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Ballistic conductance of a quantum sphere

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Abstract
The conductance of a quantum sphere with two one-dimensional wires attached to it is investigated. An explicit form for the conductance as a function of the chemical potential is found from first principles. The form and positions of the resonance maxima on the plot of the conductance are studied.

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1. Introduction

Recent progress in nanotechnology has stimulated interest in the study of electron properties of curved and non-flat nanostructures. A number of new physical phenomena have been discussed in the last few years. We mention, for example, the Aharonov–Bohm oscillations in quantum rings, the conductance quantization for a two-dimensional electron gas in a frustum of a sphere [1], resistance oscillations in a circular quasiballistic interferometer [2], and so forth. The two-dimensional electron gas on a small sphere may be considered as the simplest example of quantum systems with non-flat geometry [3, 4].

The purpose of this paper is a theoretical study of the ballistic electron transport in a nanodevice consisting of a sphere with two wires attached to it. We consider an idealized model in which the wires are taken to be one dimensional. This crucial simplification is based on the possibility of describing the electron motion in nanowires only by means of the longitudinal part of the wavefunctions. The considered idealization is possible only when the cross-section of the real wire is much less than the typical sizes of the system. In particular, our model works only in the case of relatively large distance r between the points of gluing the wires to the sphere; for example, we shall suppose r is vastly larger than the Fermi wavelength λ_F.

The central problem with the systems of the considered type is the finding of a procedure to match wavefunctions at the points of the junction of the wires and the nanosphere. There are two approaches to the problem. The most widespread method is based on introducing

an '*a priori*' scattering matrix at the points of the junction in such a way that the current conservation law and the time reversal symmetry are satisfied. In the simplest case of two wires, this scattering matrix is determined by six real parameters; the selection of these parameters requires additional assumptions: reality of matrix elements, the specific smallness for certain of them, and so on (we refer to [5] for a detailed discussion). Another way of looking at the problem of finding the scattering matrix has been proposed in [6, 7], it has already been used for analysing the ballistic transport in [8–10]. In the framework of this approach, the scattering matrix at the points of the junction is introduced in the usual way as the scattering matrix for a perturbation of the free Hamiltonian H^0 of the device (H^0 is the direct sum of the free Hamiltonians of an electron on the sphere and in the wires). This perturbation is determined by the boundary conditions at the points of the junctions. Therefore, the elements of the scattering matrix are expressed in terms of boundary conditions, which have a direct physical interpretation similar to those in the zero-range potential theory. In turn, these boundary conditions lead to the appearance of phenomenological parameters in the scattering matrix such as the scattering length for a zero-range potential [11–13]. We use this alternative approach to the scattering problem in the present paper. A useful mathematical formalization of the approach considered here is founded on the Krein resolvent formula [13], and gives the scattering matrix in terms of the renormalized Green functions for the free Hamiltonians on the sphere and in the wires.

2. Hamiltonian of the device

Consider a nanodevice consisting of a conducting sphere $\mathbf{S}$ of radius a and two wires $\mathbf{R}_1^+$ and $\mathbf{R}_2^+$ attached to $\mathbf{S}$ at points q_1 and q_2, respectively, by gluing the point 0 from $\mathbf{R}_j^+ = \{x : x \geqslant 0\}$ to the point q_j. If the wires are isolated from the sphere, then the electron Hamiltonian H^0 of the device is the direct sum of the Hamiltonian H_S of a free electron on the sphere and the Hamiltonians H_j ($j = 1, 2$) of non-interacting free electrons in the wires: $H^0 = H_S \oplus H_1 \oplus H_2$. For convenience, we choose the Neumann boundary conditions at the point 0 for H_j; as to H_S, we recall that $H_S = (2m^*a^2)^{-1}\boldsymbol{L}^2$, where $\boldsymbol{L}$ is the angular momentum operator and m^* is the electron effective mass. A wavefunction ψ of the device consists of three parts: ψ_S, ψ_1, ψ_2, where ψ_S is a function on $\mathbf{S}$, and ψ_j ($j = 1, 2$) are functions on $\mathbf{R}_j^+$. It is convenient to consider ψ as a one-column matrix

