MASTER THESIS

Numerical Calculation of Conductance by the Virtual-Site Method

仮想サイトを用いた転送行列からの電気伝導度の数値計算

Yukiko Hosoda

細田由喜子

(35102035)

Department of Physics,
Graduate School of Science and Engineering,
Aoyama Gakuin University

Supervisors: Kenn Kubo and Naomichi Hatano
指導教官：久保健・羽田野直道

2003

論　　文　　要　　旨
（和　文）

提 出 年 度： **2003**
提　　出　　日： **2004/02/10**
専　　　　　攻： 物理学
学 生 番 号： **35102035**
学 生 氏 名： 細田由喜子
研究指導教員：久保健・羽田野直道

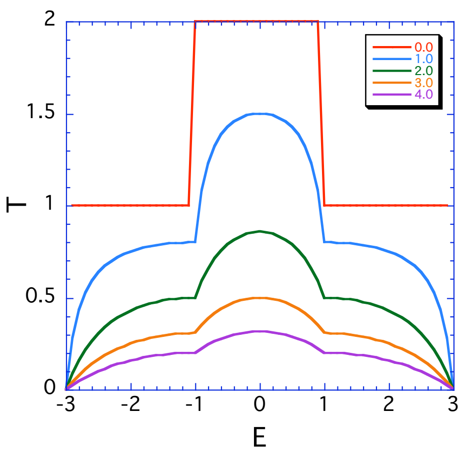
（論文題目）
カーボン系物質の電気伝導度の転送行列計算

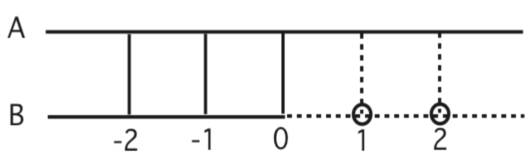
（内容の要旨）

本論文では、カーボン系物質の電気伝導度を計算する。カーボン系物質は、ナノエレクトロニクスにおいてシリコン系物質が迎える限界を超えると期待されている。現在のナノデバイスの主流であるシリコン系物質では材料を削る製法（トップダウン）がとられている。半導体や電気回路の更なる集積化が必要な今、ナノ材料を積み上げていく製法（ボトムアップ）のとれる物質が求められている。その点で、カーボン系物質が注目されているのである。１９８５年にフラーレン、１９９１年にナノチューブが発見されて以来、ナノスケールでのカーボン系物質が多く存在する事がわかっている。

カーボン系物質の最も注目されている性質として、電気特性が挙げられる。その中でもナノチューブは、半径やカイラリティによって、金属的であったり半導体的であったりする事がわかっている。これらのナノ物質を電気回路に応用できれば、分子サイズの回路が出現する期待も持てる。そこで、様々な形状のカーボン系物質の電気伝導度を数値計算する必要性がある。

本研究では、太さが一定でないカーボンナノチューブ様の物質の電気伝導度を転送行列を用いて数値計算する。太さが一定でないと、場所によってチャンネル数が変化する。そこで、仮想サイトという概念を導入するのが本研究の新しい点である。チャンネル数が変化する場合は、チャンネル数が一定の場合（左図）の計算方法は使えず、田村-塚田らが特殊な条件付き転送行列法を提案していた**[1]**。我々は、仮想サイトを導入して仮想的に太さを一定にする事によって、チャンネル数が変化する場合も従来と同じ方法で扱う方法を提案する（右図）。仮想サイトを用いて、１次元鎖と梯子格子を接合した場合の数値計算の結果を紹介する。





左図：梯子格子に一つの不純物がある場合の透過確率。

右図：仮想サイトを用いた１次元鎖と梯子格子の接合格子。これにより、梯子格子と同様に扱える。

[1] R. Tamura and M. Tsukada, Phys. Rev. B 61, 8548 (2000)

Academic Year of 2003, Submitted on Feb, 25, 2004

Graduate School of Science and Engineering, Aoyama Gakuin University

Conductance of the Carbon-Based Materials

Yukiko Hosoda (35102035)
Department of Physics, Master course
Supervisors: Ken Kubo and Naomichi Hatano

We propose a new method of calculating the conductance of carbon-based materials from the transfer matrix with virtual sites. The electronics on a nanometer scale, so called the nanoelectronics, is now one of the most important and anticipated technologies along with the information technology and biotechnology. One of the most hopeful materials for the nanoelectronicsis is carbon-based materials. It is silicon that has played the most important role through the history of the electronics in the twentieth century. However, the techniques of forming electronic devices on a nanometer scale of silicon have almost reached the limit. Carbon-based materials are expected to break the limit, because carbon generally forms crystals of smaller size than silicon does.

