Scattering matrix of a three-terminal junction in one dimension

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We study the transport characteristics of a three-terminal junction of quantum wires through a one-dimensional formalism. A single-mode S matrix is derived by the tight-binding formulation and its relation with the scattering matrix approach is clarified. By using this S matrix, the transport characteristics of quantum interference devices are reproduced in a single-mode regime. This formulation helps us to introduce realistic junctions in one-dimensional analyses of quantum wires.

Quantum effects can be observed in semiconductors when the size of the structures reaches the coherence length. This condition can be easily accomplished by modern epitaxial and lithographical techniques. Among quantum effects, tunneling phenomena can be analyzed in one dimension as a first approximation. However, to analyze other quantum interference effects in electron waveguides such as the *A-B* effect, junctions should be introduced.

To perform this task, two-dimensional (2D) analyses of electron waveguides have been performed by numerical methods such as the mode matching method[1–4] or the tight-binding (recursive) Green function method.[5–7] Although these numerical analyses are easy to perform for specific examples, it is not always easy to acquire general characteristics from numerical results. To obtain an analytic representation of conductance, one-dimensional (1D) analyses have been applied by using a single-mode S matrix at a junction.[8–20] Furthermore, one-dimensional analyses are of particular importance when one intends to incorporate many-body effects into analyses,[21] because it is very difficult to analyze quantum wires in two dimensions and in the Hilbert space of more than one electron. By using one-dimensional formalism, the qualitative features of quantum oscillations are described in an *AB* ring or a *T*-stub structure[11,13,14] in a single-mode regime. However, these one-dimensional approaches are phenomenological and have been discussed mainly from a theoretical interest, because the applicability of these approximations is not clear. In this paper, we clarify the relation between the S matrix approach and tight-binding formulation and derive an S matrix which corresponds to an energy-dependent extension of that S matrix.

We consider a 1D system which describes a three-terminal junction. When the problem is mapped to 1D from 2D, information about the direction is naturally lost and assumptions must be made to describe such a system. Because the only indispensable restriction is unitarity, there is some freedom in choosing an S matrix.[10,18] At a three-terminal junction, an outgoing wave $\psi = {}^t(\psi_M, \psi_O, \psi_I)$ and an incoming wave $\varphi = {}^t(\varphi_M, \varphi_O, \varphi_I)$ are related by the following linear equation:

$$\psi = \mathbf{S}\varphi, \tag{1}$$

where $\mathbf{S}$ is a 3×3 scattering matrix $\{S_{PQ}\}$. Here, I, O, and M denote the indices of an input, output, and intermediate lead, respectively. In the following discussion, we only consider junctions in which two of the three leads are equivalent. ψ_P (φ_P) is the amplitude of the outgoing (incoming) wave from (to) the junction through a lead P. And S_{PQ} is a scattering amplitude from a lead Q to a lead P.

Büttiker *et al.*[10] derived the scattering matrix from a unitarity condition and an artificial assumption that the S matrix of the junction is real. Using a free parameter ϵ ($0 \le \epsilon \le 1/2$), the scattering matrix of the junction was described as

$$\mathbf{S} = \begin{pmatrix} -(a+b) & \sqrt{\epsilon} & \sqrt{\epsilon} \\ \sqrt{\epsilon} & a & b \\ \sqrt{\epsilon} & b & a \end{pmatrix}, \tag{2}$$

where

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \pm\frac{1}{2}(\sqrt{1-2\epsilon}-1) \\ \pm\frac{1}{2}(\sqrt{1-2\epsilon}+1) \end{pmatrix}, \begin{pmatrix} \pm\frac{1}{2}(\sqrt{1-2\epsilon}+1) \\ \pm\frac{1}{2}(\sqrt{1-2\epsilon}-1) \end{pmatrix}.$$

This S matrix has an advantage in that it can describe various junctions by changing a single parameter and has been widely used.[11,12,14,20] When $\epsilon = 4/9$, it describes a homogeneous junction and is equivalent to the formulation of Xia, in which matching of the wave function was used.[13,16,22] When $\epsilon = 1/2$, $S_{MM} = 0$ and corresponds to the S matrix introduced by Shapiro.[8,9]

However, it is not clear to what extent this S matrix can be used as a model to describe realistic junctions. Even if energy is kept fixed in the analyses, the value of ϵ should be determined from phenomenological arguments.