$$\psi = \begin{pmatrix} \psi_S \\ \psi_1 \\ \psi_2 \end{pmatrix}. \tag{1}$$

The gluing of the wires to the sphere involves the appearance of non-trivial boundary conditions for ψ_S, ψ_1 and ψ_2 at points q_j. The role of boundary values for ψ_1 and ψ_2 is played, of course, by $\psi_j(0)$ and $\psi_j'(0)$. The zero-range potential theory shows that the role of boundary values for ψ_S is played by coefficients of asymptotics of ψ_S near the points q_j [11, 12]. More precisely, let $G_S(x, y; z)$ be the Green function for the Hamiltonian H_S. Then

$$G_S(x, q_j; z) = -m^*(\pi\hbar^2)^{-1} \ln \rho(x, q_j) + F_1(x, q_j; z) + o(1) \tag{2}$$

as $x \to q_j$, where $\rho(x, y)$ is the geodesic distance between points x and y on the sphere, and $F_1(x, y; z)$ is a continuous function of (x, y). According to equation (2), the component ψ_S of an eigenfunction ψ for the Hamiltonian H of the device has the following asymptotic behaviour near the point q_j:

$$\psi_S(x) = -m^*(\pi\hbar^2)^{-1} a_j(\psi_S) \ln \rho(x, q_j) + b_j(\psi_S) + o(1). \tag{3}$$

The complex coefficients a_j and b_j play the role of boundary values for ψ_S at the points q_j. We will consider the Hamiltonians H which are determined by the boundary conditions of the form

$$\begin{cases} b_j(\psi_S) = \sum_{k=1}^{2} [\beta_{jk} a_k(\psi_S) + \alpha_{jk} \psi_k(0)] \\ \psi_j'(0) = \sum_{k=1}^{2} [\alpha_{jk} a_k(\psi_S) + \gamma_{jk} \psi_k(0)] \end{cases} \tag{4}$$

where $a_k(\psi_S)$ and $b_j(\psi_S)$ are defined by equation (3). The parameters α_{jk}, β_{jk} and γ_{jk} in equation (4) form 2×2 matrices A, B and C, respectively, such that the 4×4 matrix

$$P = \begin{bmatrix} B & A \\ A^+ & C \end{bmatrix}$$

is Hermitian. From the point of view of the zero-range potential theory, the elements of B are the strengths of a point perturbation of H_S at the points q_j. The non-diagonal elements of this matrix correspond to a non-local tunnelling from the point q_j of the gluing to another one [13]. Therefore, if $\lambda_F \ll r \equiv \rho(q_1, q_2)$, then the matrix B has to be diagonal. Similarly, C has to be diagonal, too. In this case γ_{jj} is the strength of a point perturbation of H_j at the point 0 from $\mathbf{R}_j^+$. As for the matrix A, it is responsible for the transmission from the wires to the sphere. Indeed, if $A = 0$, then boundary conditions (4) decompose. This means that there is no transmission from the wires into the sphere. Therefore, the parameters α_{jj} determine the transmission probability from the wires $\mathbf{R}_j^+$ to the sphere $\mathbf{S}$ through the point q_j. If $\alpha_{jk} \neq 0$ for $j \neq k$ there are non-trivial boundary conditions which connect the wire $\mathbf{R}_j^+$ with the point q_k; therefore, we must suppose A to be diagonal. Further we will consider in detail the case of scalar matrices A, B and C:

$$\alpha_{11} = \alpha_{22} \equiv \alpha \qquad \beta_{11} = \beta_{22} \equiv \beta \qquad \gamma_{11} = \gamma_{22} \equiv \gamma. \tag{5}$$

In this case the wires $\mathbf{R}_j^+$ are glued to the sphere alike. In the general case of diagonal matrices B and C, their elements β_{jj} and γ_{jj} are expressed in terms of scattering lengths λ_j^b and λ_j^c on the corresponding zero-range potentials: $\gamma_{jj} = -m^* \lambda_j^c / 2\hbar^2$ [13], $\beta_{jj} = -m^* \ln(\lambda_j^b) / \pi\hbar^2$ [12]. If $\beta_{11} = \beta_{22}$ (respectively, $\gamma_{11} = \gamma_{22}$), then we will denote simply $\lambda_{jj}^b \equiv \lambda^b$ (respectively, $\lambda_{jj}^c \equiv \lambda^c$). It will be convenient to express $|\alpha_{jj}|$ in terms of a quantity with the dimension of length: $|\alpha_{jj}|^2 = m^{*2} \lambda_j^a / \hbar^4$ (and denote $\lambda_j^a \equiv \lambda^a$, if $\alpha_{11} = \alpha_{22}$).

