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The scattering matrix method for quantum waveguides

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Abstract. A scattering matrix method for investigating the electron transport in quantum waveguides is presented. By dividing the structure into a number of transverse slices, the global scattering matrix is obtained by the composition of the individual scattering matrices associated with each interface. Complicated geometries and inhomogeneous external potentials are included in the formulation. It is shown that the proposed scattering matrix method possesses many advantages over the traditional mode-matching and transfer matrix methods, especially in treating the electron wave propagation in complicated geometries. Justification for the method is provided by the unitarity of the calculated scattering matrix, and the consistency of the results with those obtained by the recursive Green's function method.

1. Introduction

Recent technological advances in nanometre-scale lithography and atomic-layer epitaxy which can provide semiconductor microstructures smaller than the inelastic and elastic mean scattering lengths have attracted much attention to studies of mesoscopic systems, especially since the discovery of the quantized conductance phenomenon [1, 2]. One of the most important problems in mesoscopic physics is that of obtaining an understanding of the electron transport in a quasi-one-dimensional system where the electrons are confined in a narrow channel. For a structure with transverse dimensions comparable to the electron wavelength, the transport problems can be treated as a quantum ballistic scattering process. Thus the nature of the problems becomes that of a scalar quantum waveguide. Because of the prospects for device applications, a large amount of both experimental and theoretical research on ballistic electron transport in quantum waveguides with various configurations has been reported over the past few years [3, 4]. Many experimental studies of the conductance versus the gate voltage in split-gate geometry for a heterojunction structure have been reported, and a lot of interesting effects in ballistic transport have been found in double- and multiple-constriction, single-bend or multiple-bend geometric structures [5].

Over the past few years, several analytical and numerical approaches to ballistic transport have become well established. In the theoretical studies, the single-electron and effective-mass approximations are usually applied, and it is often supposed that the waveguide structures have hard potential walls which would not allow any penetration of the electron wave function into the lateral barriers. In general, the electron wave propagation in waveguide structures is studied by the mode-matching (boundary-matching) method [6, 7] and other methods [8, 9] including the recursive Green's function method [10, 11]. For complicated geometries, the problems are usually studied through numerical simulation of

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the Schrödinger wave equation—for example, in the time-dependent approach [12, 13], and the quantum transmitting-boundary method [14].

The transfer matrix approach [15, 16] is another important tool in the investigation of electron transport in low-dimensional systems, especially in the studies of coherent tunnelling in quantum-well structures. Using the transfer matrix method, many interesting effects, such as universal conductance fluctuations and weak localization, can be elegantly analysed. In addition, the transfer matrix method proves to be very efficient in studies of disordered systems, while the transfer matrix technique is unfortunately numerically singular for structures with dimensions larger than the electron Fermi wavelength [17]. In the transfer matrix formalism, numerical errors due to the exponential behaviour of the evanescent modes arise unavoidably [18]. The problem in the transfer matrix method can be removed by the scattering matrix algorithm. For systems with quasi-one-dimensional disorder, several scattering matrix methods have been proposed by Bandyopadhyay and Cahay [17] and Tamura and Ando [19], while for general two-dimensional mesoscopic systems, to the best of our knowledge, a scattering matrix method has not been established. In this paper, we present a comprehensive scattering matrix method for the electron transport in two-dimensional mesoscopic systems. The single-electron and the effective-mass approximations are applied as is usual in the literature. In general, we assume that the waveguide structures have hard potential walls, and that the proposed formulation can also be used to analyse electron transport in soft wall structures.

The paper is organized as follows. In the next section, the general formalism of the scattering matrix approach is presented. In section 3, the method for calculating the scattering matrix is presented. In section 4, we perform the numerical implementation of the proposed method and compare our results with those obtained by the RGF method. In section 5, we propose a generalized algorithm for treating multiple-terminal structures. Finally, a brief summary is presented.

2. General formalism

We start from the two-dimensional Schrödinger equation

$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+U_c(x,y)+U_{ex}(x,y)\right]\Phi(x,y)=E\Phi(x,y) \qquad (1)$$

where m^* is the electron effective mass, $U_c(x,y)$ is the lateral confining potential, $U_{ex}(x,y)$ is an external potential, and E is the Fermi energy of the two-dimensional electron gas.

For a general waveguide structure with complicated geometries, one often divides the cavity into a number of uniform sections—see figure 1. Therefore, the wave functions at an arbitrary position in the cavity would be constructed as linear combinations of transverse modes in the pertinent section. At an arbitrary position x assumed to be located in the mth section, we have the following expansion of the wave function:

$$\Phi(x,y)=\sum_{n=1}^{N_m}(a_n e^{ik_n^m x}+b_n e^{-ik_n^m x})\phi_n^m(y) \qquad (2)$$

$$(\phi_1^m,\phi_2^m,\ldots,\phi_{N_m}^m)^{\mathrm{T}}=\mathbf{C}_m(\varphi_1^m,\varphi_2^m,\ldots,\varphi_{N_m}^m)^{\mathrm{T}} \qquad (3)$$

$$\varphi_n^m(y)=\sqrt{2/D_m}\sin(n\pi y/D_m) \qquad (4)$$

where D_m is the section width, N_m is the number of channels involved in transport in the section, $\mathbf{C}_m$ is an N_m-dimensional matrix, and k_n^m is the longitudinal wavelength for the nth mode in the mth section. Here, we assume hard-wall confinement for simplicity.

