/\hbar^2)\begin{pmatrix} 0 \\ 0 \\ 0 \\ \delta(z - z') \end{pmatrix} \tag{27}$$

we get the $G^{\uparrow\downarrow}$, $G^{\downarrow\downarrow}$ as the first and the third elements of the column:

$$G(z > z') = (2Ma_0/\hbar^2)F(z)\begin{pmatrix} 0 \\ 0 \\ F^{-1}(z')_{34} \\ F^{-1}(z')_{44} \end{pmatrix} \tag{28}$$

$$G(z < z') = -(2Ma_0/\hbar^2)F(z)\begin{pmatrix} F^{-1}(z')_{14} \\ F^{-1}(z')_{24} \\ 0 \\ 0 \end{pmatrix}. \tag{29}$$

These are the desired solutions of equation (1).

3. GF for a segmented nanowire with a non-ideal surface

In this section we construct the GF for a cylindrical nanowire consisting of three segments with weak spin-dependent electron scattering at the lateral interface. The one-electron GF $G^\sigma(\vec{r}, \vec{r}')$ for a nanowire of radius R_0 and segment lengths c_j ($j = 1, 3$ for the ferromagnetic segments and $j = 2$ for the paramagnetic spacer) obeys the following equation in the jth segment:

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2} + E^{j\sigma} - \frac{2M}{\hbar^2}V^{j\sigma}\delta(r - r_0)\right)G^\sigma(\vec{r}, \vec{r}') = \frac{2Ma_0}{\hbar^2}\frac{\delta(r - r')}{r}\delta(\theta - \theta')\delta(z - z'). \tag{30}$$

We use cylindrical coordinates, z pointing along the nanowire axis. M is the mass of an electron, a_0 is the lattice constant, $r_0 = R_0 - a_0$. The complex parameter $E^{j\sigma}$ depends on the segment j; it is given by

$$E^{j\sigma} = \frac{2ME}{\hbar^2} + (k_{\mathrm{F}}^{j\sigma})^2 + \mathrm{i}\frac{2k_{\mathrm{F}}^{j\sigma}}{l^{j\sigma}} \tag{31}$$

where E is the energy relative to the Fermi energy, $l^{j\sigma}$ is the mean free path and $k_F^{j\sigma}$ is the Fermi momentum of electrons with spin projection σ in the j-layer. The real part of the bulk coherent potential is included in the Fermi energy. The surface potential is positioned inside the wire at a distance of one lattice parameter from the nanowire surface. Zero boundary conditions are imposed on the GF at the lateral surface:

$$G^\sigma(r = R_0, r', z, z', \theta, \theta') = G^\sigma(r, r' = R_0, z, z', \theta, \theta') = 0. \tag{32}$$

An eigenfunction expansion is used to construct the GF. Starting with the expansion in θ variables:

$$G^\sigma(\vec{r}, \vec{r}') = \sum_n G_n^\sigma(r, r', z, z')\mathrm{e}^{\mathrm{i}n(\theta-\theta')} \tag{33}$$

$G_n^\sigma(r, r', z, z')$ obeys the equation

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{n^2}{r^2} + \frac{\partial^2}{\partial z^2} + \frac{2M}{\hbar^2}E - \frac{2M}{\hbar^2}V^{j\sigma}\delta(r - r_0)\right) G_n^\sigma(r, r', z, z') = \frac{2Ma_0}{\hbar^2}\frac{\delta(r - r')}{r}\delta(z - z'). \tag{34}$$

There are two complications if this is compared to the analogous equation for a multilayer [4]. The first one is the two-dimensional nature of the boundary problem. Moreover, since the imaginary part of the surface potential $V^{j\sigma}$ will be in general nonzero, we deal with a non-selfadjoint boundary problem. In that case one must use a biorthogonal expansion to construct the solution of the corresponding problem [9]. The eigenfunctions of the differential operator

$$\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{n^2}{r^2} - \frac{2M}{\hbar^2}V^{j\sigma}\delta(r - r_0) \tag{35}$$

corresponding to the eigenvalue $-(\nu_{nm}^{j\sigma}/R_0)^2$ are expressed through the Bessel functions of the first and the second kinds:

$$\phi_{nm}(r, j) = \begin{cases} r < r_0 & a_{nm}J_n\left(\nu_{nm}^{j\sigma}\dfrac{r}{R_0}\right) \\ r > r_0 & b_{nm}\left(J_n\left(\nu_{nm}^{j\sigma}\dfrac{r}{R_0}\right) - \dfrac{J_n(\nu_{nm}^{j\sigma})}{Y_n(\nu_{nm}^{j\sigma})}Y_n\left(\nu_{nm}^{j\sigma}\dfrac{r}{R_0}\right)\right). \end{cases} \tag{36}$$