Now using the Krein resolvent formula [13] we are able to get an explicit form for the Green function G for H in terms of the Green function G^0 for H^0 and the matrix of boundary conditions P. First of all, using the matrix notation (1) for the wavefunctions we represent G^0 as the following 3×3 matrix

$$G^0(x, y; z) = \begin{pmatrix} G_S(x, y; z) & 0 & 0 \\ 0 & G_1(x, y; z) & 0 \\ 0 & 0 & G_2(x, y; z) \end{pmatrix} \tag{6}$$

where G_j $(j = 1, 2)$ are the Green functions of H_j. We need below the so-called Krein $\mathcal{Q}$-function $Q(z)$. In our case it is an analytic matrix-valued function of the spectral parameter z with the following block structure:

$$Q(z) = \begin{pmatrix} Q_S(z) & 0 & 0 \\ 0 & G_1(0, 0; z) & 0 \\ 0 & 0 & G_2(0, 0; z) \end{pmatrix} \tag{7}$$

where $Q_S(z)$ is a 2×2 matrix with elements

$$Q_S^{jk}(z) = \begin{cases} F_1(q_j, q_k; z) & \text{if} \quad j = k \\ G_S(q_j, q_k; z) & \text{otherwise} \end{cases} \tag{8}$$

(recall that F_1 is given by equation (2)). Now the Krein resolvent formula reads

$$G(x, y; z) = G^0(x, y; z) - \Gamma(z)[Q(z) - P]^{-1}\Gamma^+(z^*). \tag{9}$$

We call attention to the form of the Green function G. Since a state vector for H has the form of the one-column matrix (1), G is represented as a 3×3 matrix with operator elements. In equation (9) G^0 is a diagonal matrix of form (6), and the second term in equation (9) is a finite-dimensional operator of the form

$$\sum_{j,k=1}^{3} \xi_{jk}(z)|\tilde{\varphi}_j(x; z)\rangle\langle\varphi_k(y; z)|.$$

To get the terms of the last sum it is necessary to multiply the scalar 4×4 matrix $[Q_S(z) - P]^{-1}$ by the 3×4 matrix $\Gamma(z)$ and the 4×3 matrix $\Gamma^+(z^*)$ with operators as elements. Here

$$\Gamma(x; z) = \begin{pmatrix} |G_S(x, q_1; z)\rangle & |G_S(x, q_2; z)\rangle & 0 & 0 \\ 0 & 0 & |G_1(x, 0; z)\rangle & 0 \\ 0 & 0 & 0 & |G_2(x, 0; z)\rangle \end{pmatrix} \tag{10}$$

therefore

$$\Gamma^+(x; z^*) = \begin{pmatrix} \langle G_S(q_1, y; z)| & 0 & 0 \\ \langle G_S(q_2, y; z)| & 0 & 0 \\ 0 & \langle G_1(0, y; z)| & 0 \\ 0 & 0 & \langle G_2(0, y; z)| \end{pmatrix}. \tag{11}$$

The use of the Krein formula is based on knowledge of the explicit forms of the matrices G^0 and Q. Indeed,

$$G_S(x, y; z) = \frac{m^*}{2\hbar^2 \cos(\pi t)} \mathcal{P}_{t-\frac{1}{2}}(\cos(\rho(x, y)/a)). \tag{12}$$

Here $\mathcal{P}_\nu(x)$ is the Legendre function and $t(k) = \sqrt{a^2k^2 + 1/4}$, where $k = \sqrt{2m^*z/\hbar^2}$ is the electron wave vector [14]. The Green functions for the wires have the form

$$G_1(x, y; k^2) = G_2(x, y; k^2) = \frac{\mathrm{i}m^*}{\hbar^2 k} (\exp(\mathrm{i}k|x - y|) + \exp(\mathrm{i}k(x + y)). \tag{13}$$