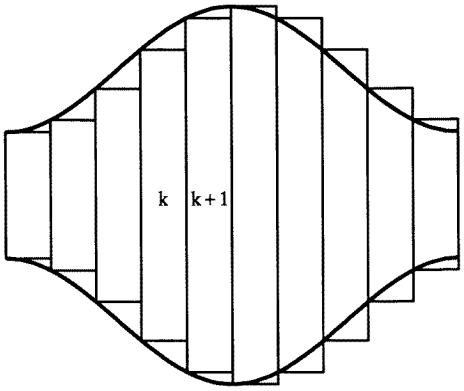

Figure 1. A schematic view of a two-dimensional cavity which is divided into a number of transverse slices along the longitudinal direction.

Although the evanescent modes are found to play an important role in the electron wave propagation, in the terminals one can still consider just the propagating mode [20], while in each section of the cavity one should consider four evanescent modes or more. Therefore, N_m should be determined by k_n^m. By solving the following eigenvalue problem, $\mathbf{C}_m$ and k_n^m can be obtained:

$$\sum_{j=1}^{N'_m} H_{ij}^m (\mathbf{C}'_m)_{nj} = [E - \hbar^2 (k_n^m)^2 / 2m^*](\mathbf{C}'_m)_{ni} \tag{5}$$

$$H_{ij}^m = \int_0^{D_m} \varphi_i^m(y) \left[-\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial y^2} + U_{ex}(x_m, y) \right] \varphi_j^m(y)\, \mathrm{d}y \tag{6}$$

where N'_m should be sufficiently large in order to obtain a convergent result for k_n^m for $1 \leqslant n \leqslant N_m$. The desired N_m-dimensional matrix $\mathbf{C}_m$ is taken from the N'_m-dimensional matrix $\mathbf{C}'_m$, so it is not a unit matrix in the presence of an external potential [15]. In the absence of external potentials, the above formulations can be much simplified: $k_n^m = \sqrt{2m^* E/\hbar^2 - (n\pi/D_m)^2}$ and $\boldsymbol{C}_m$ reduces to a unit matrix.

All of the waveguide structures considered in this paper are supposed to be divided into two kinds of region: the straight terminals and the cavities to which the terminals attach along the longitudinal direction. In general, neither the scattering matrix method nor the transfer matrix method is suitable for those waveguide structures which cannot be divided into intervals along the longitudinal direction.

In a waveguide structure, the wave function at position x can be represented by a $2N(x)$-dimensional column vector $\boldsymbol{A}(x)$ which is given by

$$\boldsymbol{A}(x) = [\boldsymbol{A}^+(x), \boldsymbol{A}^-(x)]^{\mathrm{T}} \tag{7}$$

$$\boldsymbol{A}^+(x) = [a_1 \mathrm{e}^{\mathrm{i}k_1 x}, a_2 \mathrm{e}^{\mathrm{i}k_2 x}, \ldots, a_n \mathrm{e}^{\mathrm{i}k_n x}]^{\mathrm{T}} \tag{8}$$

$$\boldsymbol{A}^-(x) = [b_1 \mathrm{e}^{-\mathrm{i}k_1 x}, b_2 \mathrm{e}^{-\mathrm{i}k_2 x}, \ldots, b_n \mathrm{e}^{-\mathrm{i}k_n x}]^{\mathrm{T}}. \tag{9}$$

The components of the vectors $\boldsymbol{A}^+(x)$ and $\boldsymbol{A}^-(x)$ denote the flux amplitudes of the right-going and left-going waves, respectively. If x is in the input lead, we have further notation: $\boldsymbol{A}^+(x) = \boldsymbol{A}^i(x)$ and $\boldsymbol{A}^-(x) = \boldsymbol{A}^0(x)$, because a right-going wave is coming into the cavity and a left-going wave is going out from the cavity in the input lead. Similar notation can be used for the output lead.

For two different positions $x_1 < x_2$, the relations between the vectors $\boldsymbol{A}(x_1)$ and $\boldsymbol{A}(x_2)$ are expressed by a scattering matrix formulation:

$$\begin{bmatrix} \boldsymbol{A}^-(x_1) \\ \boldsymbol{A}^+(x_2) \end{bmatrix} = \mathbf{S}(x_1, x_2) \begin{bmatrix} \boldsymbol{A}^+(x_1) \\ \boldsymbol{A}^-(x_2) \end{bmatrix} \tag{10}$$

where $\mathbf{S}(x_1, x_2)$ is an $(N(x_1)+N(x_2))$-dimensional scattering matrix. If the interval between x_1 and x_2 is uniform, we have $N(x_1) = N(x_2) = N$, and the corresponding matrix $\mathbf{S}$ can be written readily:

$$\mathbf{S}(x_2 - x_1) = \begin{bmatrix} \mathbf{0} & \mathbf{P} \\ \mathbf{P} & \mathbf{0} \end{bmatrix} \tag{11}$$

where $\mathbf{P}$ is an N-dimensional diagonal matrix with diagonal elements $P_{mm} = \mathrm{e}^{\mathrm{i}k_m(x_2-x_1)}$.

