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S-matrix formulation of mesoscopic systems and evanescent modes

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Abstract

Validity of the Landauer–Buttiker formalism for studying linear transport in mesoscopic systems is well established theoretically as well as experimentally. Akkermans *et al* (1991 *Phys. Rev. Lett.* **66** 76) have shown that the formalism can be extended to study thermodynamic properties like persistent currents. This extension was verified for simple one-dimensional systems. We study the applicability of Akkermans *et al*'s formula for quasi-one-dimensional systems with several conducting channels. In the case that all modes are propagating the formula is still valid but in the case of evanescent modes it requires reinterpretation.

1. Introduction

Due to technological advances in nanofabrication, it is possible to realize very small systems in which the quantum mechanical coherence length of the electron extends throughout the length of the sample. Quantum interference phenomena and fluctuations are important in determining the thermodynamic and transport properties of these systems [1]. They are frequently referred to as mesoscopic systems.

Mesoscopic phenomena can occur in canonical systems as well as in grand canonical systems. The systems are often so small that even measuring probes (like voltage probes and current probes) can change the system from canonical to grand canonical [2]. While a canonical system is well described by the Hamiltonian of an isolated system, that is not the case for a grand canonical system. A grand canonical mesoscopic system, by definition, is coupled to a reservoir with which it can exchange electrons. The reservoir can drastically change the quantum states of the system and this has to be explicitly accounted for [3]. This can be done by solving the Schrödinger equation of the whole system, including the leads. The system is open and has to be solved as a scattering problem. This method is known as the Landauer–Buttiker formalism.

If an Aharonov–Bohm flux is applied through the center of a ring, the ring gets magnetized and a persistent current is generated in the ring [4]. This current arises because of the

vector potential that changes the phase of the wavefunction in the ring [5]. Persistent current is an example of mesoscopic phenomena: the magnetization is determined by quantum interference effects. Persistent currents have been studied for more than a decade, theoretically as well as experimentally [5]. In an isolated ring the persistent current is carried by the eigenstates. However, if the ring is connected to reservoirs, the persistent current is carried by the resonant and non-resonant scattering states. Several such grand canonical systems have been studied, like a quantum ring connected to a single reservoir or to many reservoirs [6]. If it is connected to many reservoirs with different chemical potentials, then non-equilibrium currents can coexist with equilibrium persistent currents. In such open systems several interesting effects have been predicted, like current magnification in the presence of transport [7–9], directional dependence of persistent currents [10] and the current magnification effect in equilibrium systems in the absence of transport current [11].

In order to realize a mesoscopic grand canonical system we connect the ring to reservoirs that are at fixed chemical potentials as is schematically shown in figure 1. The left reservoir has a chemical potential μ_1 and the right one has a chemical potential μ_2 . The reservoirs can also be at a finite temperature *T*. The ring is threaded by an Aharonov–Bohm flux. If $\mu_1 > \mu_2$, then there is a transport current (which is



Figure 1. A ring connected to an infinite wire. A δ function potential is present in the ring at position X. A chemical potential difference $(\mu_1 - \mu_2)$ between the left reservoir (LR) and the right reservoir (RR) drives a transport current through regions I and II. The ring is pierced by an Aharonov–Bohm flux ϕ that drives an equilibrium current called the persistent current in the ring. α is the Aharonov–Bohm phase an electron picks up in region IV and β is that in region V. In all expressions for physically observable quantities we only encounter the sum $\alpha + \beta = \frac{2\pi\phi}{\phi_0}$, where ϕ_0 is the flux constant.

a non-equilibrium current) through regions I and II. There is, however, no transport current in the ring. The ring will carry a persistent current which is an equilibrium current. Thus, in the present geometry, the equilibrium persistent currents and non-equilibrium transport currents are spatially separated.