While the above treatments contain specific assumptions on the elements of the scattering matrix, the tight-binding formulation leads to an energy-dependent and complex scattering matrix without any assumptions except for a tight-binding lattice. Guinea and Vergés[23] directly obtained transmission coefficients of quantum wires with junctions. However, we will show that the S matrix obtained from this formulation can be used to describe realistic junctions, without the restriction of the lattice.

In this formulation, the Hamiltonian is given by

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$$H = H_0 + H', \tag{3}$$

$$H_0 = -t \sum_{i=\ldots,-2,-1,0,1,2,\ldots} (|i\rangle\langle i+1| + |i+1\rangle\langle i|) -t \sum_{j=1',2',\ldots} (|j\rangle\langle j+1| + |j+1\rangle\langle j|), \tag{4}$$

$$H' = -t(|0\rangle\langle 1'| + |1'\rangle\langle 0|). \tag{5}$$

The sites are shown in the inset to Fig. 1. H_0 represents transfer terms within an infinite lead and within a half-infinite lead. H' connects these two leads. All the hopping matrix elements are set to be $-t$. Using the Green functions for each part and connecting them by solving the Dyson equation,[5,24] Green functions for the total system can be analytically determined. By using the formula by Fisher and Lee,[25] the S matrix can be derived as

$$\mathbf{S} = \begin{pmatrix} \alpha & \beta & \beta \\ \beta & \alpha & \beta \\ \beta & \beta & \alpha \end{pmatrix}, \tag{6}$$

where

$$\alpha = \frac{-e^{ika}}{2e^{ika} - e^{-ika}}, \quad \beta = \frac{2i \sin ka}{2e^{ika} - e^{-ika}},$$

where k is the wave number and is related to energy by the formula $E = 2t(1 - \cos ka)$. This expression is equivalent to that of Xia[13] when $ka = \pi/2$. The transmission probability $T = |\beta|^2$ and reflection probability $R = |\alpha|^2$ are plotted against wave number in Fig. 1. While any length in the system must be discrete in the tight-binding formulation, this restriction can be removed if only the above S matrix is used. It can be regarded that the energy dependence was introduced by the scale defined by the tight-binding lattice.

Though the above formulation treats all leads as equivalent ones as that of Xia, by introducing another transmission element t' in (3), this formulation can be extended to describe a junction in which one of the three leads is connected by a different transfer term.

$$H' = -t'(|0\rangle\langle 1'| + |1'\rangle\langle 0|). \tag{7}$$

By following the same procedure as the previous case,

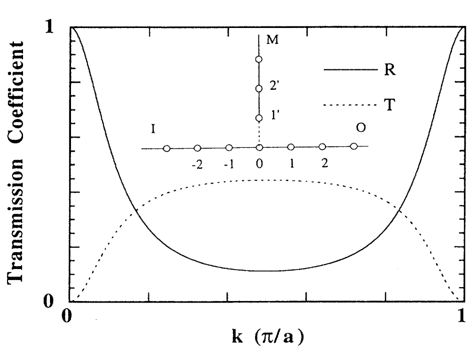

FIG. 1. Transmission and reflection coefficients in the 1D homogeneous tight-binding junction ($\mu = 1$). Inset: 1D tight-binding sites for a three-terminal junction. The solid line represents H_0, while the dotted line represents H'.

