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Solution of Dyson's equation in a quasi-1D wire

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Abstract. We obtain the current transmission amplitudes as a function of Fermi energy for electrons scattering from a defect in a quasi-one-dimensional wire by solving Dyson's equation for the single-electron Green function. Dyson's equation in a confined geometry includes both mode conversion and coupling to all the evanescent modes in the wire. After obtaining the Green functions, we use Fisher and Lee's relationship between the single-electron Green functions and the current transmission amplitudes through the defect to find all the intersubband and intrasubband transmission probabilities. In agreement with a previous calculation of the transmission amplitudes performed by simply matching wavefunctions at the defect boundary, evanescent modes are shown to dominate the scattering properties whenever the Fermi energy approaches either a new confinement subband or a quasi-bound state splitting off from the higher-lying confinement subbands.

1. Introduction

Electron scattering in a confined geometry is qualitatively different from scattering in an open geometry due to the existence of evanescent modes introduced by the confinement [1]. Figure 1 shows a case where only the lowest normal mode is incident on a defect in a wire. In figure 1 the second and higher normal modes are evanescent waves which decay along the x direction of propagation. The scattering defect couples propagating modes in the wire both to each other and to all the evanescent modes through the scattering boundary conditions. Therefore, for a steady current flow incident on a defect in the wire, a localised mode will build up around the defect even if the scatterer is repulsive. These extra stored electrons cannot collect around a single defect in an open geometry where the electrons must scatter into a travelling wave which propagates away from the defect.

In this paper we consider the scattering from a single delta function defect in a quasi-one-dimensional wire. Dyson's equation for the single-electron Green function is exactly soluble for this special potential. Mode conversion as well as scattering into all the evanescent modes from each higher-lying confinement subband are included in the Dyson equation describing scattering in a confined geometry. We have already examined this problem using a simpler method of matching wavefunctions and their derivatives at the defect [1]. Here we show that the same transmission and reflection coefficients result from the solution of Dyson's equation. Some additional insight can be gained into the resulting unusual scattering properties [1–4] by considering the class of scattering diagrams which dominate our solution of Dyson's equation.

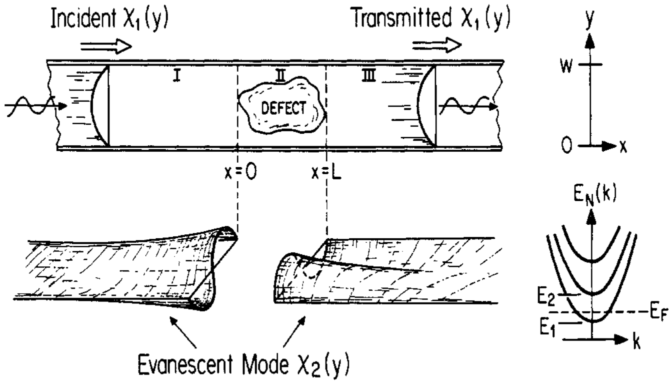

Figure 1. A single scattering defect in a quasi-one-dimensional wire. The wire is assumed to be infinitely long on either side of the defect. For carriers incident only in the lowest subband as shown, evanescent waves build up on either side of the defect in the second and higher normal modes. The building up and storage of electrons around a single scatterer is a unique feature of scattering in a confined geometry such as a wire.

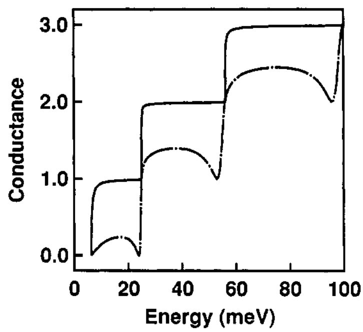

Figure 2. Two-probe Landauer conductance versus electron Fermi energy through a repulsive delta function defect (full curve) and an attractive delta function defect (chain curve) in a quasi-1D wire. A point of 'perfect transparency', where the conductance is equal to its ballistic value of $(n-1)$ times $2e^2/h$, appears immediately below the nth subband minima. The extra drops in the conductance through the attractive potential correspond to extra quasi-bound states in the wire which have split off from the confinement subbands.