The Landauer–Buttiker approach proposes that an equilibrium phenomenon, like persistent current in such an open system as that in figure 1, can be obtained from solving the scattering problem [3]. Akkermans *et al* [12] related the persistent current IS to the S-matrix by the following formula:

$$IS = \frac{1}{2\pi i} \frac{\partial \log[\det(S)]}{\partial \phi}.$$
 (1)

Such a simple mathematical relation between the persistent current inside the ring and the S-matrix obtained from the wavefunction far away from the ring is rather novel and resulted in a flurry of theoretical activity [13]. While it is established (from theoretical and experimental points of view) that conductance (a non-equilibrium phenomenon) can be obtained from the S-matrix, Akkermans' approach may prove to be the first step to obtain any equilibrium phenomenon from the S-matrix. Hence Akkermans et al's formula is a step towards a mesoscopic version of fluctuationdissipation theorem [13]. The work by Dashen *et al* [14] is the most seminal work in this area that elaborates the connection between statistical mechanics and S-matrix theory. For nonlinear response and AC response an important role is played by the partial density of states [15] rather than the density of states and this too has been formulated in terms of the S-matrix [16]. The correctness of equation (1) has been explicitly verified in one dimension (1D) but not in quasione dimension (Q1D). Complexities due to the presence of evanescent modes in Q1D has been observed recently [17, 18] but they are not yet well known [19]. For example, the Friedel sum rule [17] and the Buttiker–Thomas–Pertre formula [18] break down in the presence of evanescent modes.

In this work we undertake the task of verifying the validity of the Akkermans formula, equation (1), in the case of Q1D systems. We show analytically how the evanescent modes complicate things. Earlier works [17, 18] on different formulae are essentially numerical verifications. Persistent current in the geometry of figure 1 has been studied earlier, but always using the wavefunction formalism. The *S*-matrix was never used and comparison was not made between Akkermans *et al*'s approach and the usual wavefunction approach. In this paper we show explicitly that the 1D result cannot be straightforwardly extended to Q1D in the presence of evanescent modes.

2. Model and method

As shown in figure 1, we consider a ring coupled to a wire. The scattering solution for this geometry is discussed in detail in our earlier work [6]. Here we outline some points with respect to calculating the RHS of equation (1) which was not done earlier. There is a δ -potential impurity present in the ring at an arbitrary position X (figure 1). We apply an Aharonov–Bohm flux ϕ through the ring, perpendicular to the plane of the paper. We consider two modes of propagation because it will show the shortcomings of Akkermans *et al*'s formula. The Schrödinger equation for a Q1D wire in the presence of a δ potential at x = 0, $y = y_i$ (the third degree of freedom, i.e. the *z* direction, is usually frozen by creating a strong quantization [1]) is

$$\begin{bmatrix} -\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + V_c(y) \\ + \gamma \delta(x, y - y_i) \end{bmatrix} \Psi(x, y) = E \Psi(x, y).$$
(2)

Here the *x* coordinate is along the wire and the *y* coordinate is perpendicular to the wire, m^* is the electron mass and *E* is the electron energy. $V_c(y)$ is the confining potential perpendicular to the wire. The wavefunction in the ring can be obtained by solving the above equation with periodic boundary conditions where we assume the ring to be so large that its curvature can be neglected. The magnetic field appears just as a phase of $\Psi(x, y)$ and will be accounted for while applying the boundary conditions. Away from the δ potential (i.e. $x \neq 0$ and $y \neq y_i$), equation (2) can be separated as

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi(x)}{dx^2} = \frac{\hbar^2k^2}{2m^*}\psi(x)$$
(3)

and

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dy^2} + V_{\rm c}(y)\right]\chi_n(y) = E_n\chi_n(y).$$
 (4)

Here we consider that the electron is propagating along the x direction. This means in regions I and II of figure 1 the x direction is along the arrows. In region III, the x direction is along the line joining P and Q. And in regions IV and V, the x direction is along the perimeter of the ring. One can choose different axes in the different regions as the matrix equations obtained from mode matching are independent of this choice [6]. The confinement potential $V_c(y)$ in different

regions is in the y (transverse) direction. It can be seen from equations (3) and (4) that

$$E = E_n + \frac{\hbar^2 k_n^2}{2m^*}.$$
 (5)