Here, we notice that only the wave component $\mathrm{e}^{\mathrm{i}k_m\,\delta x}$ is taken into account in the scattering matrix formalism, while in the transfer matrix method, both wave components $\mathrm{e}^{\mathrm{i}k_m\,\delta x}$ and $\mathrm{e}^{-\mathrm{i}k_m\,\delta x}$ should be taken into consideration. For an evanescent mode, if the index m or δx is large, $\mathrm{e}^{\mathrm{i}k_m\,\delta x}$ would become very small while $\mathrm{e}^{-\mathrm{i}k_m\,\delta x}$ would become very large. Therefore, numerical errors would inevitably occur in the calculations. In the scattering matrix method, this kind of numerical error would not emerge.

For three different positions $x_1 < x_2 < x_3$, supposing that the scattering matrices $\mathbf{S}(x_1, x_2)$ and $\mathbf{S}(x_2, x_3)$ are known, the scattering matrix connecting x_1 and x_3 is determined by the composition law [19]

$$\mathbf{S}(x_1, x_3) = \mathbf{S}(x_1, x_2) \otimes \mathbf{S}(x_2, x_3). \tag{12}$$

For a general two-terminal cavity structure which is not uniform along the longitudinal direction, one usually divides it into a number of transverse slices (see figure 1). The number of slices should be large enough that each slice can be considered as a uniform segment. The global scattering matrix for the cavity is constructed by the composition of the individual scattering matrices associated with each slice. Supposing the number of transverse slices is M and x_k is the coordinate of the left-hand end of the kth slice, the global scattering matrix $\mathbf{S}$ is determined by

$$\mathbf{S} = \mathbf{S}(x_0^-, x_M^+) = \prod_{k=0}^{M-1} \mathbf{S}(x_k^+, x_{k+1}^-) \otimes \mathbf{S}(x_{k+1}^-, x_{k+1}^+) \tag{13}$$

where $\mathbf{S}(x_{k+1}^-, x_{k+1}^+)$ is the scattering matrix associated with the interface between the kth and the $(k+1)$th slices. The wave functions in the two terminals which are labelled L and R can be related by the global scattering matrix:

$$\begin{bmatrix} \boldsymbol{A}_{\mathrm{L}}^- \\ \boldsymbol{A}_{\mathrm{R}}^+ \end{bmatrix} = \mathbf{S} \begin{bmatrix} \boldsymbol{A}_{\mathrm{L}}^+ \\ \boldsymbol{A}_{\mathrm{R}}^- \end{bmatrix}. \tag{14}$$

In order to obtain the transmission coefficients, it should be noted that the definition of the scattering matrix defined in equation (13) is slightly different from a standard one [10] because the closed channels are involved. Supposing the number of open channels is N_0, what represent the flux amplitudes of the right-going (left-going) waves in open channels are the first N_0 components of the vector $\boldsymbol{A}^+$ ($\boldsymbol{A}^-$). To obtain the transmission coefficients, we should calculate the elements that emerge in the first N_0 lines and columns of the N-dimensional matrices $\mathbf{S}_{ij}$ $(i, j = 1, 2)$, where the $\mathbf{S}_{ij}$ are the submatrices of the scattering matrix $\mathbf{S}$. For each submatrix $\mathbf{S}_{ij}$ these elements construct a new N_0-dimensional matrix $\check{\mathbf{S}}_{ij}$. A $2N_0$-dimensional scattering matrix $\check{\mathbf{S}}$ can be constructed with four matrices

$\check{\mathbf{S}}_{ij}$. Bearing in mind that evanescent states do not exist in the incoming waves, the last $N - N_0$ elements of $\boldsymbol{A}_{\mathrm{L}}^{+}$ and $\boldsymbol{A}_{\mathrm{R}}^{-}$ vanish; therefore, we have

$$\begin{bmatrix} \boldsymbol{A}_{\mathrm{L}}^{0} \\ \boldsymbol{A}_{\mathrm{R}}^{0} \end{bmatrix} = \begin{bmatrix} \check{\mathbf{S}}_{11} & \check{\mathbf{S}}_{12} \\ \check{\mathbf{S}}_{21} & \check{\mathbf{S}}_{22} \end{bmatrix} \begin{bmatrix} \boldsymbol{A}_{\mathrm{L}}^{i} \\ \boldsymbol{A}_{\mathrm{R}}^{i} \end{bmatrix} \tag{15}$$

where $\boldsymbol{A}_{\mathrm{L}}^{0}$, $\boldsymbol{A}_{\mathrm{R}}^{0}$, $\boldsymbol{A}_{\mathrm{L}}^{i}$, and $\boldsymbol{A}_{\mathrm{R}}^{i}$ are N_0-dimensional column vectors which are constructed from the first N_0 elements of the vectors $\boldsymbol{A}_{\mathrm{L}}^{-}$, $\boldsymbol{A}_{\mathrm{R}}^{+}$, $\boldsymbol{A}_{\mathrm{L}}^{+}$, and $\boldsymbol{A}_{\mathrm{R}}^{-}$ respectively. Current conservation requires the unitarity of the $\check{\mathbf{S}}$-matrix, $\check{\mathbf{S}}\check{\mathbf{S}}^{\dagger} = \check{\mathbf{S}}^{\dagger}\check{\mathbf{S}} = \mathbf{1}$. The unitarity of the $\check{\mathbf{S}}$-matrix serves as an important criterion for the validity of the results in the numerical computations. In the calculations, we evaluate the diagonal elements of $\check{\mathbf{S}}\check{\mathbf{S}}^{\dagger}$ which should each be 1. In all of the results presented in this paper, the deviation from this expectation is no more than 10^{-3}. The transmission coefficient T_{ij}^{mn} which denotes the norm of the probability amplitude with which an electron coming from the lead i in the transverse mode m is transmitted into the mode n in the lead j can be readily written down:

$$T_{ij}^{mn} = |(\check{\mathbf{S}}_{ij})_{mn}|^2. \tag{16}$$

If $i = j$, T_{ij}^{mn} becomes the reflection coefficient R_i^{mn}. Supposing electrons are incident from the left-hand lead L in which all of the open channels are equivalently occupied, we have $\boldsymbol{A}_{\mathrm{L}}^{i} = \{1, 1, \ldots, 1\}^{\mathrm{T}}$ and $\boldsymbol{A}_{\mathrm{R}}^{i} = \{0, 0, \ldots, 0\}^{\mathrm{T}}$; then the total transmission coefficient T and reflection coefficient R are given by

$$T = \left| \check{\mathbf{S}}_{21} \boldsymbol{A}_{\mathrm{L}}^{i} \right| \tag{17}$$

$$R = \left| \check{\mathbf{S}}_{11} \boldsymbol{A}_{\mathrm{L}}^{i} \right| \tag{18}$$

where $|\cdots|$ denotes the inner product of a column vector. Although the formulation is given for the two-probe structure, generalizing it to the multi-terminal structure is straightforward. In the next section, we will provide a method for evaluating the scattering matrix.

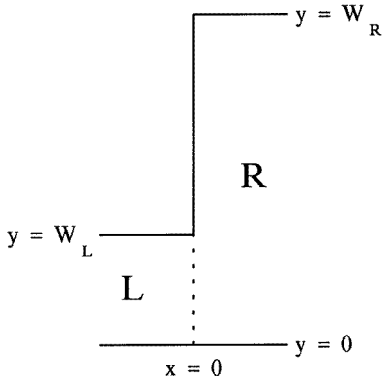

Figure 2. A schematic view of two linked segments with different widths.

3. The method of calculation

In this section, we provide a method for calculating the scattering matrix associated with an interface at which the boundaries of two linked segments are discontinuous. The coordinates

of the calculation are shown in figure 2. When the difference between the width of the left-hand segment W_L and that of the right-hand segment W_R is not large, one can take the numbers of transverse modes in the two segments to be the same as each other, i.e., $N_L = N_R = N$. At the interface, the wave functions in the two segments are represented by two N-dimensional column vectors $\boldsymbol{A}_L$ and $\boldsymbol{A}_R$, respectively, which are related by a scattering matrix $\mathbf{S} = \mathbf{S}(0^-, 0^+)$:

$$\begin{bmatrix} \boldsymbol{A}_L^- \\ \boldsymbol{A}_R^+ \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{11} & \mathbf{S}_{12} \\ \mathbf{S}_{21} & \mathbf{S}_{22} \end{bmatrix} \begin{bmatrix} \boldsymbol{A}_L^+ \\ \boldsymbol{A}_R^- \end{bmatrix}. \tag{19}$$

At the interface, supposing $x = 0$, the continuity of the wave functions and their first derivatives requires that

$$\sum_{m=1}^{N_L} (a_m^L + b_m^L)\phi_m^L(y) = \sum_{n=1}^{N_R} (a_n^R + b_n^R)\phi_n^R(y) \tag{20}$$

$$\sum_{m=1}^{N_L} (a_m^L - b_m^L)k_m^L\phi_m^L(y) = \sum_{n=1}^{N_R} (a_n^R - b_n^R)k_n^R\phi_n^R(y). \tag{21}$$

Insertion of equation (3) into the above expressions gives

$$\sum_{m=1}^{N_L} \varphi_m^L(y) \sum_{m'=1}^{N_L} C_{m'm}^L (a_{m'}^L + b_{m'}^L) = \sum_{n=1}^{N_R} \varphi_n^R(y) \sum_{n'=1}^{N_R} C_{n'n}^R (a_{n'}^R + b_{n'}^R) \tag{22}$$

$$\sum_{m=1}^{N_L} \varphi_m^L(y) \sum_{m'=1}^{N_L} C_{m'm}^L k_{m'}^L (a_{m'}^L - b_{m'}^L) = \sum_{n=1}^{N_R} \varphi_n^R(y) \sum_{n'=1}^{N_R} C_{n'n}^R k_{n'}^R (a_{n'}^R - b_{n'}^R). \tag{23}$$

We should be very careful to eliminate the transverse modes in the above formulations when there is an appreciable difference between W_L and W_R, as has been clarified in reference [21]. In the case where $W_L < W_R$, we multiply both sides of equations (22) and (23) by $\varphi_n^R(y)$ and $\varphi_m^L(y)$ respectively, integrate with respect to y, and obtain

$$\sum_{m=1}^{N_L} D_{mn} \sum_{m'=1}^{N_L} C_{m'm}^L (a_{m'}^L + b_{m'}^L) = \sum_{n'=1}^{N_R} C_{n'n}^R (a_{n'}^R + b_{n'}^R) \tag{24}$$

$$\sum_{m'=1}^{N_L} C_{m'm}^L k_{m'}^L (a_{m'}^L - b_{m'}^L) = \sum_{n=1}^{N_R} D_{mn} \sum_{n'=1}^{N_R} C_{n'n}^R k_{n'}^R (a_{n'}^R - b_{n'}^R) \tag{25}$$

where the D_{mn} are the coefficients which denote the coupling between the transverse modes in the two regions, and are given by

$$D_{mn} = \int \varphi_m^L(y)\varphi_n^R(y)\, \mathrm{d}y. \tag{26}$$

The integration should be performed in the region with smaller width; here, it is the left-hand region.