We can also write the eigenfunctions for the adjoint problem:

$$\phi^*_{nm}(r, j) = \begin{cases} r < r_0 & a^*_{nm}J_n\left((\nu_{nm}^{j\sigma})^*\dfrac{r}{R_0}\right) \\ r > r_0 & b^*_{nm}\left(J_n\left((\nu_{nm}^{j\sigma})^*\dfrac{r}{R_0}\right) - \dfrac{J_n(\nu_{nm})}{Y_n((\nu_{nm}^{j\sigma})^*)}Y_n\left((\nu_{nm}^{j\sigma})^*\dfrac{r}{R_0}\right)\right). \end{cases} \tag{37}$$

The constants $a_{nm}, b_{nm}, a^*_{nm}, b^*_{nm}$ and the eigenvalues are defined by the continuity of the eigenfunctions and the jump of the first derivative at $r = r_0$:

$$\begin{aligned} &a_{nm}J_n\left(\nu_{nm}^{j\sigma}\frac{R_0 - a_0}{R_0}\right) = b_{nm}\left(J_n\left(\nu_{nm}^{j\sigma}\frac{R_0 - a_0}{R_0}\right) - \frac{J_n(\nu_{nm}^{j\sigma})}{Y_n(\nu_{nm}^{j\sigma})}Y_n\left(\nu_{nm}^{j\sigma}\frac{R_0 - a_0}{R_0}\right)\right) \\ &b_{nm}\left(J'_n\left(\nu_{nm}^{j\sigma}\frac{R_0 - a_0}{R_0}\right) - \frac{J_n(\nu_{nm}^{j\sigma})}{Y_n(\nu_{nm}^{j\sigma})}Y'_n\left(\nu_{nm}^{j\sigma}\frac{R_0 - a_0}{R_0}\right)\right) - a_{nm}J'_n\left(\nu_{nm}^{j\sigma}\frac{R_0 - a_0}{R_0}\right) \\ &\quad = \frac{2MV}{\hbar^2}a_{nm}J_n\left(\nu_{nm}^{j\sigma}\frac{R_0 - a_0}{R_0}\right). \end{aligned} \tag{38}$$

Equating the determinant of the homogeneous system to zero we find (for a given n) the corresponding numbers $\nu_{nm}^{j\sigma}, \quad m = 1, 2, \ldots$. Similarly, the parameters of the adjoint problem are determined by the systems of equations:

$$a_{nm}^* J_n\left((\nu_{nm}^{j\sigma})^* \frac{R_0 - a_0}{R_0}\right) = b_{nm}^* \left(J_n\left((\nu_{nm}^{j\sigma})^* \frac{R_0 - a_0}{R_0}\right) - \frac{J_n((\nu_{nm}^{j\sigma})^*)}{Y_n((\nu_{nm}^{j\sigma})^*)} Y_n\left((\nu_{nm}^{j\sigma})^* \frac{R_0 - a_0}{R_0}\right)\right)$$

$$b_{nm}^* \left(J_n'\left((\nu_{nm}^{j\sigma})^* \frac{R_0 - a_0}{R_0}\right) - \frac{J_n((\nu_{nm}^{j\sigma})^*)}{Y_n((\nu_{nm}^{j\sigma})^*)} Y_n'\left((\nu_{nm}^{j\sigma})^* \frac{R_0 - a_0}{R_0}\right)\right) \tag{39}$$

$$-a_{nm}^* J_n'\left((\nu_{nm}^{j\sigma})^* \frac{R_0 - a_0}{R_0}\right) = \frac{2MV}{\hbar^2} a_{nm}^* J_n\left((\nu_{nm}^{j\sigma})^* \frac{R_0 - a_0}{R_0}\right)$$

in these formulae $J_n'(\nu_{nm}^{j\sigma} \frac{R_0 - a_0}{R_0})$ means $(\mathrm{d}/\mathrm{d}r) J_n(\nu_{nm}^{j\sigma} \frac{r}{R_0})|_{r=R_0-a_0}$.