In the present thesis, we use the transfer matrix method with virtual sites in order to calculate the conductance of deformed carbon-based materials, where the channel number changes from place to place. Our new point is to introduce virtual sites. The case where the channel number changes was conventionally analyzed by a special method called the constrained transfer-matrix method. By introducing the virtual sites, we treat the cases of the uniform channel number and the non-uniform channel number in the same way. We show, as tutorial examples, the results for the chain lattice and the ladder lattice with uniform channel numbers as well as a chain connected a ladder with a non-uniform channel number. Finally, we discuss an application to carbon-based materials.

MASTER THESIS
Numerical Calculation of Conductance by the Virtual-Site Method

Yukiko Hosoda
(35102035)
Department of Physics,
Graduate School of Science and Engineering,
Aoyama Gakuin University
5-10-1 Fuchinobe, Sagamihara, Kanagawa 229-0006, Japan

Supervisors: Kenn Kubo and Naomichi Hatano

February 25, 2004

Abstract

We propose a new method of calculating the conductance of carbon-based materials with non-uniform channel numbers. Carbon-based materials is one of the most hopeful materials for the nanoelectronics. By the present method, we can calculate the conductance in the same way no matter the channel number changes or not. We demonstrate the method in several examples.

Contents

1 Introduction

The electronics on a nanometer scale, so called the nanoelectronics, is now one of the most important and anticipated technologies along with the information technology and biotechnology. The development of the electronics has been the development of techniques of making electronic devices smaller and smaller. For example, the most important requirement for LSI (Large Scale Integration), which is essential in our life, is to make its size much smaller to the range of nanometers.

One of the most hopeful materials for the nanoelectronics is carbon-based materials [1, 2]. It is silicon that has played the most important role through the history of the electronics in the twentieth century. However, the techniques of forming electronic devices on a nanometer scale of silicon have almost reached the limit. Carbon-based materials are expected to break the limit, because carbon generally forms crystals of smaller size than silicon does.

The carbon-based materials have several advantages over silicon. One of the advantages is that carbon has a much wider variety of network structure; carbon can form not only the sp^3-hybridized orbital but also the sp^2-hybridized orbital. Carbon atoms of sp^3-hybridized orbitals form the diamond crystal as well as molecules of saturated hydrocarbons, such as methane, ethane, and so on. On the other hand, carbon atoms of sp^2-hybridized orbitals form the graphite crystal as well as molecules of aromatic hydrocarbons, such as benzene, naphthalene, and so on. Another advantage of carbon is a possibility of electronic conduction by π electrons in the case of carbon materials with sp^2-hybridized atoms.

The discoveries of fullerene (C_{60}) in 1985 and of nanotube in 1991 caused a breakthrough in the work of a series of materials made of sp^2-hybridized carbon atoms; a number of materials of sp^2-hybridized carbon atoms with interesting forms were formed, such as cages and tubes. The most hopeful material as an electronic device is carbon nanotube. The carbon nanotube is intrinsically a quantum wire, whereas lithography is necessary to from a quantum wire of silicon. In addition, the nanotubes show metallic or semiconducting properties depending on the radius and the chirality.

Another carbon-based material of focused attention is carbon nanohorn. The carbon nanohorn has been already in the stage of application as an electrode of fuel cells for mobile computers. Thus we need to study the electronic conductivity of the carbon-based materials for the further development of the nanoelectronics.

In the present thesis, we propose a new method of computing the conductance of carbon-based materials. In Sec. 2 we present the general method of calculation used in this study. We introduce in Sec. 2.1 the Landauer formula, which yields the conductance of mesoscopic materials from the transmission coefficient. In Sec. 2.2 we present the transfer-matrix method of obtaining the transmission coefficient. In Sec. 3 we show tutorial examples: a chain lattice, a ladder lattice and a chain connected to ladder. The last example, in particular, describes a case where the channel number is not uniform through the material. This is relevant to various carbon-based materials. In order to treat such a case, we introduce a new method using virtual sites. In Sec. 4 we show how to apply the virtual-site method to carbon-based materials. Finally, in Sec. 5 we give the summary.

2 Calculation method

In this section, we introduce the Landauer formula and the transfer-matrix method. We adopt the tight-binding model for numerical calculations.

2.1 Landauer formula

The Landauer formula has been used to calculate the conductance of mesoscopic conductors [3]. The formula expresses a concept that has proved very useful in understanding mesoscopic transport; the current flow through a conductor is proportional to the **transmission coefficient**, which describes the ease of transmit of electrons through the conductor.

It is well-known that the conductance G of a large conductor of width $W$and of length L obeys the ohmic scaling law:

$$G = \sigma W/L, \tag{1}$$

where the conductivity σ is a material constant independent of its dimensions. Mesoscopic conductors, however, do not show the behavior of Eq. (1) because its dimensions are much smaller than the mean free path and the phase-relaxation length. The conductance of mesoscopic systems is given by

$$G = \frac{2e}{h} \sum_{i,j} |t_{ij}|^2, \tag{2}$$

where t_{ij} denotes the transmission coefficient from the ith channel to the jth channel. This is the Landauer formula.