After rewriting equations (24) and (25) in the form of a matrix, we obtain

$$\mathbf{D}^T\mathbf{C}_L^T(\boldsymbol{A}_L^+ + \boldsymbol{A}_L^-) = \mathbf{C}_R^T(\boldsymbol{A}_R^+ + \boldsymbol{A}_R^-) \tag{27}$$

$$\mathbf{C}_L^T\mathbf{K}_L(\boldsymbol{A}_L^+ - \boldsymbol{A}_L^-) = \mathbf{D}\mathbf{C}_R^T\mathbf{K}_R(\boldsymbol{A}_R^+ - \boldsymbol{A}_R^-) \tag{28}$$

where $\mathbf{K}_L$ is a N_L-dimensional diagonal matrix with

$$(\mathbf{K}_L)_{mm} = k_m^L \tag{29a}$$

and $\mathbf{K}_R$ is an N_R-dimensional diagonal matrix with

$$(\mathbf{K}_R)_{mm} = k_m^R \tag{29b}$$

and $\mathbf{D}$ is an $N_L \times N_R$ matrix with elements D_{mn}. Equations (27) and (28) enable us to obtain the following matrices if $N_L = N_R$:

$$\mathbf{S}_{11} = -(\mathbf{M}_1 + \mathbf{M}_2)^{-1}(\mathbf{M}_1 - \mathbf{M}_2) \tag{30}$$

$$\mathbf{S}_{12} = 2(\mathbf{M}_1 + \mathbf{M}_2)^{-1} \tag{31}$$

$$\mathbf{S}_{21} = 2(\mathbf{M}_3 + \mathbf{M}_4)^{-1} \tag{32}$$

$$\mathbf{S}_{22} = -(\mathbf{M}_3 + \mathbf{M}_4)^{-1}(\mathbf{M}_3 - \mathbf{M}_4) \tag{33}$$

where

$$\mathbf{M}_1 = \mathbf{D}^T\mathbf{C}_L^T \tag{34}$$

$$\mathbf{M}_2 = (\mathbf{D}\mathbf{C}_R^T\mathbf{K}_R)^{-1}\mathbf{K}_L \tag{35}$$

$$\mathbf{M}_3 = (\mathbf{D}^T\mathbf{C}_L^T)^{-1} \tag{36}$$

$$\mathbf{M}_4 = \mathbf{K}_L^{-1}\mathbf{D}\mathbf{C}_R^T\mathbf{K}_R. \tag{37}$$

When the difference between the widths of the two segments is very large, N_L and N_R should not be the same as each other. In this case, the conventional transfer matrix method and the above procedures cannot be applied, while the problem can be treated by our scattering matrix method. Combining equations (27) and (28) into one, we obtain

$$\mathbf{M}_L\boldsymbol{A}_L = \mathbf{M}_R\boldsymbol{A}_R \tag{38}$$

where

$$\mathbf{M}_L = \begin{bmatrix} \mathbf{D}^T\mathbf{C}_L^T \\ \mathbf{C}_L^T\mathbf{K}_L \end{bmatrix} \tag{39}$$

$$\mathbf{M}_R = \begin{bmatrix} \mathbf{C}_R^T \\ \mathbf{D}\mathbf{C}_R^T\mathbf{K}_R \end{bmatrix}. \tag{40}$$

The matrices $\mathbf{M}_L$ and $\mathbf{M}_R$ can be rewritten in terms of four blocks:

$$\mathbf{M}_L = \begin{bmatrix} (\mathbf{M}_L)_{11} & (\mathbf{M}_L)_{12} \\ (\mathbf{M}_L)_{21} & (\mathbf{M}_L)_{22} \end{bmatrix} \tag{41}$$

$$\mathbf{M}_R = \begin{bmatrix} (\mathbf{M}_R)_{11} & (\mathbf{M}_R)_{12} \\ (\mathbf{M}_R)_{21} & (\mathbf{M}_R)_{22} \end{bmatrix} \tag{42}$$

where $(\mathbf{M}_L)_{11}$ and $(\mathbf{M}_L)_{12}$ are $N_R \times N_L$ matrices, $(\mathbf{M}_L)_{21}$ and $(\mathbf{M}_L)_{22}$ are N_L-dimensional matrices, $(\mathbf{M}_R)_{11}$ and $(\mathbf{M}_R)_{12}$ are N_R-dimensional matrices, and $(\mathbf{M}_R)_{21}$ and $(\mathbf{M}_R)_{22}$ are $N_L \times N_R$ matrices. By tedious matrix algebra we obtain the desired matrices:

$$\mathbf{S}_{11} = \mathbf{M}_1\left[\mathbf{M}_2(\mathbf{M}_L)_{11} - (\mathbf{M}_L)_{21}\right] \tag{43}$$

$$\mathbf{S}_{12} = \mathbf{M}_1\left[(\mathbf{M}_R)_{22} - \mathbf{M}_2(\mathbf{M}_R)_{12}\right] \tag{44}$$