For the case of weak surface scattering,

$$\frac{2MV^{j\sigma} a_0^2}{\hbar^2 R_0} \ll 1$$

we get

$$\nu_{nm}^{j\sigma} \approx \nu_{nm}^{(0)} + \frac{2MV^{j\sigma} a_0}{\hbar^2} \frac{a_0}{R_0} \nu_{nm}^{(0)} \left(1 + \frac{2MV^{j\sigma} a_0}{\hbar^2}\right) \tag{40}$$

where $\nu_{nm}^{(0)}$ is the mth root of the Bessel function $J_n(r)$.

Now we represent the GF as

$$G^\sigma(\vec{r}, \vec{r}') = \sum_{nm} \frac{G_{nm}^\sigma(z, z')}{2\pi \|\cdot\|_{nm}} \phi_{nm}^{j\sigma}(r) \phi_{nm}^{j'\sigma *}(r') \mathrm{e}^{\mathrm{i}n(\theta - \theta')} \tag{41}$$

with the norm

$$\|\cdot\|_{nm} = \int_0^{R_0} \phi_{nm}^{j\sigma}(r) \phi_{nm}^{j\sigma *}(r) r \, \mathrm{d}r \tag{42}$$

and $G_{nm}^\sigma(z, z')$ is the solution of the equation:

$$\left(-\left(\frac{\nu_{nm}^{j\sigma}}{R_0}\right)^2 + \frac{2M}{\hbar^2} E + \frac{\partial^2}{\partial z^2}\right) G_{nm}^\sigma(z, z') = \frac{2Ma_0}{\hbar^2} \delta(z - z'). \tag{43}$$

There is an essential difference from the case of an ideal lateral surface which originates from the fact that

$$\int_0^{R_0} \phi_{nm}(r, j) \phi_{nl}^*(r, k) r \, \mathrm{d}r = \delta_{lm}$$

only for $j = k$ whereas for different segments there is no such orthonormality. In other words the biorthogonal systems ϕ, ϕ^* depend on the segment to which the coordinate z belongs.

We now construct the approximate GF in the entire region. Let us divide the plane $\{z, z'\}$ into the following sections: $z = 0$, $z = c_2$, $z' = 0$, $z' = c_2$.
The region where $z < 0$, $z' < 0$ is marked as '11',
the region where $0 < z < c_2$, $z' < 0$ is marked as '21',
the region where $c_2 < z$, $z' < 0$ is marked as '31',
the region where $z < 0$, $0 < z' < c_2$ is marked as '12',

the region where $0 < z < c_2$, $0 < z' < c_2$ is marked as '22',
the region where $c_2 < z$, $0 < z' < c_2$ is marked as '32',
the region where $z < 0$, $c_2 < z'$ is marked as '13',
the region where $0 < z < c_2$, $c_2 < z'$ is marked as '23',
the region where $c_2 < z$, $c_2 < z'$ is marked as '33'.

The angle dependence $\exp\{\mathrm{i}n(\theta - \theta')\}$ is the same for all components of the GF. Thus for all k, j (k, j mark the segments to which the coordinates z and z' belong, respectively) we have

$$G^{\sigma kj}(r, r', z, z', \theta, \theta') = \sum_n G_n^{\sigma kj}(r, r', z, z') \exp\{\mathrm{i}n(\theta - \theta')\}. \tag{44}$$

We find that the diagonal functions have the following form:

$$G_n^{\sigma kk}(r, r', z, z') = \sum_{nm} G_{nm}^{\sigma kk}(z, z')\phi_{nm}(r, k)\phi_{nm}^*(r', k) \tag{45}$$

and the $G_{nm}^{\sigma kk}(z, z')$ are in the region where $z < 0$ and $z' < 0$:

$$\begin{aligned} G_{nm}^{\sigma 11}(z > z') &= \mathrm{e}^{-\mathrm{i}Q_{nm}^{1\sigma} z'}\left(a_{nm}^{11}\mathrm{e}^{\mathrm{i}Q_{nm}^{1\sigma} z} + b_{nm}^{11}\mathrm{e}^{-\mathrm{i}Q_{nm}^{1\sigma} z}\right) \\ G_{nm}^{\sigma 11}(z < z') &= \mathrm{e}^{-\mathrm{i}Q_{nm}^{1\sigma} z}\left(a_{nm}^{11}\mathrm{e}^{\mathrm{i}Q_{nm}^{1\sigma} z'} + b_{nm}^{11}\mathrm{e}^{-\mathrm{i}Q_{nm}^{1\sigma} z'}\right) \end{aligned} \tag{46}$$