From equations (2) and (12), we get the diagonal elements of $Q_S(z)$

$$Q_S^{11} = Q_S^{22} = -\frac{m^*}{\pi\hbar^2} \left[\Psi\left(\frac{1}{2} + t\right) - \frac{\pi}{2} \tan(\pi t) - \ln(2a) + C_E \right] \tag{14}$$

where $\Psi(x)$ is the logarithmic derivative of the Euler Γ-function (i.e. the digamma function) and C_E is the Euler constant. For convenience, we mention the other elements of the matrix $Q(z)$

$$Q_S^{12}(z) = Q_S^{21}(z) = -\frac{m^*}{2\hbar^2} \frac{1}{\cos(\pi t)} \mathcal{P}_{t-\frac{1}{2}}(-\cos(r/a)) \tag{15}$$

and

$$G_1(0, 0; k^2) = G_2(0, 0; k^2) = 2\mathrm{i}m^*(\hbar^2 k)^{-1}. \tag{16}$$

3. Scattering matrix

The Krein formula (9) shows immediately that the general form of the wavefunction for H is the following

$$\psi = \psi^0 - \Gamma(z)[Q(z) - P]^{-1}\Gamma^+(z^*)(H^0 - z)\psi^0 \tag{17}$$

where $\operatorname{Im} z \neq 0$, and ψ^0 is an arbitrary wavefunction of H^0. Substituting in equation (17) ψ^0 of the form (1) with $\psi_S^0 = \psi_2^0 = 0$, $\psi_1^0(x) = \exp(\mathrm{i}kx) + \exp(-\mathrm{i}kx)$, we find a state vector ψ for H which is the superposition of an incoming and outgoing wave in the channel $\mathbf{R}_1^+$ and an outgoing wave in the channel $\mathbf{R}_2^+$. In the most important case $\gamma_{11} = \gamma_{22}$, we get the scattering matrix $S(E)$ in the form

$$S(E) = \left[C + A^*(Q_S(E) - B)^{-1}A + \frac{2m^*\mathrm{i}}{\hbar^2 k}\right]\left[C + A^+(Q_S(E) - B)^{-1}A - \frac{2m^*\mathrm{i}}{\hbar^2 k}\right]^{-1} \tag{18}$$

(recall that $k = \sqrt{2m^*E/\hbar^2}$). It is easy to show that the matrix S is unitary; it is symmetric if and only if the numbers α_{jj} are real. Thus, in our model the scattering on the sphere is described by means of the six real parameters α_{jj}, β_{jj} and γ_{jj}. Note, that in the case of a two-dimensional system, the zero-range perturbation vanishes in the limit $\beta_{jj} \to \infty$; equation (18) shows that in this limit $S_{12}(E) \to 0$, as might be expected.

After some cumbersome algebra, the transmission amplitude $S_{12}(E)$ from the wire $\mathbf{R}_1^+$ to the wire $\mathbf{R}_2^+$ can be written in the form

$$S_{12}(E) = \frac{\mathrm{i}\hbar^2 k\alpha_{11}^*\alpha_{22}Q_S^{12}(E)}{m^*\Delta(E)} \tag{19}$$

where

$$\Delta(E) = \left(\frac{\hbar^2 k}{2m^*}\right)^2 |\alpha_{11}\alpha_{22}|^2 - \frac{\mathrm{i}\hbar^2 k}{2m^*}\left(1 + \frac{\mathrm{i}\hbar^2 k\gamma}{2m^*}\right)\left[|\alpha_{22}|^2\left(Q_S^{11} - \beta_{11}\right) + |\alpha_{11}|^2\left(Q_S^{22} - \beta_{22}\right)\right]$$
$$- \left(1 + \frac{\mathrm{i}\hbar^2 k\gamma}{2m^*}\right)^2\left[\left(Q_S^{11} - \beta_{11}\right)\left(Q_S^{22} - \beta_{22}\right) - \left|Q_S^{12}\right|^2\right]. \tag{20}$$