The paradigm for calculating conductivity in phase coherent structures has shifted almost exclusively to the viewpoint of Landauer and the various Landauer conductance formulae [5]. Derivations of these conductance formulae from linear response theory have been criticised by Landauer [6] for failure to include the necessary adiabatic widening from a narrow to a wide region. These criticisms can be further appreciated by comparing the electrostatic and electrochemical potentials for a geometry with and without a constriction, given in figure 1 and figure 2 of [7], to the geometries without a constriction considered in [8–10]. For the geometries considered in [8–10] it is difficult to understand how the necessary electrostatic potential drop associated with the quantum contact resistance can develop, for at what point in space can the electrostatic potential $V(x)$ in the perfect leads correspond to that in figure 1 of [7]?

However, in these same studies of conductance using linear response theory [8–10], a relation has been derived between the one-particle Green functions and the current transmission amplitudes through a disordered region beginning with the work of Fisher and Lee [8] and also discussed in [9–11]. Here we confirm that the Fisher–Lee relationship is satisfied for the special case of a delta function potential in a quasi-1D wire by explicit calculation of both the single-particle Green functions and the transmission amplitudes. 'Two-probe' Landauer formulae can therefore be used to calculate conductance when the transmission probabilities are obtained either by straightforwardly matching wavefunctions and their derivatives at the disordered regions or by the more complicated recursive evaluation of Dyson's equation for the single-particle Green functions [12]. Detailed background and bibliography of previous work on the conductance of phase-coherent electron devices can be obtained from the citations in [1–11].

2. Dyson's equation in a quasi-1D wire

Consider again the quasi-one-dimensional wire having electrons confined along the y direction but free to move along the x direction shown in figure 1. The two-dimensional 'wire' of this paper is a reasonable approximation to real physical systems where the confinement along z, usually normal to a semiconductor heterojunction interface, is much stronger than the 'lateral' confinement along y. Furthermore, if the additional confinement along z is taken into account the results for the transmission coefficients presented in section 4 do not change substantially, so it is adequate to work with the simpler two-dimensional 'wire'.

The equation of motion for the Green function G in the quasi-1D wire of figure 1 is

$$\left\{E - \left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mathrm{d}^2}{\mathrm{d}y^2}\right) + V_{\mathrm{c}}(y) + V_{\mathrm{d}}(x,y)\right]\right\} G(xy;x'y') = \delta(x-x')\delta(y-y') \tag{1}$$

where the confinement potential $V_{\mathrm{c}}(y)$ depends only on the transverse direction y and $V_{\mathrm{d}}(x,y)$ is the potential of any defects or impurities in the wire. Throughout our discussion we assume propagation at a constant energy E and do not write the energy argument in the Green functions. $G(xy;x'y')$ from (1) has the standard interpretation as being the 'transmission amplitude' that a unit impulse of probability amplitude originally deposited at position (x',y') will propagate to position (x,y). The one-dimensional Schrödinger equation along y including only the confinement potential $V_{\mathrm{c}}(y)$

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}y^2} + V_{\mathrm{c}}(y)\right)\chi_n(y) = E_n\chi_n(y) \tag{2}$$

gives rise to a set of normal modes $\chi_n(y)$ and subband energies E_n where n is the subband index. In addition to their standard completeness property, the $\chi_n(y)$ can be chosen real and obey the useful relation

$$\sum_n \chi_n(y)\chi_n(y') = \delta(y-y'). \tag{3}$$

Multiplying (1) on the left by $\chi_a(y)$, on the right by $\chi_c(y)$, and applying the useful equation (3), we obtain the equation of motion for the Green function in a Q1D wire as

$$\sum_b \left\{ \left[E - E_b - \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \right) \right] \delta_{ab} - V_{ab}(x) \right\} G(xb; x'c) = \delta(x - x')\delta_{ac}. \tag{4}$$