in the region where $c_2 < z$ and $c_2 < z'$:

$$\begin{aligned} G_{nm}^{\sigma 33}(z > z') &= \mathrm{e}^{\mathrm{i}Q_{nm}^{3\sigma} z}\left(a_{nm}^{33}\mathrm{e}^{\mathrm{i}Q_{nm}^{3\sigma} z'} + b_{nm}^{33}\mathrm{e}^{-\mathrm{i}Q_{nm}^{3\sigma} z'}\right) \\ G_{nm}^{\sigma 33}(z < z') &= \mathrm{e}^{\mathrm{i}Q_{nm}^{3\sigma} z'}\left(a_{nm}^{33}\mathrm{e}^{\mathrm{i}Q_{nm}^{3\sigma} z} + b_{nm}^{33}\mathrm{e}^{-\mathrm{i}Q_{nm}^{3\sigma} z}\right) \end{aligned} \tag{47}$$

and in the region '22', where $0 < z < c_2$, $0 < z' < c_2$:

$$G_{nm}^{\sigma 22}(z > z') = \mathrm{e}^{\mathrm{i}Q_{nm}^{2\sigma} z}\left(a_{nm}^{22}\mathrm{e}^{\mathrm{i}Q_{nm}^{2\sigma} z'} + \tilde{a}_{nm}^{22}\mathrm{e}^{-\mathrm{i}Q_{nm}^{2\sigma} z'}\right) + \mathrm{e}^{-\mathrm{i}Q_{nm}^{2\sigma} z}\left(b_{nm}^{22}\mathrm{e}^{\mathrm{i}Q_{nm}^{2\sigma} z'} + \tilde{b}_{nm}^{22}\mathrm{e}^{-\mathrm{i}Q_{nm}^{2\sigma} z'}\right). \tag{48}$$

We introduced the notation:

$$Q_{nm}^{j\sigma} = \sqrt{(k_{\mathrm{F}}^{j\sigma})^2 - \left(\frac{\nu_{nm}^{(0)} + \kappa_{nm}^{j\sigma}}{R_0}\right)^2 + \frac{2\mathrm{i}k_{\mathrm{F}}^{j\sigma}}{l^{j\sigma}}} \tag{49}$$

and $G_{nm}^{\sigma 22}(z < z')$ can be obtained from $G_{nm}^{\sigma 22}(z > z')$ by interchanging the variables z and z'. The nondiagonal GFs (we write them only in the region $z > z'$ because of the symmetry of the GF) have the following form:
In the region $0 < z < c_2$, $z' < 0$:

$$G_n^{\sigma 21} = \sum_{ml}\left(A_{nml}^{21}\mathrm{e}^{-\mathrm{i}Q_{nl}^{1\sigma} z'}\mathrm{e}^{\mathrm{i}Q_{nm}^{2\sigma} z} + B_{nml}^{21}\mathrm{e}^{-\mathrm{i}Q_{nl}^{1\sigma} z'}\mathrm{e}^{-\mathrm{i}Q_{nm}^{2\sigma} z}\right)\phi_{nm}(r, 2)\phi_{nl}^*(r, 1) \tag{50}$$

in the region $c_2 < z$, $0 < z' < c_2$:

$$G_n^{\sigma 32} = \sum_{ml}\left(A_{nml}^{32}\mathrm{e}^{\mathrm{i}Q_{nm}^{3\sigma} z}\mathrm{e}^{\mathrm{i}Q_{nl}^{2\sigma} z'} + B_{nml}^{32}\mathrm{e}^{\mathrm{i}Q_{nm}^{3\sigma} z}\mathrm{e}^{-\mathrm{i}Q_{nl}^{2\sigma} z'}\right)\phi_{nm}(r, 3)\phi_{nl}^*(r, 2) \tag{51}$$

and in the region $c_2 < z, z' < 0$:

$$G_n^{\sigma 31} = \sum_{ml} A_{nml}^{31} \mathrm{e}^{\mathrm{i}Q_{nm}^{3\sigma} z} \mathrm{e}^{-\mathrm{i}Q_{nl}^{1\sigma} z'} \phi_{nm}(r,3)\phi_{nl}^*(r,1). \tag{52}$$

The supposed form (46)–(52) of the GF makes it possible to calculate it to first order of V. The coefficients A and B can be calculated from the conditions of the continuity of $G_n(r, r', z, z')$ and their derivatives.