where

$$\mathbf{M}_1 = \left[(\mathbf{M}_L)_{22} - \mathbf{M}_2(\mathbf{M}_L)_{12}\right]^{-1} \tag{45}$$

$$\mathbf{M}_2 = (\mathbf{M}_R)_{21}(\mathbf{M}_R)_{11}^{-1} \tag{46}$$

and

$$\mathbf{S}_{21} = \mathbf{M}_3\left[(\mathbf{M}_L)_{11} - \mathbf{M}_4(\mathbf{M}_L)_{21}\right] \tag{47}$$

$$\mathbf{S}_{22} = \mathbf{M}_3\left[\mathbf{M}_4(\mathbf{M}_R)_{22} - (\mathbf{M}_R)_{12}\right] \tag{48}$$

where

$$\mathbf{M}_3 = \left[(\mathbf{M}_R)_{11} - \mathbf{M}_4(\mathbf{M}_R)_{21}\right]^{-1} \tag{49}$$

$$\mathbf{M}_4 = (\mathbf{M}_L)_{12}(\mathbf{M}_L)_{22}^{-1}. \tag{50}$$

In the above, we suppose that the width of the left-hand segment is not larger than that of the right-hand segment. If $W_L > W_R$, we can proceed with the following procedures to obtain the corresponding scattering matrix. First, we interchange all of the quantities with subscript L and those with subscript R. Then we perform the above procedures and obtain a scattering matrix $\mathbf{S}$. In the case where $W_L > W_R$, the desired scattering matrix $\mathbf{S}'$ is given by

$$\mathbf{S}' = \begin{bmatrix} \mathbf{S}_{22} & \mathbf{S}_{21} \\ \mathbf{S}_{12} & \mathbf{S}_{11} \end{bmatrix}. \tag{51}$$

4. Numerical implementation

In this section, we perform numerical calculations of the transmission for several kinds of two-terminal waveguide structure using the proposed scattering matrix method. In the numerical calculations, five or more evanescent modes are involved for each segment. Our scattering matrix method has no limitation as regards the number of transverse modes because numerical errors due to the exponential behaviour of the evanescent modes do not exist in the method. The number of divided segments should be large enough that the desired results are obtained. We find that it is sufficient to set the number to be 50.

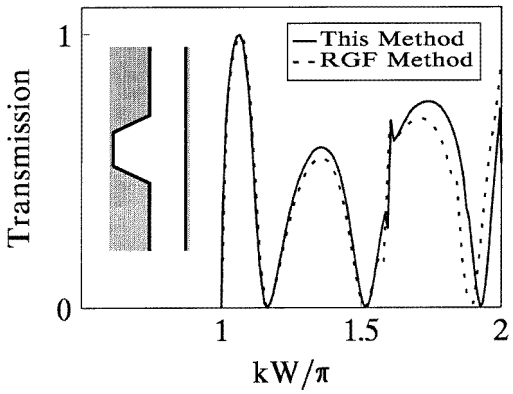

Figure 3. Transmission coefficients versus kW/π calculated by our method (solid line) and the RGF method (dotted line).

First, we make a comparison of the results obtained by our method and the RGF method for the structure with a trapezoid-shaped cavity as shown in the inset of figure 3. From the figure, we find that the two results are in excellent agreement with each other, which can be taken as a justification of our scattering matrix method.

In order to realize quantum-modulated transistor action in an electron waveguide structure, one often resorts to a multiple-stub structure [11, 16]. Quantum wire with a periodic serial structure has been studied by Wu *et al* [16] using a transfer matrix method. Just as pointed out in reference [16], we also find that the total transfer matrix becomes numerically singular when the length of channel linking the two adjacent stubs is large. In fact, we think that no transfer matrix method is suitable for the study of periodic quantum dot structures. For the periodic multiple-stub structure, the total transfer matrix $\mathbf{T}$ is determined by the transfer matrix $\mathbf{T}_1$ for a single-stub, i.e., $\mathbf{T} = \mathbf{T}_1^n$, where n is the number of stubs. Let the diagonalized form of $\mathbf{T}_1$ be labelled $\boldsymbol{\lambda}$ and the matrix $\mathbf{P}$ be the transformation matrix

which diagonalizes $\mathbf{T}_1$ such that

$$\mathbf{P}^{-1}\mathbf{T}_1\mathbf{P} = \boldsymbol{\lambda}. \tag{52}$$

Then the total transfer matrix is expressed as

$$\mathbf{T} = \mathbf{T}_1^n = \mathbf{P}\boldsymbol{\lambda}^n\mathbf{P}^{-1}. \tag{53}$$

For a diagonal element of the matrix $\boldsymbol{\lambda}$, λ_j, λ_j^n would be become either very small if $|\lambda_j| < 1$ or very large if $|\lambda_j| > 1$, which is to say, numerical errors would be accumulated in the transfer matrix algorithm for the multiple-stub structure.

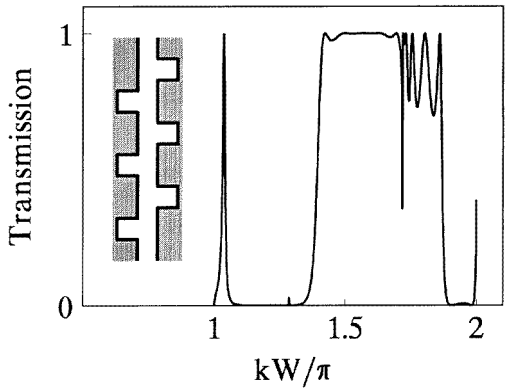

Figure 4. Transmission coefficients versus kW/π for a multiple-stub structure shown in the inset.