To shorten our notations, we introduce the matrix $\tilde{Q}$ with dimensionless elements $\tilde{Q}(E) = \hbar^2(Q_S(E) - B)/m^*$. Using these notations we obtain for the transmission coefficient $T_{12}(E) = |S_{12}(E)|^2$ from the first wire to the second one

$$T_{12}(E) = \left|\frac{16k\sqrt{\lambda_1^a\lambda_2^a}\tilde{Q}^{12}}{4\lambda_1^a\lambda_2^a k^2 - 2\mathrm{i}k(4 - \mathrm{i}k\lambda^c)\left(\lambda_2^a\tilde{Q}^{11} + \lambda_1^a\tilde{Q}^{22}\right) - (4 - \mathrm{i}k\lambda^c)^2\det\tilde{Q}}\right|^2. \tag{21}$$

It is significant that expression (21) for $T_{12}(E)$ contains only dimensionless combinations of scattering parameters ka, $k\lambda_j^a$, $k\lambda_j^b$ and $k\lambda^c$. Equation (21) gives the possibility of analysing the ballistic conductance of the considered device at the condition $r \gg \lambda_F$. We stress that at $r = 0$ equation (21) is inapplicable since in this case the aforementioned condition is violated. Nevertheless, we can get the proper limit ($|S_{12}(E)| \to 1$ as $r \to 0$) using more general boundary conditions than those in equation (4).

4. Transmission coefficient

Here we consider in detail the case of scalar matrices A, B and C (see notations in equation (5)). In addition, we set for simplicity $\lambda^a = \lambda^b = \lambda^c \equiv \lambda$. In the case $r \neq a\pi$, the dependence T_{12} on $k\lambda$ is shown in figure 1.

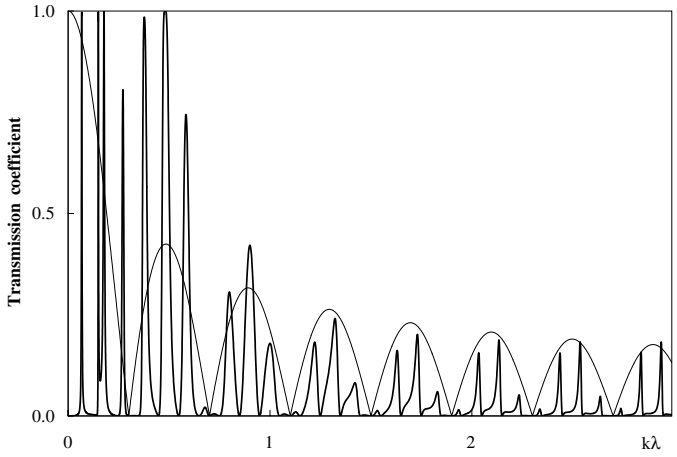

Figure 1. The transmission coefficient T_{12} (thick line) and the absolute value of the Legendre function (thin line) as functions of $k\lambda$; $r = 0.75\pi a$, $a = 10\lambda$.

As this figure shows, there is a series of sharp peaks between the points of vanishing of $T_{12}(E)$. Note, that if $r \neq \pi a$, there are two kinds of zeros of T_{12}. The zeros of the first kind coincide with the eigenvalues $E_l = \hbar^2 l(l+1)/(2m^* a^2)$ of H_S. Indeed, at $E = E_l$, the numerator in equation (21) has a pole of the first order, whereas the denominator has a double pole. It is clear that the position of the zeros of the first kind is independent of r. The zeros of the second kind are determined by the equation $\tilde{Q}^{12}(E) = 0$ (i.e. by the zeros of the Legendre function), their position depends on r. The shape of the curve in figure 1 is determined by the number of zeros of the first kind situated between the zeros of the Legendre function (the thin line in figure 1 is the graph of the absolute value of the Legendre function). We show that the absolute value of the Legendre function determines the height of the peaks. Because of this, the peaks in figure 1 join in packets, the width of a packet is equal to the distance between two neighbouring zeros of the Legendre function. The numerical analysis shows that the form of the graph $T_{12}(k)$ has only a weak dependence on β and γ.