For simplicity we take $V_{c}(y)$ to be a square well potential of width W, which gives $\chi_n(y) = \sin[\frac{n\pi}{W}(y + \frac{W}{2})]$. So $E_n = \frac{\hbar^2 n^2 \pi^2}{2m^* W^2}$. Hence, in the first mode

$$k_1 = \sqrt{\frac{2m^*E}{\hbar^2} - \frac{\pi^2}{W^2}}$$
(6)

is the propagating wavevector and in the second mode

$$k_2 = \sqrt{\frac{2m^*E}{\hbar^2} - \frac{4\pi^2}{W^2}}$$
(7)

is the propagating wavevector.

When electrons are incident along region I (in figure 1) in the first mode the scattering problem can be solved exactly. The solution to equation (3) in region I becomes

$$\psi_{\rm I} = \frac{1}{\sqrt{k_1}} {\rm e}^{{\rm i}k_1 x} + \frac{r'_{11}}{\sqrt{k_1}} {\rm e}^{-{\rm i}k_1 x} + \frac{r'_{12}}{\sqrt{k_2}} {\rm e}^{-{\rm i}k_2 x}.$$
 (8)

Similarly, in regions II, III, IV and V we get

$$\psi_{\rm II} = \frac{g_{11}}{\sqrt{k_1}} {\rm e}^{{\rm i}k_1 x} + \frac{g_{12}}{\sqrt{k_2}} {\rm e}^{{\rm i}k_2 x} \tag{9}$$

$$\psi_{\rm III} = \frac{A e^{i k_1 x}}{\sqrt{k_1}} + \frac{B e^{-i k_1 x}}{\sqrt{k_1}} + \frac{C e^{i k_2 x}}{\sqrt{k_2}} + \frac{D e^{-i k_2 x}}{\sqrt{k_2}}$$
(10)

$$\psi_{\rm IV} = \frac{E e^{ik_1 x}}{\sqrt{k_1}} + \frac{F e^{-ik_1 x}}{\sqrt{k_1}} + \frac{G e^{ik_2 x}}{\sqrt{k_2}} + \frac{H e^{-ik_2 x}}{\sqrt{k_2}}$$
(11)

$$\psi_{\rm V} = \frac{J e^{ik_1(x-l_2)}}{\sqrt{k_1}} + \frac{K e^{-ik_1(x-l_2)}}{\sqrt{k_1}} + \frac{L e^{ik_2(x-l_2)}}{\sqrt{k_2}} + \frac{M e^{-ik_2(x-l_2)}}{\sqrt{k_2}},$$
(12)

where $r'_{11}, r'_{12}, g'_{11}, g'_{12}, A, B, C, D, E, F, G, H, J, K, L$ and *M* are to be determined by mode matching.

Note that at P and Q we have a three-legged junction that is schematically shown in figure 2. In a previous work [6] we proposed a junction scattering matrix $S_{\rm J}$ for a two-channel junction that can be easily generalized to any number of channels. For the δ potential impurity at X we use the scattering matrix $S_{\rm b}$ that was derived by Bagwell [20]. One can match the wavefunctions and conserve the currents by using these S-matrices that give us a set of linear equations. We calculate the coefficients A, B, C, D, E, F, G, H, J, K, L and *M* numerically by matrix inversion.

Persistent current can be computed from the wavefunction

$$IW^{(k_1)} = \int_{-\frac{W}{2}}^{\frac{W}{2}} \frac{\hbar}{2\mathrm{i}m^*} (\psi^{\dagger}\vec{\nabla}\psi - \psi\vec{\nabla}\psi^{\dagger}) \,\mathrm{d}y.$$
(13)

Here the index k_1 implies that this is the current due to an incident electron in the k_1 channel from the left. Similarly currents are generated due to incident electrons in the k_1



Figure 2. A three-legged junction.

channel from the right, the k_2 channel from the left and the k_2 channel from the right. So the net observable persistent current is

$$IW = 2IW^{(k_1)} + 2IW^{(k_2)}.$$
(14)