the S matrix is obtained as

$$\mathbf{S} = \begin{pmatrix} \delta & \beta & \beta \\ \beta & \alpha & \gamma \\ \beta & \gamma & \alpha \end{pmatrix}, \tag{8}$$

$$\alpha = \frac{1}{\Delta} i\mu^2 e^{ika},$$

$$\beta = \frac{2\mu}{\Delta} \sin ka,$$

$$\gamma = \frac{2}{\Delta} \sin ka,$$

$$\delta = \frac{1}{\Delta}(-2 \sin ka + i\mu^2 e^{-ika}),$$

where $\mu = t'/t$ and $\Delta = 2 \sin ka - i\mu^2 e^{ika}$. By changing t', it is possible to change the coupling between the half-infinite lead and the infinite lead. This S matrix amounts to a natural extension of the homogeneous S matrix (6). Moreover, when $ka = \pi/2$, this expression reduces to the first branch of the expressions in (2) when $\epsilon = 4\mu^2/(\mu^2 + 2)^2$.[27] The condition $0 \le \epsilon \le 1/2$ is naturally satisfied for a real μ. As a result, the above formulation corresponds to an energy-dependent extension of the S matrix (2). Therefore, when the S matrix of (2) is used, we can consider that the configuration of the junction is changed by changing the parameter ϵ, while the energy is kept fixed. In particular, $\mu = 1$ corresponds to a homogeneous case, and $\mu = \sqrt{2}$ corresponds to the strong coupling case of $\epsilon = 1/2$ in (2); thus the S matrix used by Shapiro[8] can be achieved for $ka = \pi/2$.

The transmission probability $|\beta|^2, |\gamma|^2$ and reflection probability $|\alpha|^2, |\delta|^2$ are plotted against wave number in Fig. 2(a) for $\mu = 3/4$. For reference, the same values in a 2D T junction depicted in the inset to Fig. 2(b) are shown in Fig. 2(b) in a single mode regime. The transmission coefficients, $T_{PQ} = |(S_{PQ})_{11}|^2$, are numerically obtained by the tight-binding (recursive) Green function method.[6,26] Though quantitative agreement is not achieved in this simple formulation, qualitative characteristics are reproduced in $ka < \pi/2$, if we regard a as W and ignore the threshold energy of propagation in 2D. It is expected that various configurations of 2D junctions can be described by changing the single parameter μ.

Finally, as simplest applications, the above formulation is applied to quantum interference devices in which one of the three leads is terminated by an infinite potential barrier. The symmetric structure, in which the lead M is terminated and symmetric about an input and an output lead, corresponds to a T-stub structure.[5] The asymmetric structure, in which the lead O is terminated, corresponds to a bend structure.[28] In the symmetric structure, the transmission amplitude is obtained as

$$t = \gamma + \alpha p \alpha + \alpha p \delta p \alpha + \cdots = \frac{2(1+p)\sin k}{2(1+p)\sin k - i\mu^2(e^{ik} + pe^{-ik})}. \tag{9}$$

Here, p is the factor obtained while propagating through the terminated lead and equal to $-e^{2ikL}$, where L is the length of that lead. In this expression, it is readily seen that zeros of the transmission occur for $p = -1$ and $k =$

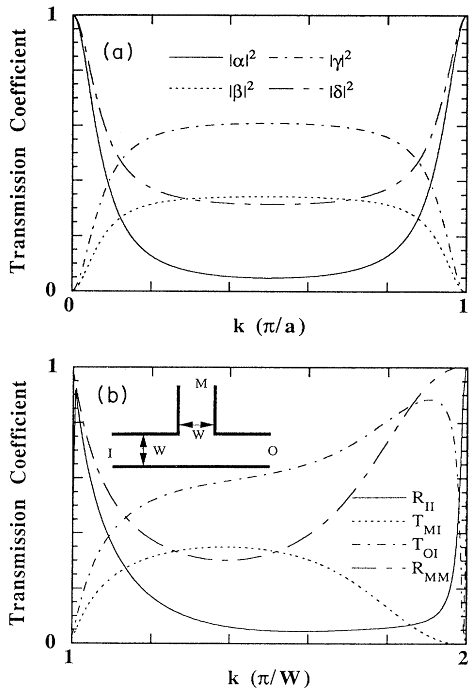

FIG. 2. (a) Transmission and reflection coefficients in the 1D tight-binding junction for $\mu = 3/4$. (b) Transmission and reflection coefficients in the 2D T junction. Inset: the T junction.