Although the transfer matrix technique is very efficient for structures whose dimensions are not very large, it is numerically singular for structures with dimensions much larger than the electron de Broglie wavelength [17], while the same problem does not exist in the scattering matrix method and we find that numerical errors would not be accumulated in the composition of scattering matrices. In figure 4, we provide the results for a multiple-stub structure shown in the inset of the figure. The length of channel linking the two adjacent stubs on one side of the main wire is set to be $2W$, where W is the width of the terminal as well as the width and height of the stub. Similar structures are found to exhibit perfect quantum-modulated transistor action.

As can be seen in the last section, external potentials can be incorporated in the scattering matrix formulation. In fact, the so-called external potentials do not always imply that external potentials, such as electric fields and magnetic fields, actually exist. For example, disorder would be considered as a kind of external potential and can be treated by the method. In figure 5, we provide the results for the structure with a circular obstacle in its symmetric semicircular cavity. The circular obstacle lies at the centre in the cavity and its radius is equal to half of the lead width W. The circular obstacle can be described by the following expression:

$$U_{ex}(x, y) = \begin{cases} 10E_1 & x^2 + y^2 < (W/2)^2 \\ 0 & \text{elsewhere in the cavity} \end{cases} \tag{54}$$

where $E_1 = (\hbar\pi/W)^2/2m^*$ and the original point is set to be at the centre of the cavity. From the figure, it is found that the effect of the obstacle on the transmission is enhanced with the increase of the electron energy, which can be well understood when the relationship

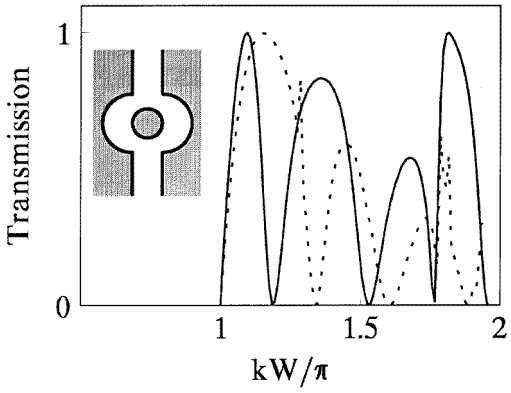

Figure 5. For the structure with a circular obstacle in its cavity, the transmission coefficient versus kW/π. The solid line is for the case in which the obstacle is not taken into account and the dotted line is for the case in which the obstacle is included in the calculations.

between the electron wavelength and the dimensions of the obstacle is taken into account. The 2D propagation vector for the fundamental propagating mode at the terminal k_1 is given by $k_1 W/\pi = \sqrt{(kW/\pi)^2 - 1}$, and the corresponding wavelength is given by $\lambda_1 = 2\pi/k_1$. When kW/π is increased from 1 to 2, the electron wavelength λ_1 is decreased from ∞ to $1.15W$. As the electron energy is close to the first threshold, the longitudinal wavelength is so long that the obstacle has little effect on the electron transmission. In figure 5, it is found that the two results are very close to each other when kW/π is close to 1. As the electron energy is close to the second threshold, the electron wavelength becomes close to the dimensions of the obstacle, and it is found that the effects of the obstacle on the transmission are very notable.

5. Multi-terminal structure

Treating the scattering problem in a multi-terminal structure is very difficult whatever method one uses. Except numerical methods based on the finite-difference or the finite-element technique, only the RGF method can be used to treat general multi-terminal structures, while it is unfortunately the case that the pertinent algorithm has to be reformulated from the beginning for each structure. For those multi-terminal structures in which all of the terminals are parallel to each other, our scattering matrix method can be applied.

In this section, we provide the scattering matrix formulations for treating a typical four-terminal structure as shown in the inset of figure 7. In the four-terminal structure, there are two terminals attached to the left-hand end of the cavity and the other two terminals are attached to the right-hand end. In order to obtain the global scattering matrix, the scattering matrix associated with the interface where two terminals attach to the left-hand end of the cavity should be calculated first. As shown in figure 6, the two left-hand terminals are labelled L_1 and L_2, and the left-hand end of the cavity is labelled R. The wave functions in the three regions are related to each other by a scattering matrix $\mathbf{S}$:

$$\begin{bmatrix} \boldsymbol{A}^-_{L_1} \\ \boldsymbol{A}^-_{L_2} \\ \boldsymbol{A}^+_{R} \end{bmatrix} = \mathbf{S} \begin{bmatrix} \boldsymbol{A}^+_{L_1} \\ \boldsymbol{A}^+_{L_2} \\ \boldsymbol{A}^-_{R} \end{bmatrix}. \tag{55}$$

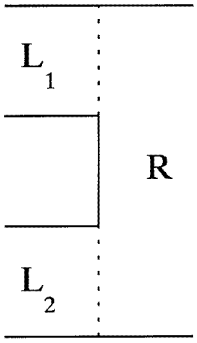

Figure 6. A schematic view of two terminals attached to one end of the cavity.