Let us turn to the case $r = \pi a$ (the wires are attached to the opposite poles of the sphere). In this case, it is convenient to represent $T_{12}(k)$ in the form $T_{12}(k) = (1 + \tau^2(k))^{-1}$ where

$$\tau(k) = \frac{[(k\lambda)^2 + 16] \det \tilde{Q} + 4(k\lambda)^2(1 - \tilde{Q}^{11})}{16k\lambda \tilde{Q}^{12}}. \tag{22}$$

It is clear that the transmission coefficient vanishes at the poles of $\tau(k)$, on the other hand, it has peaks at zeros of $\tau(k)$ (here the maximum of $T_{12}(k)$ is equal to 1). In the considered case, at $E = E_l$, the second-order poles in $\det \tilde{Q}$ are cancelled. Therefore, the numerator and the denominator in $\tau(k)$ have poles of the same order, and $\tau(k)$ has no poles at $E = E_l$. Moreover, $\tilde{Q}^{12}$ does not vanish since $\mathcal{P}_\nu(-1) \equiv 1$. Therefore, the zeros of T_{12} of both kinds disappear, and the minima of $T_{12}(k)$ lie above the axis of abscissae (figure 2(*a*)). More precisely, the points of minimum lie on an enveloping curve which is determined by the equation $f = k^2/\left(c_1 k^2 + c_2 k + c_3\right)^2$ where the coefficients c_1, c_2 and c_3 depend only slightly on k (see equation (22)). A small deviation of the distance r from the value $r = \pi a$ causes the crossover from the singular transport regime at $r = \pi a$ to the generic regime (figures 2(*a*)–(*c*)).

It is easy to estimate the distance between adjacent minima at large l: $\Delta k = (1 + o(1/l))a^{-1}$. Hence, if $l \gg 1$, then the oscillation period with respect to k is practically

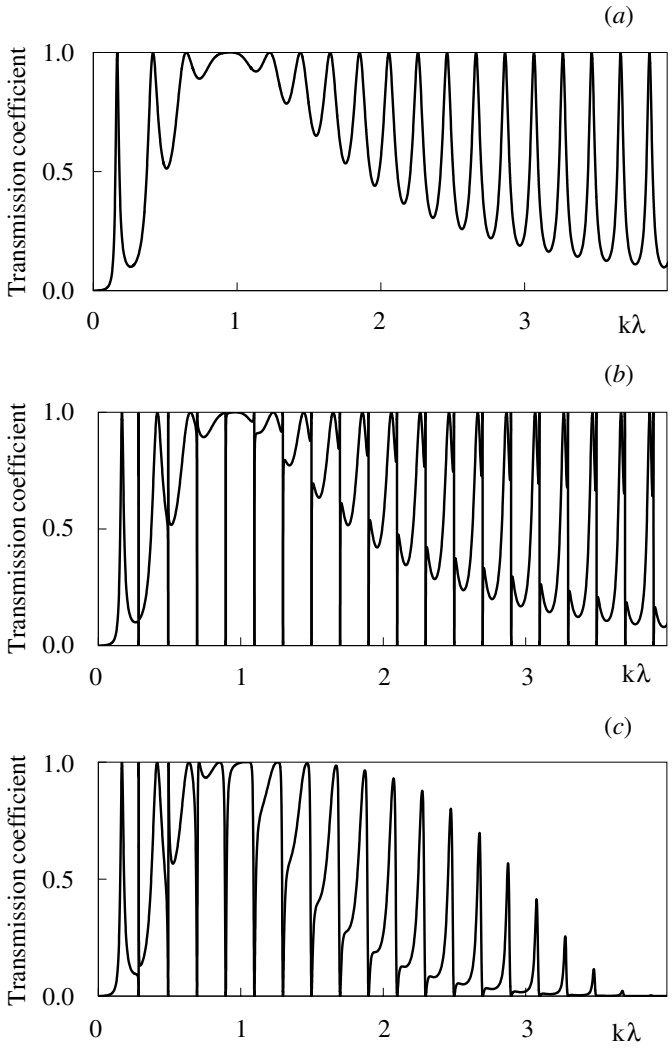

Figure 2. The transmission coefficient as a function of $k\lambda$ at $a = 10\lambda$: (*a*) $r = \pi a$; (*b*) $r = 0.98\pi a$; (*c*) $r = 0.96\pi a$.

constant: $\Delta k = a^{-1}$. Figure 2 shows that the height of peaks of $T_{12}(k)$ is exactly equal to 1. On the other hand, if $r \neq \pi a$, then it is not necessarily the case. To explain this behaviour of the peaks, we note that the asymptotics of $\tau(k)$ at $k\lambda \gg 1$ has the form

$$\tau(k) = \eta(k)\cos(\pi t + \theta(k)) \tag{23}$$

where the amplitude $\eta(k)$ and the phase $\theta(k)$ vary slowly with k.