As an example we present the calculation for the boundary '22' ↔ '21':

$$\sum_m [(a_{nm}^{22} + \tilde{a}_{nm}^{22})\mathrm{e}^{\mathrm{i}Q_{nm}^{2\sigma} z} + (b_{nm}^{22} + \tilde{b}_{nm}^{22})\mathrm{e}^{-\mathrm{i}Q_{nm}^{2\sigma} z}]\phi_{nm}(r,2)\phi_{nm}^*(r,2)$$
$$= \sum_{ml} [A_{nml}^{21} \mathrm{e}^{\mathrm{i}Q_{nm}^{2\sigma} z} + B_{nml}^{21} \mathrm{e}^{-\mathrm{i}Q_{nm}^{2\sigma} z}]\phi_{nm}(r,2)\phi_{nl}^*(r,1). \tag{53}$$

Since the same basis function $\phi_{nm}(r, 2)$ appears in both parts, we can multiply the equation by $\phi_{nm}^*(r, 2)r$ and integrate over r from 0 to R_0. We obtain

$$\begin{aligned} (a_{nm}^{22} + \tilde{a}_{nm}^{22})\phi_{nm}^*(r,2) &= \sum_l A_{nml}^{21}\phi_{nl}^*(r,1) \\ (b_{nm}^{22} + \tilde{b}_{nm}^{22})\phi_{nm}^*(r,2) &= \sum_l B_{nml}^{21}\phi_{nl}^*(r,1). \end{aligned} \tag{54}$$

Similarly, multiplying both sides by $\phi_{nm}(r, 2)r'$ and integrating over r' from 0 to R_0 we get

$$\begin{aligned} a_{nm}^{22} + \tilde{a}_{nm}^{22} &= \sum_l A_{nml}^{21} \int \phi_{nm}(r,2)\phi_{nl}^*(r,1)r'\,\mathrm{d}r' \\ b_{nm}^{22} + \tilde{b}_{nm}^{22} &= \sum_l B_{nml}^{21} \int \phi_{nm}(r,2)\phi_{nl}^*(r,1)r'\,\mathrm{d}r'. \end{aligned} \tag{55}$$

The equations for the continuity of derivatives have the form:

$$\begin{aligned} \mathrm{i}Q_{nm}^{2\sigma}(a_{nm}^{22} - \tilde{a}_{nm}^{22})\phi_{nm}^*(r,2) &= \sum_l (-\mathrm{i}Q_{nl}^{1\sigma})A_{nml}^{21}\phi_{nl}^*(r,1) \\ \mathrm{i}Q_{nm}^{2\sigma}(b_{nm}^{22} - \tilde{b}_{nm}^{22})\phi_{nm}^*(r,2) &= \sum_l (-\mathrm{i}Q_{nl}^{1\sigma})B_{nml}^{21}\phi_{nl}^*(r,1) \end{aligned} \tag{56}$$

or, after the same integration:

$$\begin{aligned} a_{nm}^{22} - \tilde{a}_{nm}^{22} &= \sum_l \left(\frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right) A_{nml}^{21}\Phi_{nml}^{21} \\ b_{nm}^{22} - \tilde{b}_{nm}^{22} &= \sum_l \left(\frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right) B_{nml}^{21}\Phi_{nml}^{21} \end{aligned} \tag{57}$$

where the following notations are introduced:

$$\Phi_{nml}^{kj} = \int_0^R \phi_{nm}(r|k)\phi_{nl}^*(r|j)r\,\mathrm{d}r. \tag{58}$$

Therefore, we find

$$
\begin{aligned}
a_{nm}^{22} &= \frac{1}{2}\sum_{l}\left(1-\frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right)A_{nml}^{21}\Phi_{nml}^{21} \\
\tilde{a}_{nm}^{22} &= \frac{1}{2}\sum_{l}\left(1+\frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right)A_{nml}^{21}\Phi_{nml}^{21} \\
b_{nm}^{22} &= \frac{1}{2}\sum_{l}\left(1-\frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right)B_{nml}^{21}\Phi_{nml}^{21} \\
\tilde{b}_{nm}^{22} &= \frac{1}{2}\sum_{l}\left(1+\frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right)B_{nml}^{21}\Phi_{nml}^{21}.
\end{aligned}
\tag{59}
$$