The matrix elements of the defect potential in (4) are

$$V_{ab}(x) = \int \mathrm{d}y\, \chi_a(y) V_\mathrm{d}(x, y) \chi_b(y) \tag{5}$$

and the matrix elements of the Green function are

$$G(xb; x'c) = \int \mathrm{d}y \int \mathrm{d}y'\, \chi_b(y) G(xy; x'y') \chi_c(y'). \tag{6}$$

$G(xb; x'c)$ from (6) has the interpretation as being the 'transmission amplitude' that a unit impulse of probability amplitude originally deposited at position x' in normal mode c will propagate to position x in normal mode b. Also, the 'free' Green function in the absence of a defect potential obeys an equation of motion

$$\left\{ E - E_a - \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \right) \right\} G^0(xa; x'c) = \delta(x - x')\delta_{ac} \tag{7}$$

so $G^0(xa; x'c)$ is diagonal in the mode indices a and c as $G^0(xa; x'c) = G^0_a(x; x')\delta_{ac}$.

By standard manipulations of (4) and (7), repeatedly applying (3), we obtain the Dyson equation for a Q1D wire as

$$G(xa; x'c) = G^0(xa; x'c) + \sum_{bd} \int \mathrm{d}x''\, G^0(xa; x''b) V_{bd}(x'') G(x''d; x'c). \tag{8}$$

This Dyson equation can be given its usual interpretation of summing over the probability amplitudes of all the possible scattering processes for a particle starting at position x' in normal mode c arriving at position x in normal mode a.

3. Delta function scatterer

We choose the scattering potential $V_\mathrm{d}(x, y)$ to be a delta function

$$V_\mathrm{d}(x, y) = \gamma\delta(x)\delta(y - y_i) \tag{9}$$

so that its matrix elements $V_{ab}(x)$ from (5) are

$$V_{ab}(x) = \delta(x)\gamma\chi_a(y_i)\chi_b(y_i). \tag{10}$$

The weight γ can be either positive or negative.

Now let us iterate the Dyson equation (8) assuming initially for simplicity that only the lowest two normal modes are present. The infinite series for $G(x1;x'1)$ is

$$\begin{aligned} G(x1;x'1) = {} & G_1^0(x;x') + G_1^0(x;0)V_{11}G_1^0(0;x') \\ & + G_1^0(x;0)V_{11}G_1^0(0;0)V_{11}G_1^0(0;x') \\ & + G_1^0(x;0)V_{12}G_2^0(0;0)V_{21}G_1^0(0;x') \\ & + G_1^0(x;0)V_{11}G_1^0(0;0)V_{11}G_1^0(0;0)V_{11}G_1^0(0;x') \\ & + G_1^0(x;0)V_{11}G_1^0(0;0)V_{12}G_2^0(0;0)V_{21}G_1^0(0;x') \\ & + G_1^0(x;0)V_{12}G_2^0(0;0)V_{21}G_1^0(0;0)V_{11}G_1^0(0;x') \\ & + G_1^0(x;0)V_{12}G_2^0(0;0)V_{22}G_2^0(0;0)V_{21}G_1^0(0;x') + \cdots \end{aligned} \tag{11}$$

where $V_{ab} = \gamma\chi_a(y_i)\chi_b(y_i)$. Equation (11) can be regrouped as a power series

$$\begin{aligned} G(x1;x'1) = {} & G_1^0(x;x') + G_1^0(x;0)V_{11}G_1^0(0;x')[1 + \left(V_{11}G_1^0(0;0) + V_{22}G_2^0(0;0)\right)^1 \\ & + \left(V_{11}G_1^0(0;0) + V_{22}G_2^0(0;0)\right)^2 \\ & + \left(V_{11}G_1^0(0;0) + V_{22}G_2^0(0;0)\right)^3 + \cdots] \end{aligned} \tag{12}$$

and summed as

$$G(x1;x'1) = G_1^0(x;x') + \frac{G_1^0(x;0)V_{11}G_1^0(0;x')}{1 - \left(V_{11}G_1^0(0;0) + V_{22}G_2^0(0;0)\right)}. \tag{13}$$

Equation (13) is valid for any energy of the incident electron. That is, equation (13) is valid when modes one and two are either propagating modes or evanescent modes. We later discuss the convergence of the power series (12) leading to (13), and show that the resulting equation (13) is better than the method used to obtain it.