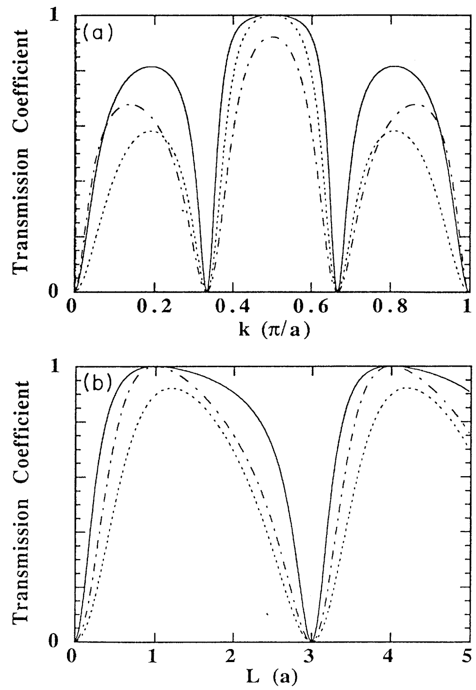

FIG. 3. (a) Wave number dependence for $L = 3a$ and (b) length dependence for $k = \pi/(3a)$ of transmission coefficients in symmetric and asymmetric quantum interference devices. Solid line: $\mu = 3/4$ and symmetric structure; dotted line: $\mu = 1$ and symmetric structure; and dot-dashed line: $\mu = 3/4$ and asymmetric structure.

$n\pi$. In contrast, the transmission maximum occurs when $p = -e^{-2ik}$ and the maximum always reaches the value of 1 regardless of the value of μ.

Similarly, in the asymmetric structure, the transmission amplitude is described as

$$t = \alpha + \alpha p\gamma + \alpha p\beta p\gamma + \cdots = \frac{2\mu \sin k(1+p)}{2\sin k - i\mu^2 e^{ik}(1+p)}. \tag{10}$$

While the zeros occur at the same parameter as in the symmetric case, the transmission maximum occurs at a different value from (9). From (10), the following equation is derived:

$$\frac{1}{|t|^2} = \frac{(\mu^2+1)^2}{4\mu^2} + \frac{1}{4\mu^2}(\cot kL - \mu^2 \cot k)^2 \geq \frac{(\mu^2+1)^2}{4\mu^2} \geq 1. \tag{11}$$

Therefore the transmission coefficient $|t|^2$ is always less than 1 as long as $\mu \neq 1$. In other words, the symmetry between the input and the output lead is necessary to obtain maximum modulation.[16] Wave number dependence and length dependence of the transmission coefficient for three different parameters are depicted in Figs. 3(a) and 3(b), respectively. In spite of the simplicity of the formulation, the general characteristics are qualitatively reproduced. The results smoothly change when L is not an integer multiple of the lattice unit a, and they become periodic with one-half of the wavelength. Though the conductance is periodic with one-half of the wavelength in a single-mode regime, it oscillates with many frequencies in a multimode regime,[26] and this reflects the existence of many transverse modes and cannot be dealt with by a simple model as described above.

In conclusion, we have studied the transport properties of the junctions in one-dimensional formulations. We clarified the relation between the 1D tight-binding Hamiltonian and the 1D scattering matrix approach. The energy-dependent S matrix was derived from the tight-binding formalism and was shown to be an energy-dependent extension of the phenomenological S matrix introduced by Büttiker *et al.*[10] This formulation is expected to be useful for incorporating realistic junctions in quantum wires within a 1D approximation.

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