Similar equations can be written for the other boundaries. The number of equations is more than the number of unknown coefficients: nevertheless, the system is consistent. We find that

$$
\begin{aligned}
A_{nml}^{31} = A_{nll}^{31}\delta_{ml} = (2\mathrm{e}^{-\mathrm{i}Q_{nl}^{3\sigma}c_2})\Bigg\{\mathrm{i}\sum_{m}(Q_{nm}^{2\sigma})^{-1}\big\{(Q_{nl}^{1\sigma}-Q_{nm}^{2\sigma})(Q_{nm}^{2\sigma}-Q_{nl}^{3\sigma})\mathrm{e}^{\mathrm{i}Q_{nm}^{2\sigma}c_2} \\
+(Q_{nl}^{1\sigma}+Q_{nm}^{2\sigma})(Q_{nm}^{2\sigma}+Q_{nl}^{3\sigma})\mathrm{e}^{-\mathrm{i}Q_{nm}^{2\sigma}c_2}\big\}\Phi_{nlm}^{32}\Phi_{nml}^{21}\Bigg\}^{-1}
\end{aligned}
\tag{60}
$$

$$
A_{nml}^{21} = \frac{1}{2}\left(1+\frac{Q_{nl}^{3\sigma}}{Q_{nm}^{2\sigma}}\right)\mathrm{e}^{\mathrm{i}(Q_{nl}^{3\sigma}-Q_{nm}^{2\sigma})c_2}\Phi_{nlm}^{32}A_{nll}^{31}
\tag{61}
$$

$$
B_{nml}^{21} = \frac{1}{2}\left(1-\frac{Q_{nl}^{3\sigma}}{Q_{nm}^{2\sigma}}\right)\mathrm{e}^{\mathrm{i}(Q_{nl}^{3\sigma}-Q_{nm}^{2\sigma})c_2}\Phi_{nlm}^{32}A_{nll}^{31}
\tag{62}
$$

$$
A_{nml}^{32} = \frac{1}{2}\left(1-\frac{Q_{nm}^{1\sigma}}{Q_{nl}^{2\sigma}}\right)\Phi_{nlm}^{21}A_{nmm}^{31}
\tag{63}
$$

$$
B_{nml}^{32} = \frac{1}{2}\left(1+\frac{Q_{nm}^{1\sigma}}{Q_{nl}^{2\sigma}}\right)\Phi_{nlm}^{21}A_{nmm}^{31}
\tag{64}
$$

$$
\begin{aligned}
a_{nm}^{33} = \frac{1}{4}\sum_{l}\Bigg\{\left(1+\frac{Q_{nl}^{2\sigma}}{Q_{nm}^{3\sigma}}\right)\left(1-\frac{Q_{nm}^{1\sigma}}{Q_{nl}^{2\sigma}}\right)\mathrm{e}^{\mathrm{i}(Q_{nl}^{2\sigma}-Q_{nm}^{3\sigma})c_2} \\
+\left(1-\frac{Q_{nl}^{2\sigma}}{Q_{nm}^{3\sigma}}\right)\left(1+\frac{Q_{nm}^{1\sigma}}{Q_{nl}^{2\sigma}}\right)\mathrm{e}^{-\mathrm{i}(Q_{nl}^{2\sigma}+Q_{nm}^{3\sigma})c_2}\Bigg\}\Phi_{nlm}^{21}\Phi_{nml}^{32}A_{nmm}^{31}
\end{aligned}
\tag{65}
$$