We can derive the transmission coefficient t_{ij} from the scattering matrix S. Consider a scattering problem in one dimension (Fig. 1(a)). The S-matrix is the matrix that relates the amplitudes of the scattering waves $\mathbf{b}$ to the incident wave amplitudes $\mathbf{a}$:

$$\begin{pmatrix} b_{\mathrm{L}} \\ b_{\mathrm{R}} \end{pmatrix} = S \begin{pmatrix} a_{\mathrm{R}} \\ a_{\mathrm{L}} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} a_{\mathrm{R}} \\ a_{\mathrm{L}} \end{pmatrix}, \tag{3}$$

where the subscripts L and R denote the left-going and right-going waves, respectively. The S matrix is a unitary matrix because of the flux conservation. We use the transfer matrix to write down the S matrix in the next subsection.

Meanwhile, the usual scattering problem has an incident wave, a reflection wave and a transmission wave (Fig. 1(b) and (c)). They are related in the following ways:

$$\begin{aligned} \Psi_{\mathrm{R}} + r\Psi_{\mathrm{L}} &= t\Phi_{\mathrm{R}} && \text{for an incident wave from the left,} \\ \Phi_{\mathrm{L}} + r'\Phi_{\mathrm{R}} &= t'\Psi_{\mathrm{L}} && \text{for an incident wave from the right,} \end{aligned} \tag{4}$$

where the factors t and t' are the transmission coefficients and r and r' are the reflection coefficients, while $\Psi(\Phi)$ denotes the wave function on the left (right) side. We rewrite Eq. (4) as follows:

$$\begin{aligned} \Psi_{\mathrm{R}} &= -r\Psi_{\mathrm{L}} + t\Phi_{\mathrm{R}}, \\ \Phi_{\mathrm{L}} &= t'\Psi_{\mathrm{L}} - r'\Phi_{\mathrm{R}}, \end{aligned} \tag{5}$$

from which we obtain

$$\begin{pmatrix} \Psi_{\mathrm{R}} \\ \Phi_{\mathrm{L}} \end{pmatrix} = \begin{pmatrix} -r & t \\ t' & -r' \end{pmatrix} \begin{pmatrix} \Psi_{\mathrm{L}} \\ \Phi_{\mathrm{R}} \end{pmatrix} \equiv A \begin{pmatrix} \Psi_{\mathrm{L}} \\ \Phi_{\mathrm{R}} \end{pmatrix} \tag{6}$$

Comparing Fig. 1(a)–(c), we have

$$\begin{aligned} a_{\mathrm{R}} &= \Psi_{\mathrm{R}}, \\ a_{\mathrm{L}} &= \Phi_{\mathrm{L}}. \end{aligned} \tag{7}$$

We then notice in Eqs. (6) and (3) that the matrix A is, in fact, the inverse of the S matrix:

$$A = S^{-1} = S^{\dagger} \tag{8}$$

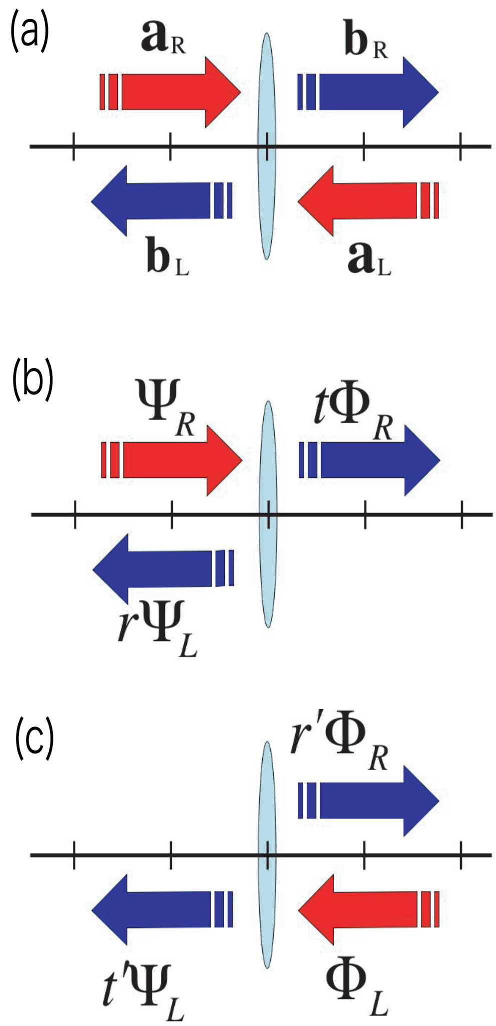


Figure 1: (a) The definition of the S-matrix; $\mathbf{a}$ and $\mathbf{b}$ represent the amplitudes of the incident waves and the scattering waves. (b) The incident wave Ψ_{R} from the left is split into the transmission wave $t\Phi_{\mathrm{R}}$ and the scattering wave $r\Psi_{\mathrm{L}}$. (c) The incident wave Φ_{L} from the right is split into the transmission wave $t'\Psi_{\mathrm{L}}$ and the scattering wave $r'\Phi_{\mathrm{R}}$.