By analogy with our calculation of G_{11} from (13), the result for an arbitrary intrasubband Green function $G(xa;x'a)$ including all the normal confinement modes is

$$G(xa;x'a) = G_a^0(x;x') + G_a^0(x;0)V_{aa}G_a^0(0;x')\left[1 - \left(\sum_n V_{nn}G_n^0(0;0)\right)\right]^{-1}. \tag{14}$$

Detailed discussion of one-dimensional results similar to (14) are given in [13–14]. The expression for the intersubband Green function $G(xa;x'b)$ again including all the normal confinement modes is

$$G(xa;x'b) = +G_a^0(x;0)V_{ab}G_b^0(0;x')\left[1 - \left(\sum_n V_{nn}G_n^0(0;0)\right)\right]^{-1}. \tag{15}$$

Equations (14) and (15) are the exact solutions of the Dyson equation (8) with the scattering potential (9), and can be obtained by straightforward algebra after inserting (9) into (8). The iteration proceedure in (11), which fails if the Fermi energy is equal to a subband minimum but is useful for visualizing the possible scattering processes, is not necessary to solve (8).

Equations (14) and (15) can be evaluated by noting that the 'free' Green function for normal mode a is [13]

$$G_a^0(x;x') = -\frac{m}{\hbar^2\kappa_a}\exp\left(-\kappa_a|x-x'|\right) \qquad E < E_a \tag{16}$$

if mode a is an evanescent mode where

$$\kappa_a = +\sqrt{\frac{2m(E_a - E)}{\hbar^2}} \tag{17}$$

and

$$G_a^{0\pm}(x;x') = \mp\mathrm{i}\frac{m}{\hbar^2 k_a}\exp\left(\pm\mathrm{i}k_a(x-x')\right) \qquad E > E_a \tag{18}$$

if mode a is a propagating mode where

$$k_a = +\sqrt{\frac{2m(E - E_a)}{\hbar^2}}. \tag{19}$$

From (16) and (18) we see that $G_a^0(0,0)$, which occurs repeatedly in the power series (12) and corresponds diagrammatically to the particle repeatedly looping around the delta function [14], is simply proportional to the density of propagating or evanescent states for mode a. Thus, the series in the denominator of (14) and (15) of the form $\sum_n V_{nn}G_n^0(0;0)$ should be interpreted as a Golden Rule amplitude involving the square root of the initial density of states, a matrix element connecting initial to final state, and the square root of the density of final states. Taking the square magnitude of this denominator will yield an infinite series of Golden-Rule-type scattering terms between all possible normal modes. The numerators of (14) and (15) can also be interpreted in this way.

4. Transmission coefficients

Let us evaluate the Green functions for the special case where x and x' are on opposite sides of the scatterer and hence $x' < 0 < x$. Since we are interested in transmission through the scatterer from left to right we consider only G^+. Because we work with the time-independent form of the Green functions, implicitly assumed in all our calculations is that a constant applied incident current is imposed on the scatterer from the left. If this were not true the scattering problem could not reach a time-independent solution. We must leave on the applied current long enough that evanescent modes can build up around the scatterer until a steady state is reached as described in the introduction and in [1].

To evaluate the intrasubband Green function from (14), we use the identity

$$G_a^{0+}(x;0)G_a^{0+}(0;x') = G_a^{0+}(0;0)G_a^{0+}(x;x') \tag{20}$$

to rewrite (14) as

$$G^+(xa;x'a) = t_{aa}(E)\,G_a^{0\,+}(x;x'). \tag{21}$$

Here $t_{aa}(E)$ is the current transmission amplitude through the defect

$$t_{aa}(E) = \left(1 + \sum_n^{\mathrm{e}} V_{nn} \frac{m}{\hbar^2 \kappa_n} + \mathrm{i} \sum_{n \neq a}^{\mathrm{p}} V_{nn} \frac{m}{\hbar^2 k_n}\right) \times \left(1 + \sum_n^{\mathrm{e}} V_{nn} \frac{m}{\hbar^2 \kappa_n} + \mathrm{i} \sum_n^{\mathrm{p}} V_{nn} \frac{m}{\hbar^2 k_n}\right)^{-1} \tag{22}$$