$$
\begin{aligned}
b_{nm}^{11} = \frac{1}{4}\sum_{l}\Bigg\{\left(1-\frac{Q_{nl}^{2\sigma}}{Q_{nm}^{1\sigma}}\right)\left(1+\frac{Q_{nm}^{3\sigma}}{Q_{nl}^{2\sigma}}\right)\mathrm{e}^{\mathrm{i}(Q_{nm}^{3\sigma}-\mathrm{i}Q_{nl}^{2\sigma})c_2} \\
+\left(1+\frac{Q_{nl}^{2\sigma}}{Q_{nm}^{1\sigma}}\right)\left(1-\frac{Q_{nm}^{3\sigma}}{Q_{nl}^{2\sigma}}\right)\mathrm{e}^{\mathrm{i}(Q_{nm}^{3\sigma}+Q_{nl}^{2\sigma})c_2}\Bigg\}\Phi_{nml}^{32}\Phi_{nlm}^{21}A_{nmm}^{31}
\end{aligned}
\tag{66}
$$

$$
a_{nm}^{22} = \frac{1}{4}\sum_{l}\left(1+\frac{Q_{nl}^{3\sigma}}{Q_{nm}^{2\sigma}}\right)\left(1-\frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right)\mathrm{e}^{\mathrm{i}(Q_{nl}^{3\sigma}-Q_{nm}^{2\sigma})c_2}\Phi_{nlm}^{32}\Phi_{nml}^{21}A_{nll}^{31}
\tag{67}
$$

$$
\tilde{a}_{nm}^{22} = \frac{1}{4}\sum_{l}\left(1+\frac{Q_{nl}^{3\sigma}}{Q_{nm}^{2\sigma}}\right)\left(1+\frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right)\mathrm{e}^{\mathrm{i}(Q_{nl}^{3\sigma}-Q_{nm}^{2\sigma})c_2}\Phi_{nlm}^{32}\Phi_{nml}^{21}A_{nll}^{31}
\tag{68}
$$

$$b_{nm}^{22} = \frac{1}{4}\sum_l \left(1 - \frac{Q_{nl}^{3\sigma}}{Q_{nm}^{2\sigma}}\right)\left(1 - \frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right) \mathrm{e}^{\mathrm{i}(Q_{nl}^{3\sigma}+Q_{nm}^{2\sigma})c_2} \Phi_{nlm}^{32}\Phi_{nml}^{21}A_{nll}^{31} \tag{69}$$

$$\tilde{b}_{nm}^{22} = \frac{1}{4}\sum_l \left(1 + \frac{Q_{nl}^{1\sigma}}{Q_{nm}^{2\sigma}}\right)\left(1 - \frac{Q_{nl}^{3\sigma}}{Q_{nm}^{2\sigma}}\right) \mathrm{e}^{\mathrm{i}(Q_{nl}^{3\sigma}-Q_{nm}^{2\sigma})c_2} \Phi_{nlm}^{32}\Phi_{nml}^{21}A_{nll}^{31}. \tag{70}$$

Thus we have constructed a one-particle GF for the problem (30). The deviation from the delta function in the right-hand side (43) is as small as $2MVa_0^2/(\hbar^2 R_0)$.

For the case of an ideal surface, i.e. zero surface potential, the equations for the coefficients reduce to the equation obtained for infinite multilayers by Vedyayev *et al* [4].

4. Conclusion

The problem of GF matching arises in various physical situations. The specific form of the problem depends on the model and the approach. We note that both problems considered here go back to the laterally infinite trilayer problem with collinear magnetization exhibiting GMR. At the same time the transport characteristics of these systems for which we constructed the GFs demonstrate new features if compared to simple multilayers. In our work reported here we constructed exact one-electron GF for the problem (1). In this model the intrinsic potential and exchange splitting of the conducting electron band is taken into account by different Fermi momenta for spin-up and spin-down electrons in the ferromagnetic layers and by their difference from the Fermi momentum in the paramagnetic layers. The role of the exchange splitting of the conducting band as well as the role of the intrinsic potential in the mechanism of GMR can be quite noticeable (see correspondingly [8] and [10]). The transport characteristics as functions of external magnetic field display a great diversity of behaviour, depending on the specific choice of the paramagnetic layers' thicknesses [11].

We also constructed approximate GF for the problem (30). The segmented nanowires are intensively studied objects [12]. The role of the surface spin-dependent scattering can be very important, particularly for nanowires of small radii. The complex surface potential transforms the problem into a two-dimensional one in contrast with the case of laterally infinite multilayers. Our calculations [13] show that, even for weak surface scattering, the GMR displays a complicated behaviour due to the interplay between spin-dependent electron scattering in the bulk and at the lateral interface.

The form of the GFs obtained here permits us to numerically investigate the transport characteristics of the systems.

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