Thus we arrive at

$$\begin{pmatrix} -r & t \\ t' & -r' \end{pmatrix} = S^\dagger = \begin{pmatrix} S_{11}^* & S_{21}^* \\ S_{12}^* & S_{22}^* \end{pmatrix}. \tag{9}$$

2.2 Transfer matrix

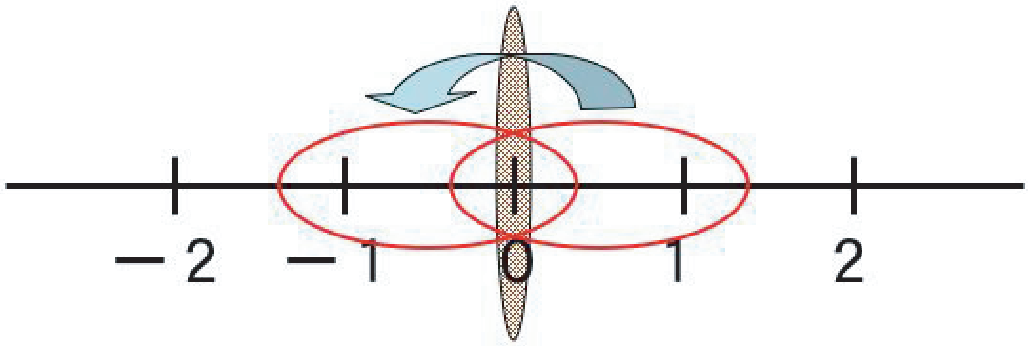


Figure 2: A chain with a potential at $x = 0$. We obtain the states at $x = -1$ and $x = 0$ by transferring the states at $x = 0$ and $x = 1$.

Consider, for example, a scattering problem in one dimension with the potential V_0 at $x = 0$ (Fig. 2). The Hamiltonian is that of the tight-binding model:

$$\mathcal{H} = \sum_x \left(|\psi_{x+1}\rangle\langle\psi_x| + |\psi_x\rangle\langle\psi_{x+1}|\right) + V_0|\psi_0\rangle\langle|\psi_0| \tag{10}$$

We define the transfer matrix in the form

$$\begin{pmatrix} \psi_{-1} \\ \psi_0 \end{pmatrix} = T_0 \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}. \tag{11}$$

Let us write down the transfer matrix T_0. From the Schrödinger equation $\mathcal{H}|\psi_0\rangle = E|\psi_0\rangle$, we obtain

$$|\psi_1\rangle + |\psi_{-1}\rangle + V_0|\psi_0\rangle = E|\psi_0\rangle, \tag{12}$$

or

$$|\psi_{-1}\rangle = (E - V_0)\,|\psi_0\rangle - |\psi_1\rangle. \tag{13}$$

By adding a trivial condition

$$|\psi_0\rangle = |\psi_0\rangle, \tag{14}$$

we have

$$\begin{pmatrix} \psi_{-1} \\ \psi_0 \end{pmatrix} = \begin{pmatrix} E - V_0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} \equiv T_0 \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}. \tag{15}$$

Thus we obtain the transfer matrix T_0. We can also write the transfer matrix for $x \neq 0$ in the same way:

$$\begin{pmatrix} \psi_{x-1} \\ \psi_x \end{pmatrix} = \begin{pmatrix} E & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_x \\ \psi_{x+1} \end{pmatrix} \equiv T \begin{pmatrix} \psi_x \\ \psi_{x+1} \end{pmatrix} \tag{16}$$

We now relate the transfer matrix to the S matrix. Consider the situations shown in Fig. 3(a) and (b). It is quite difficult to transfer the incident wave plus the reflection wave to the transmission wave, because we do not know the coefficients r and $r' apriori$. Instead, we transfer in the opposite direction. Now consider the situations in Fig. 3(c) and (d). We transfer the transmission wave $\Phi_{\mathrm{R}}(\Psi_{\mathrm{L}})$ to the left (right) to obtain the incident wave and the reflection wave. The three waves in Fig. 3(c) and (d) are related in the following ways:

$$\begin{aligned} \Phi_{\mathrm{R}} &= x_{\mathrm{R}}\Psi_{\mathrm{R}} + y_{\mathrm{L}}\Psi_{\mathrm{L}} && \text{for an incident wave from the eft,} \\ \Psi_{\mathrm{L}} &= x_{\mathrm{L}}\Phi_{\mathrm{L}} + y_{\mathrm{R}}\Phi_{\mathrm{R}} && \text{for an incident wave from the right,} \end{aligned} \tag{17}$$

where the factor $\mathbf{x}$ is the incident coefficient and $\mathbf{y}$ is the reflection coefficient. We rewrite Eq. (17) as follows:

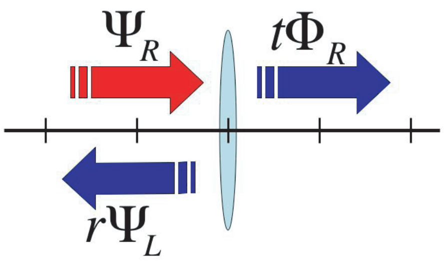
$$\begin{pmatrix} \Psi_{\mathrm{L}} \\ \Phi_{\mathrm{R}} \end{pmatrix} = \begin{pmatrix} 0 & y_{\mathrm{R}} \\ y_{\mathrm{L}} & 0 \end{pmatrix} \begin{pmatrix} \Psi_{\mathrm{L}} \\ \Phi_{\mathrm{R}} \end{pmatrix} + \begin{pmatrix} 0 & x_{\mathrm{L}} \\ x_{\mathrm{R}} & 0 \end{pmatrix} \begin{pmatrix} \Psi_{\mathrm{R}} \\ \Phi_{\mathrm{L}} \end{pmatrix}, \tag{18}$$

from which we obtain

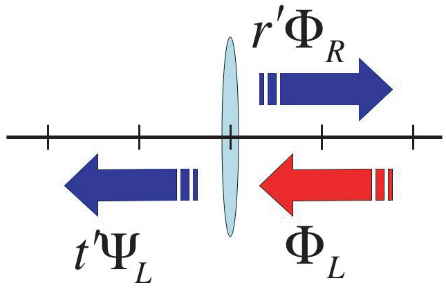
$$\begin{pmatrix} 1 & -y_{\mathrm{R}} \\ -y_{\mathrm{L}} & 1 \end{pmatrix} \begin{pmatrix} \Psi_{\mathrm{L}} \\ \Phi_{\mathrm{R}} \end{pmatrix} = \begin{pmatrix} 0 & x_{\mathrm{L}} \\ x_{\mathrm{R}} & 0 \end{pmatrix} \begin{pmatrix} \Psi_{\mathrm{R}} \\ \Phi_{\mathrm{L}} \end{pmatrix}, \tag{19}$$

followed by

$$\begin{aligned} \begin{pmatrix} \Psi_{\mathrm{R}} \\ \Phi_{\mathrm{L}} \end{pmatrix} &= \begin{pmatrix} 0 & x_{\mathrm{L}} \\ x_{\mathrm{R}} & 0 \end{pmatrix}^{-1} \begin{pmatrix} 1 & -y_{\mathrm{R}} \\ -y_{\mathrm{L}} & 1 \end{pmatrix} \begin{pmatrix} \Psi_{\mathrm{L}} \\ \Phi_{\mathrm{R}} \end{pmatrix} \\ &= \begin{pmatrix} 0 & {x_{\mathrm{R}}}^{-1} \\ {x_{\mathrm{L}}}^{-1} & 0 \end{pmatrix} \begin{pmatrix} 1 & -y_{\mathrm{R}} \\ -y_{\mathrm{L}} & 1 \end{pmatrix} \begin{pmatrix} \Psi_{\mathrm{L}} \\ \Phi_{\mathrm{R}} \end{pmatrix} \\ &= \begin{pmatrix} -{x_{\mathrm{R}}}^{-1}y_{\mathrm{L}} & {x_{\mathrm{R}}}^{-1} \\ {x_{\mathrm{L}}}^{-1} & -{x_{\mathrm{L}}}^{-1}y_{\mathrm{R}} \end{pmatrix} \begin{pmatrix} \Psi_{\mathrm{L}} \\ \Phi_{\mathrm{R}} \end{pmatrix}. \end{aligned} \tag{20}$$



(a)



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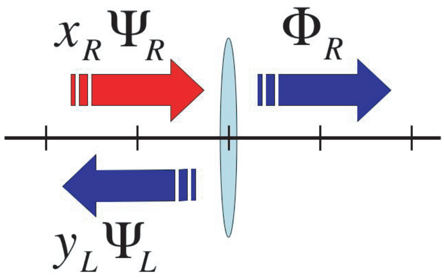
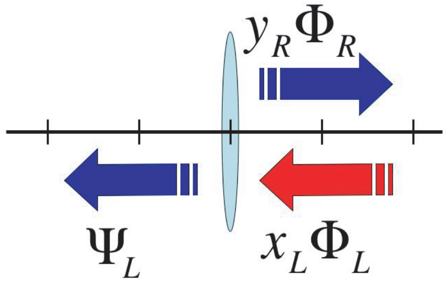