given in [1]. In (22) $\sum^{\mathrm{e}}$ denotes a sum over all the evanescent modes, $\sum^{\mathrm{p}}$ denotes a sum over the propagating modes, and mode a is assumed propagating. The ability to factor the Green function into a product of the free Green function multiplied by the transmission amplitude depends critically on the shape of the scatterer. Only for delta function scatterers is it possible to make the simple factorization in (21). In (21), the 'free' Green function keeps track of the particle's phase while $t_{aa}(E)$ gives the current transmission amplitude including any possible phase shifts. Factorization of the Green function as in (21) for the case of two delta function scatterers in one dimension (modelling a resonant tunneling problem) has been noted by Garcia-Calderón [15].

The new physics of scattering in a confined geometry, discussed in detail for all the transmission coefficients in [1], can be briefly illustrated by considering a simple case of (22) where mode one is propagating and mode two is evanescent:

$$t_{11}(E) = \frac{1 + V_{22} m/\hbar^2 \kappa_2}{1 + V_{22} m/\hbar^2 \kappa_2 + \mathrm{i} V_{11} m/\hbar^2 k_1}. \tag{23}$$

At the minima of the second subband we have $\kappa_2 = 0$ resulting in perfect transmission of the incident mode $t_{11} = 1$. This 'perfect transparency' effect, first pointed out by Chu and Sorbello [2], is a consequence of evanescent modes building up near the scattering defect [1]. In addition, the numerator of (23) is zero when the incident electron energy lines up with the quasi-bound state which has split off from the second subband [1] resulting in perfect reflection, $t_{11} = 0$. Setting the real part of the Green function's denominator in (21) to zero we recover the quasi-bound-state energy.

Evaluating the intersubband Green function from (15) yields

$$G^+(xa; x'b) = t_{ab}(E) \left(-\mathrm{i} \frac{m}{\hbar^2 \sqrt{k_a k_b}}\right) \exp(+\mathrm{i} k_a x - \mathrm{i} k_b x'). \tag{24}$$

Here $t_{ab}(E)$ is the current transmission amplitude through the defect from the incident normal mode b on the left to the transmitted normal mode a on the right

$$t_{ab}(E) = -\mathrm{i} V_{ab} \frac{m}{\hbar^2 \sqrt{k_a k_b}} \left(1 + \sum_n^{\mathrm{e}} V_{nn} \frac{m}{\hbar^2 \kappa_n} + \mathrm{i} \sum_n^{\mathrm{p}} V_{nn} \frac{m}{\hbar^2 k_n}\right)^{-1} \tag{25}$$

given in [1].

Equation (25) gives the transmission amplitudes $t_{ab} = t_{ba}$ for $a \neq b$. But for the delta function scattering potential of (9), $t_{ab} = r_{ab}$ for $a \neq b$ simply by wavefunction continuity at the scatterer [1]. Furthermore $1 + r_{aa} = t_{aa}$, so (25) gives the reflection amplitudes r_{aa} if $a = b$. These results can also be shown using the Green function approach of this paper. Therefore

$$r_{ab}(E) = -\mathrm{i}V_{ab}\frac{m}{\hbar^2\sqrt{k_a k_b}}\left(1+\sum_n^{\mathrm{e}} V_{nn}\frac{m}{\hbar^2\kappa_n}+\mathrm{i}\sum_n^{\mathrm{p}} V_{nn}\frac{m}{\hbar^2 k_n}\right)^{-1} \quad (26)$$

which holds for any two propagating normal modes a and b, should be considered the fundamental result of this paper. The two factors of (26) have a simple interpretation in terms of the Fermi Golden Rule as described in the previous section. Conversely, the intrasubband transmission from (22) appears to be a result of 'leftover' particles not deflected by the delta function, and can be obtained by applying (26) together with wavefunction continuity at the scatterer.