From equation (13) we get

$$IW^{(k_1)} = 2I_0(|E|^2 - |F|^2 + |G|^2 - |H|^2)^{(k_1)},$$
 (15)

where $I_0 = \frac{\hbar e}{2m^*W^2}$. We also calculate the scattering matrix elements r'_{11} , $r'_{12}, g'_{11}, g'_{12}, r'_{22}, r'_{21}, g'_{22}$ and g'_{21} by matrix inversion to find the scattering matrix *S* of the system:

$$S = \begin{pmatrix} r'_{11} & r'_{12} & g'_{11} & g'_{12} \\ r'_{21} & r'_{22} & g'_{21} & g'_{22} \\ g'_{11} & g'_{12} & r'_{11} & r'_{12} \\ g'_{21} & g'_{22} & r'_{21} & r'_{22} \end{pmatrix}.$$
 (16)

By substituting (16) into (1), equation (1) can also be written as a sum of four terms [15], where each term consists of scattering matrix elements due to incidence in a particular momentum channel. That is

$$IS = 2IS^{(k_1)} + 2IS^{(k_2)} \tag{17}$$

where

$$IS^{(k_{1})} = \frac{1}{2\pi} \left(|r_{11}'|^{2} \frac{\partial \arg(r_{11}')}{\partial \phi} + |r_{12}'|^{2} \frac{\partial \arg(r_{12}')}{\partial \phi} + |g_{11}'|^{2} \frac{\partial \arg(g_{11}')}{\partial \phi} + |g_{12}'|^{2} \frac{\partial \arg(g_{12}')}{\partial \phi} \right)$$
(18)

and

$$IS^{(k_2)} = \frac{1}{2\pi} \left(|r'_{21}|^2 \frac{\partial \arg(r'_{21})}{\partial \phi} + |r'_{22}|^2 \frac{\partial \arg(r'_{22})}{\partial \phi} + |g'_{21}|^2 \frac{\partial \arg(g'_{21})}{\partial \phi} + |g'_{22}|^2 \frac{\partial \arg(g'_{22})}{\partial \phi} \right).$$
(19)

Although not implied by the notation, the currents defined above (equations (14) and (17)) are differential currents in an infinitesimal energy range dE. The integration of these will give the actual measurable currents. The integration limits depend on the chemical potential μ_1 and μ_2 . Temperature can be included through the Fermi function. All expressions so far are derived for both modes being propagating. Earlier it was shown that IW = IS for a one-dimensional ring coupled to a reservoir [12]. We shall show below that, when all modes are



Figure 3. IW/I_0 and IS/I_0 versus $8\pi^2 m^* EW^2/h^2$. The two curves are identical. The system parameters are $l_1 = l_2 = l_3 = 1$, $y_i = 0.1$, $\alpha = \beta = 0.3$ and $\gamma = 4$.

propagating, then one gets IS = IW, but not when we include evanescent modes. This is because when evanescent modes are present then some expressions can be analytically continued to include evanescent modes but not all expressions.

3. Inclusion of evanescent modes

E is the energy of incidence that can be varied as an external parameter by tuning the chemical potentials of the reservoirs. When $\pi^2 \leq 2m^* E W^2/\hbar^2 < 4\pi^2$, then it can be seen from equations (7) and (8)–(12) that the k_2 mode becomes evanescent. Equations (8)–(12) are still solutions to Schrödinger's equation (3), implying electrons in the ring can be coupled to an evanescent channel due to scattering [20]. A single impurity can couple an electron to the evanescent second channel. Scattering at the junctions can also couple an electron to the evanescent second channel. No electron can be incident from (or emitted to) ∞ along the evanescent second channel. So the scattering problem has to be solved with an incident electron in the k_1 mode in the left lead and an outgoing electron in the k_1 mode in the right lead. Hence the *S* matrix becomes 2×2 and is given by

$$S = \begin{pmatrix} r'_{11} & g'_{11} \\ g'_{11} & r'_{11} \end{pmatrix}.$$
 (20)