(c)



(d)

Figure 3: (a) The same as Fig. 1(b). (b) The same as Fig. 1(c). (c) The transmission wave $\Phi_{\rm R}$ is transferred to the left side, yielding the incident wave $x_{\rm R}\Psi_{\rm R}$ and the reflection wave $y_{\rm L}\Psi_{\rm L}$. (d)The transmission wave $\Psi_{\rm L}$ is transferred to the right side, yielding the incident wave $x_{\rm L}\Phi_{\rm L}$ and the reflection wave $y_{\rm R}\Phi_{\rm R}$.

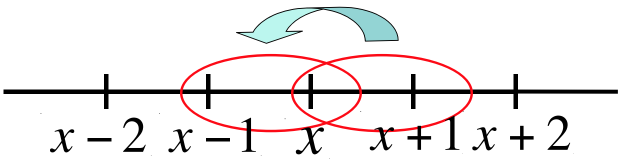


Figure 4: By transferring the states at x and $x+1$, we obtain the states at $x-1$ and x, where $x \neq 0$.

Comparing Eq. (20) with Eq. (6), we arrive at

$$A = \begin{pmatrix} -r & t \\ t' & -r' \end{pmatrix} = \begin{pmatrix} -x_{\mathrm{R}}{}^{-1} y_{\mathrm{L}} & x_{\mathrm{R}}{}^{-1} \\ x_{\mathrm{L}}{}^{-1} & -x_{\mathrm{L}}{}^{-1} y_{\mathrm{R}} \end{pmatrix} \tag{21}$$

Thus we obtain the transmission coefficients t and t' as the reciprocal of the x_{R} and x_{L}.

3 Tutorial examples

We show here several examples of deriving the conductance by the method introduced in the previous section. In Sec. 3.1 we solve the scattering problem on a chain. Next, we treat a ladder in Sec. 3.2. Finally in Sec. 3.3, we show how to treat a system where the width changes.

3.1 Chain

Consider the scattering problem in one dimension once more. Before calculating the transmission coefficient, we first need to obtain the dispersion relation for $x \neq 0$ by diagonalizing the transfer matrix in Eq. (16). Next, we write down the equation for $x = 0$ with the three waves, the incident, reflection and transmission waves.

3.1.1 Dispersion relation for $x \neq 0$

We consider the situation for $x \neq 0$ (Fig. 4). The transfer matrix is given by Eq. (16), that is,

$$\begin{pmatrix} \psi_{x-1} \\ \psi_x \end{pmatrix} = T \begin{pmatrix} \psi_x \\ \psi_{x+1} \end{pmatrix} = \begin{pmatrix} E & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_x \\ \psi_{x+1} \end{pmatrix}. \tag{22}$$

We here note the identity

$$\begin{pmatrix} {\psi_{x-1}}^\dagger & {\psi_x}^\dagger \end{pmatrix} \begin{pmatrix} \psi_{x-1} \\ \psi_x \end{pmatrix} = \begin{pmatrix} {\psi_x}^\dagger & {\psi_{x+1}}^\dagger \end{pmatrix} \begin{pmatrix} \psi_x \\ \psi_{x+1} \end{pmatrix}, \tag{23}$$

which follows from the flux conservation

$$|\psi_{x-1}|^2 = |\psi_{x+1}|^2. \tag{24}$$

Substituting Eq. (22) for Eq. (23), we have

$$T^\dagger T = I, \tag{25}$$

where I is the identity matrix. Equation (25) means that the transfer matrix T is a unitary matrix. The absolute values of the eigenvalues of a unitary matrix is unity. We also note that the elements of the transfer matrix are all real. This means the following; when we have an eigenvalue λ as in $T\mathbf{v} = \lambda\mathbf{v}$, we have

$$\lambda^* \mathbf{v}^* = T^* \mathbf{v}^* = T\mathbf{v}^*, \tag{26}$$

that is, λ^* is another eigenvalue. In other words, the eigenvalues of the transfer matrix T appears as a complex-conjugate pair. Therefore we can express the eigenvalues in the form

$$\lambda_\pm \quad = \quad e^{\mp ik}, \tag{27}$$

where $\lambda^\pm$ are the eigenvalues and k is a real number, which below turns out to be the wave number. Defining the respective eigenvector as

$$\begin{pmatrix} \psi_x^{(\pm)} \\ \psi_{x+1}^{(\pm)} \end{pmatrix}, \tag{28}$$

we have

$$\begin{aligned} \begin{pmatrix} \psi_x^{(\pm)} \\ \psi_{x+1}^{(\pm)} \end{pmatrix} &= T \begin{pmatrix} \psi_x^{(\pm)} \\ \psi_{x+1}^{(\pm)} \end{pmatrix} = \lambda_\pm \begin{pmatrix} \psi_x^{(\pm)} \\ \psi_{x+1}^{(\pm)} \end{pmatrix} \\ &= e^{\mp ik} \begin{pmatrix} \psi_x^{(\pm)} \\ \psi_{x+1}^{(\pm)} \end{pmatrix} \\ &= e^{\mp 2ik} \begin{pmatrix} \psi_{x+1}^{(\pm)} \\ \psi_{x+2}^{(\pm)} \end{pmatrix} = \cdots . \end{aligned} \tag{29}$$