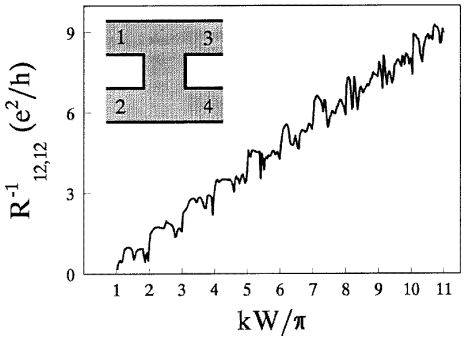

Figure 7. The inverse resistance $R^{-1}_{14,14}$ versus kW/π for the four-terminal structure shown in the inset.

Supposing that N and M are the numbers of transverse modes considered in region R and L_1 (L_2), respectively, we have

$$\mathbf{M}_{\mathrm{L}} \begin{bmatrix} \boldsymbol{A}_{\mathrm{L}_1} \\ \boldsymbol{A}_{\mathrm{L}_2} \end{bmatrix} = \mathbf{M}_{\mathrm{R}} \boldsymbol{A}_{\mathrm{R}}. \tag{56}$$

The matrices $\mathbf{M}_{\mathrm{L}}$ ($(N+2M)\times 4M$) and $\mathbf{M}_{\mathrm{R}}$ ($(N+2M)\times 2N$) are given as follows:

$$\mathbf{M}_{\mathrm{R}} = \begin{bmatrix} \mathbf{C}_{\mathrm{R}}^{\mathrm{T}} \\ \begin{bmatrix} \mathbf{D}_{\mathrm{L}_1} \\ \mathbf{D}_{\mathrm{L}_2} \end{bmatrix} \mathbf{C}_{\mathrm{R}}^{\mathrm{T}} \mathbf{K}_{\mathrm{R}} \end{bmatrix} \tag{57}$$

$$\mathbf{M}_{\mathrm{L}} = \begin{bmatrix} [\, \mathbf{D}_{\mathrm{L}_1}^{\mathrm{T}} \mathbf{C}_{\mathrm{L}_1}^{\mathrm{T}} \quad \mathbf{D}_{\mathrm{L}_2}^{\mathrm{T}} \mathbf{C}_{\mathrm{L}_2}^{\mathrm{T}} \,] \\ \begin{bmatrix} \mathbf{C}_{\mathrm{L}_1}^{\mathrm{T}} \mathbf{K}_{\mathrm{L}_1} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_{\mathrm{L}_2}^{\mathrm{T}} \mathbf{K}_{\mathrm{L}_2} \end{bmatrix} \end{bmatrix} \tag{58}$$

where the notation has a similar meaning to that in equations (38)–(40) We rewrite $\mathbf{M}_{\mathrm{L}}$ and $\mathbf{M}_{\mathrm{R}}$ in terms of $(N+2M)\times M$ blocks and $(N+2M)\times N$ blocks, respectively:

$$\mathbf{M}_{\mathrm{L}} = \left[\mathbf{M}_{\mathrm{L}_1}^{+}, \mathbf{M}_{\mathrm{L}_1}^{-}, \mathbf{M}_{\mathrm{L}_2}^{+}, \mathbf{M}_{\mathrm{L}_2}^{-}\right] \tag{59}$$

$$\mathbf{M}_{\mathrm{R}} = \left[\mathbf{M}_{\mathrm{R}}^{+}, \mathbf{M}_{\mathrm{R}}^{-}\right]. \tag{60}$$

Therefore, the scattering matrix $\mathbf{S}$ can be obtained readily:

$$\mathbf{S} = \left[\mathbf{M}_{\mathrm{L}_1}^{-}, \mathbf{M}_{\mathrm{L}_2}^{-}, -\mathbf{M}_{\mathrm{R}}^{+}\right]^{-1} \left[-\mathbf{M}_{\mathrm{L}_1}^{+}, -\mathbf{M}_{\mathrm{L}_2}^{+}, \mathbf{M}_{\mathrm{R}}^{-}\right]. \tag{61}$$

The scattering matrix associated with the right-hand end of the cavity can be obtained similarly. By the composition law, it is not difficult to calculate the global scattering matrix for the four-terminal structure.

In figure 7, we provide the calculated Büttiker resistance [22] $R_{14,14}$ for the four-terminal structure as shown in the inset of the same figure. The parameters are taken to be the same as those adopted in figure 8 of reference [23]. Comparison of our results with those in reference [23] shows that the two results are well consistent with each other as $kW/\pi < 7$. When $kW/\pi > 7$, as can seen from the two results, the profile of our results becomes more complicated while that in reference [23] becomes simpler. We think that the results for $kW/\pi > 7$ in reference [23] are not correct because the mode-mixing effect is enhanced and the interference between various modes becomes more complicated for higher electron energies. In fact, similar results to those in reference [23] would be obtained if the number of transverse modes in the cavity is not taken to be large enough for high electron energies.

6. Conclusions

In summary, we have presented a comprehensive scattering matrix method for investigating the electron transport in quantum waveguides. By dividing the structure into a number of transverse slices, the global scattering matrix is constructed by the composition of the individual scattering matrices associated with each interface. We have investigated complicated geometries and inhomogeneous external potentials using the proposed scattering matrix method. We have shown that the scattering matrix method possesses many advantages over the traditional transfer matrix method, especially in treating the electron wave propagation in complicated geometries. We have justified our method by demonstrating the unitarity of the calculated scattering matrix and the consistency of the results with those obtained by the recursive Green's function method.

Acknowledgment

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