Note that the matrix elements, like all other physically observables like current, can be analytically continued. That is r'_{11} in equation (16) under $k_2 \rightarrow i\kappa_2$ is the same as r'_{11} in equation (20). In fact, they are the same expression as a function of E but valid in different regimes $(E > \frac{4\pi^2}{W^2})$ and $E < \frac{4\pi^2}{W^2}$). But the S-matrix in equation (20) cannot be considered as an analytical continuation of that in equation (16)because their dimensions are different. So equation (1) cannot be analytically continued. Although the S matrix is 2×2 , its calculation has to be done by using the 6×6 junction Smatrix S_J that is defined in [6] and the 4 \times 4 S-matrix S_b for the δ function potential that is defined in [20]. This is essential because evanescent modes can be obtained inside the ring without violating any physical principles like conservation of energy. g'_{12}, r'_{12} , etc, are non-zero, but they do not carry any current. They are not S-matrix elements any more. Rather, they define the coupling to evanescent modes. Unitarity should imply $|r'_{11}|^2 + |g'_{11}|^2 = 1$ and indeed we get this from



Figure 4. $IS^{(k_1)}/I_0$ and $IW^{(k_1)}/I_0$ versus $8\pi^2m^*EW^2/h^2$. The two curves are identical. The system parameters are $l_1 = l_2 = l_3 = 1$, $y_i = 0.1$, $\alpha = \beta = 0.3$ and $\gamma = 4$.

the junction matrix defined by S_J . This implies that S_J is appropriate for accounting for realistic multichannel situations.

4. Results and discussions

In a real system, there are always propagating modes as well as evanescent modes. As is evident from equations (6) and (7), evanescent modes have higher transverse energy than the propagating modes. Also the higher the n value of the evanescent mode, the higher is its transverse energy. This energy is at the cost of the propagation energy which becomes more and more negative for higher *n* evanescent modes. There will be a natural cutoff as very high transverse energies cannot be realized in a quantum wire. We will first consider a case when there are two modes in the wire, both being propagating. We will then consider a case when one mode is propagating and the other is evanescent. In the first case we will verify that Akkermans et al's approach gives exactly the same result as the current calculated from the wavefunction (i.e. IS = IW). In the second case there are complexities. It will be argued that such complexities will persist in a real system where there will be many evanescent modes.

Both modes are propagating. First we consider the energy range $4\pi^2 \leq 2m^* E W^2/\hbar^2 \leq 9\pi^2$ (i.e. $39.478 \leq 2m^* E W^2/\hbar^2 \leq 88.826$). Substituting this *E* in equations (6) and (7) we can see that both the modes are propagating. The nature of the current is plotted in figure 3. The figure shows that the current *IS* obtained from Akkermans *et al*'s formula (that is, from the *S*-matrix) is identical with *IW* (that is, from the wavefunction). In fact, $IS^{(k_1)}$ and $IS^{(k_2)}$ are individually identical with $IW^{(k_1)}$ and $IW^{(k_2)}$, respectively. These are shown in figures 4 and 5. This implies that $IW^{(k_1)}$ is the same algebraic expression as $IS^{(k_1)}$. Similarly for $IW^{(k_2)}$ and $IS^{(k_2)}$. And also *IS* and *IW* are the same algebraic expressions. We have checked this analytically in Mathematica.

One mode is evanescent. Now consider the energy range $\pi^2 \leq 2m^* E W^2/\hbar^2 < 4\pi^2$ (i.e. 9.87 $\leq 2m^* E W^2/\hbar^2 \leq$ 39.477) so that $k_2 = \sqrt{\frac{2m^* E}{\hbar^2} - \frac{4\pi^2}{W^2}}$ becomes imaginary $(k_2 \rightarrow i\kappa_2)$ while $k_1 = \sqrt{\frac{2m^* E}{\hbar^2} - \frac{\pi^2}{W^2}}$ remains real. In this regime the ring contains one propagating and one evanescent



Figure 5. $IS^{(k_2)}/I_0$ and $IW^{(k_2)}/I_0$ versus $8\pi^2m^*EW^2/h^2$. The two curves are identical. The system parameters are $l_1 = l_2 = l_3 = 1$, $y_i = 0.1$, $\alpha = \beta = 0.3$ and $\gamma = 4$.