5. Conclusion

As is evident from the foregoing, the dependence of the transmission coefficient $T_{12}(E)$ of the nanodevice on the energy E has an oscillatory nature. In the generic case of $r \neq \pi a$, the oscillatory peaks join in packets; the width of each packet is equal to the distance between

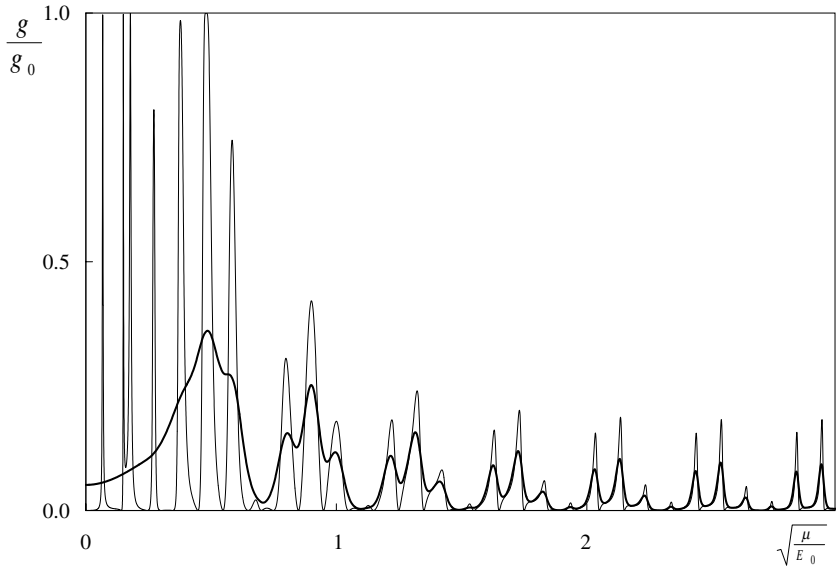

Figure 3. The conductance g as a function of the chemical potential μ at temperature $T = 0.03E_0$ (thick line) and $T = 0$ (thin line). Positions of the wires and radius of the sphere are the same as in figure 1.

adjacent zeros of the Legendre function. The height of the peaks is determined by the absolute value of the Legendre function, hence the height has the maximum in the vicinity of the maximum of this absolute value. The transmission coefficient vanishes at the points where the electron energy lies in the spectrum of the sphere as well as at the zeros of the Legendre function.

In the singular case ($r = \pi a$) the minima of the transmission coefficient $T_{12}(k)$ have an enveloping curve of the form mentioned above, whereas the maxima lie on the straight line $T_{12} = 1$, i.e. the height of the peaks is equal to 1. The peaks are practically equidistant on the curve $T_{12}(k)$, and the minimum values of $T_{12}(k)$ tend to zero as k increases. We stress that these properties are valid only if the wires $\mathbf{R}_j^+$ are glued to the sphere alike (see condition (5)). If $\alpha_{11} \neq \alpha_{22}$, then $T_{12}(k)$ has zeros of the first kind. Moreover, the numerical analysis shows that in this case, the behaviour of the peaks of $T_{12}(k)$ is similar to that in the generic case of gluing the wires to the sphere.

At a nonzero temperature T, the conductance of the device is given by the formula

$$\frac{g(\mu, T)}{g_0} = \int_0^\infty T_{12}(E) \left(-\frac{\partial f_0}{\partial E} \right) \mathrm{d}E \tag{24}$$

where $g_0 = 2e^2/h$ is the conductance quantum and f_0 is the Fermi function. The dependence of $g(\mu)$ at $T = 0.03E_0$ is shown in figure 3, where $E_0 = \hbar^2/(2m^*\lambda^2)$.

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