Thus we obtain

$$\begin{pmatrix} \psi_x^{(\pm)} \\ \psi_{x+1}^{(\pm)} \end{pmatrix} \propto \begin{pmatrix} e^{\pm ikx} \\ e^{\pm ik(x+1)} \end{pmatrix}. \tag{30}$$

By substituting Eq. (30), or $\psi_x^{\pm} \propto e^{\pm ikx}$ for the Schrödinger equation

$$\psi_{x+1}^{\pm} + \psi_{x-1}^{\pm} = E\psi_x^{\pm}, \tag{31}$$

we arrive at

$$e^{\pm ik} + e^{\mp ik} = E, \tag{32}$$

namely,

$$E = 2\cos k. \tag{33}$$

Thus we obtain the dispersion relation for $x \neq 0$ as shown in Fig. 5(a). We notice that this system has only one channel.

3.1.2 Scattering at $x = 0$

Next, we rewrite the equation at $x = 0$, Eq. (15), with the three waves, which are the transmission wave, the incident wave and the reflection wave. As was shown in Sec. 2.2, the transmission coefficient t is derived from the coefficient x_{R} in Fig. 3(c) as $t = x_{\mathrm{R}}^{-1}$.

Consider the situation where the transmission wave Φ_{R} is on the right side (Fig. 3(c)). The wave function ψ_x on both sides can be written in the form of superposition of the wave functions $\psi_x^{(\pm)}$:

$$|\psi_x\rangle = \begin{cases} |e^{ikx}\rangle & \text{on the right } (x \geq 0), \\ x_{\mathrm{R}}|e^{ikx}\rangle + y_{\mathrm{L}}|e^{-ikx}\rangle & \text{on the left } (x \leq 0). \end{cases} \tag{34}$$

Substituting Eq. (34) for Eq. (15), we have

$$\begin{pmatrix} x_{\mathrm{R}}e^{-ik} + y_{\mathrm{L}}e^{ik} \\ x_{\mathrm{R}} + y_{\mathrm{L}} \end{pmatrix} = \begin{pmatrix} E - V_0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ e^{ik} \end{pmatrix}. \tag{35}$$

Equation (35) is a simultaneous equation of x_{R} and y_{L}. Solving it, we obtain

$$x_{\mathrm{R}} = \frac{2e^{ik} - E + V_0}{2i\sin k}, \tag{36}$$

which yields

$$t = {x_{\mathrm{R}}}^{-1} = \frac{2i \sin k}{2e^{ik} - E + V_0}. \tag{37}$$

In the same way, we can obtain the transmission coefficient t' from x_{L}. Instead of Eq. (34), we have

$$|\psi_x\rangle = \begin{cases} x_{\mathrm{L}}|e^{-ikx}\rangle + y_{\mathrm{L}}|e^{ikx}\rangle & \text{on the right } (x \geq 0), \\ |e^{-ikx}\rangle & \text{on the left } (x \leq 0), \end{cases} \tag{38}$$

from which we obtain

$$x_{\mathrm{L}} = \frac{2e^{ik} - E + V_0}{2i \sin k} \tag{39}$$

and hence

$$t' = {x_{\mathrm{L}}}^{-1} = \frac{2i \sin k}{2e^{ik} - E + V_0}. \tag{40}$$

Finally, the transmission probability is given by

$$T = |t|^2 = |t'|^2 = \frac{4 \sin^2 k}{4 + (E - V_0)(E - V_0 - 4 \cos k)}. \tag{41}$$

This is shown in Fig. 5(b) for $V_0 = 0.0, 1.0, 2.0$ and 3.0. The transmission probability is, of course, $T \equiv 1$ for $V_0 = 0$.