Figure 6. IS/I_0 (solid line) and IW/I_0 (dashed line) versus $8\pi^2m^*EW^2/h^2$ of the system when the second channel is evanescent. The system parameters are $l_1 = l_2 = l_3 = 1$, $y_i = 0.1$, $\alpha = \beta = 0.3$ and $\gamma = 4$. Here IS/I_0 is obtained by substituting S given in equation (20) into equation (1).

mode. Evanescent mode current can be calculated by directly applying equation (13) to evanescent mode wavefunctions or it can be calculated by analytically continuing the propagating mode current (14) to below the barrier (that is, $k_2 \rightarrow i\kappa_2$ in (14)). We have already argued that IS and IW are the same algebraic expressions. Under the transformation $k_2 \rightarrow i\kappa_2$, applied to both IS and IW, they remain the same algebraic expression. However, Akkermans et al's formula takes a different meaning in this regime where there are evanescent modes. This is essential because Akkermans et al's formula in equation (1) is related to the S-matrix and the transformed expression $(IS_{k_2 \to i\kappa_2})$ cannot be obtained from the S-matrix. We know that no electron can be incident along the evanescent channel. So $IW^{(k_2)}$ and $IS^{(k_2)}$ are zero. So IW is now just equal to $IW^{(k_1)}$, where k_2 has been analytically continued. If one assumes that in this regime IS is equal to $IS^{(k_1)}$, where k_2 is analytically continued, then obviously once again IS = IW, as they are the same algebraic expression. However, one can see that $IS^{(k_1)}$ (see equation (18)) cannot be obtained by substituting the S-matrix (equation (20)), into Akkermans et al's formula (equation (1)). If we do this substitution, then we will get the first term and the third term in equation (18)(where of course the $k_2 \rightarrow i\kappa_2$ transformation is taken care of). We will not get the second and fourth terms as r'_{12} and g'_{12} are not S-matrix elements any more. We can see from figure 6 that the difference between *IS* and *IW* is quite large.

Since *IS* obtained from equation (1) is now reduced to just two terms, one may ask if it gives the partial current only in the





Figure 7. IS/I_0 (solid line) and $IW_1^{(k_1)}/I_0$ (dashed line) versus $8\pi^2m^*EW^2/h^2$. The system parameters are $l_1 = l_2 = l_3 = 1$, $y_i = 0.1, \alpha = \beta = 0.3$ and $\gamma = -3.7$. Here IS/I_0 is obtained by substituting *S* given in equation (20) into equation (1).

propagating channel, because this partial current also consists of two terms only. Note from equation (15) that the total current $IW^{(k_1)} = IW_1^{(k_1)} + IW_2^{(k_1)}$, where $IW_1^{(k_1)} = 2I_0(|E|^2 - |F|^2)^{(k_1)}$, E and F being the wavefunction amplitudes in the propagating channel and $IW_2^{(k_1)} = 2I_0(|G|^2 - |H|^2)^{(k_1)}$, Gand H being the wavefunction amplitudes in the evanescent channel. We have plotted $IW_1^{(k_1)}$ in figure 7. The figure shows that *IS* differs from $IW_1^{(k_1)}$. So it is confirmed that *IS* obtained from equation (1) neither gives the total measurable current of the system nor the partial current through the propagating channel.

5. Conclusions

For realistic mesoscopic rings connected to leads, there are always evanescent modes. The S-matrix is always defined by the propagating modes only. For such systems one cannot directly apply Akkermans *et al*'s formula. Instead one should start with a model where all the modes are made propagating. One should apply Akkermans *et al*'s formula to the S-matrix of this system and then analytically continue this expression for the current to the situation where an appropriate number of modes are evanescent. While the Landauer–Buttiker approach is still inevitable as the evanescent modes are obtained due to an incident electron that is scattered to evanescent modes, the formula given in equation (1) is no longer strictly valid in the presence of evanescent modes.

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