The relationship obtained by Fisher and Lee [8] between the current transmission amplitudes and the Green functions for an arbitrary defect potential is

$$t_{ab}(E) = -\mathrm{i}\hbar\sqrt{v_a v_b}G^{+}(xa;x'b)\exp(-\mathrm{i}k_a x + \mathrm{i}k_b x') \quad (27)$$

where we again require that $x' < 0 < x$. We have inserted an extra $\hbar$ in their relationship which must be there on purely dimensional grounds. The current transmission amplitudes t_{ab} through the delta function potential were explicitly calculated in [1]. In this paper we have calculated all the Green functions $G(xa;x'b)$ through the delta function defect. Both the intrasubband Green functions from (21) and the intersubband Green functions from (24) clearly obey the relation in (27) (up to an unimportant phase factor of -1). Alternately, had we not previously calculated the current transmission amplitudes using another method, we could have used the calculation in section 3 and (27) to obtain them. Therefore, we can also regard the transmission coefficients t_{aa} from (22) and t_{ab} from (25) as being obtained by solving the Dyson equation (8) and applying the Fisher–Lee relation (27).

The current transmission coefficients T_{ab} necessary to calculate the conductance through a defect we may now obtain as

$$T_{ab} = t_{ab}t^{*}_{ab} = v_a v_b|\hbar G^{+}(xa;x'b)|^2. \quad (28)$$

The-two probe Landauer conductance can then be written as

$$G = \frac{e^2}{\pi\hbar}\sum_{ab}T_{ab} = \frac{e^2}{\pi\hbar}\sum_{ab}v_a v_b|\hbar G^{+}(xa;x'b)|^2 \quad (29)$$

which is similar to the expression in [8]. Relation (27) of Fisher and Lee for the transmission coefficients, inserted into the two-probe Landauer conductance formula, gives the expression for the conductance in terms of Green functions as in (29).

The two-probe conductance versus Fermi energy from (29) for both a repulsive delta potential (full curve) having γ = 7 feV cm^2 and an attractive delta potential (chain curve) with γ = -7 feV cm^2 are shown in figure 2. Figure 2 assumes an infinite square well confinement of 30 nm width and an electron mass of 0.067 times the free electron mass appropriate for GaAs heterojunctions. Conductance through the repulsive potential (full curve) is lower than its ballistic value of n times $2e^2/h$ (where n is the subband index) due to increased reflection immediately above the bottom of the nth subband. This increased reflection rounds the shoulders of the quantised conductance steps. Immediately below the minima of the nth subband the conductance rises to its ballistic value of $(n-1)$ times $2e^2/h$ as a result of the 'perfect transparency' effect described in this section. For the two-probe conductance through an attractive defect (chain curve), a single quasi-bound state splits off from each quasi-one-dimensional subband and is visible as the extra pronounced dips in the conductance. The quasi-bound state associated with the nth subband appears when the Fermi energy lies in the $(n-1)$th subband, resulting in increased reflection and a correspondingly lower conductance near the quasi-bound-state energy. The 'perfect transparency' effect is also present when the scatterer is attractive. We have investigated the conductance through a delta function scatterer in a wire in detail in [1].

5. Conclusions

The scattering properties of electrons in a confined geometry are qualitatively different from the usual case of scattering in open geometries due to the building up and storage of electrons in evanescent waves near the scattering defect. To illustrate these properties, we solved Dyson's equation for the single-electron Green function describing electrons scattering from a delta function defect in a quasi-one-dimensional wire. We then used Fisher and Lee's relationship between the single-electron Green functions and the current transmission amplitudes to obtain the current transmission coefficients of electrons through a delta function defect in the Q1D wire. The transmission coefficients so obtained agree with those found by simply matching wavefunctions and their derivatives at the defect [1]. For the delta function scatterer, all normal modes completely 'decouple' at a new subband minimum resulting in perfect transmission despite the presence of a scatterer. If the delta function scatterer is attractive, a single quasi-bound state splits off from each confinement subband and causes increased reflection if the Fermi energy is near the quasi-bound state.

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