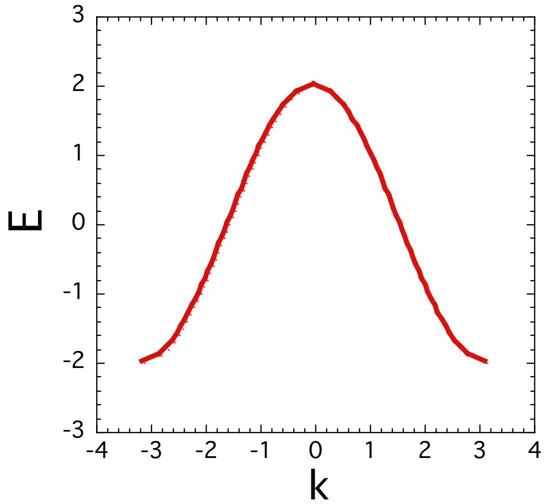
3.2 Ladder lattice

Next, we calculate the transmission coefficient on a ladder lattice shown in Fig. 6. The Hamiltonian is defined by

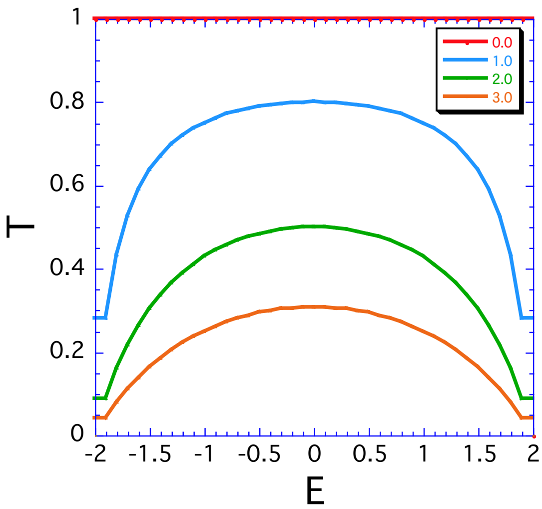
$$\begin{aligned} \mathcal{H} &= \sum_x \sum_{y=A,B} \left(|\psi_{x+1,y}\rangle\langle\psi_{x,y}| + |\psi_{x,y}\rangle\langle\psi_{x+1,y}|\right) \\ &+ \sum_x \left(|\psi_{x,B}\rangle\langle\psi_{x,A}| + |\psi_{x,A}\rangle\langle\psi_{x,B}|\right) \\ &+ V_A|\psi_{0,A}\rangle\langle|\psi_{0,A}| + V_B|\psi_{0,B}\rangle\langle|\psi_{0,B}|. \end{aligned} \tag{42}$$

From the Schrödinger equation

$$\begin{cases} \mathcal{H}|\psi_{0,A}\rangle = E|\psi_{0,A}\rangle, \\ \mathcal{H}|\psi_{0,B}\rangle = E|\psi_{0,B}\rangle, \end{cases} \tag{43}$$



(a)



(b)

Figure 5: (a) The dispersion relation for $x \neq 0$. (b) The energy dependence of the transmission probability T for $V_0 = 0.0$, 1.0, 2.0 and 3.0.

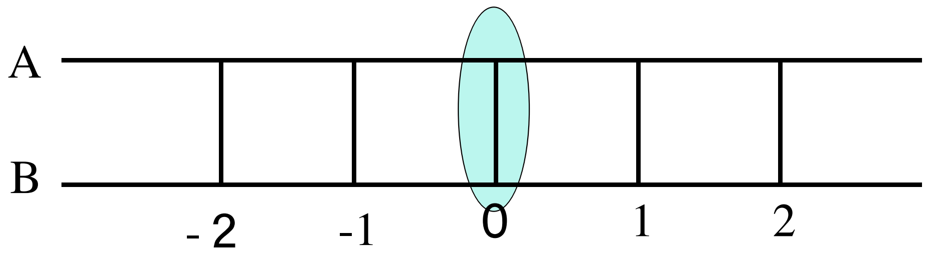


Figure 6: A ladder lattice with the potential at $(x, y) = (0, A)$ and $(0, B)$.

we obtain the following relations:

$$\begin{aligned} |\psi_{1,A}\rangle + |\psi_{-1,A}\rangle + |\psi_{0,B}\rangle + V_0|\psi_{0,A}\rangle &= E|\psi_{0,A}\rangle, \\ |\psi_{1,B}\rangle + |\psi_{-1,B}\rangle + |\psi_{0,A}\rangle + V_0|\psi_{0,B}\rangle &= E|\psi_{0,B}\rangle. \end{aligned} \tag{44}$$

By adding two trivial conditions

$$\begin{aligned} |\psi_{0,A}\rangle &= |\psi_{0,A}\rangle, \\ |\psi_{0,B}\rangle &= |\psi_{0,B}\rangle, \end{aligned} \tag{45}$$

we write down the transfer matrix as

$$\begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix} = \begin{pmatrix} E - V_A & -1 & -1 & 0 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & E - V_B & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_{0,A} \\ \psi_{1,A} \\ \psi_{0,B} \\ \psi_{1,B} \end{pmatrix} \equiv T_0 \begin{pmatrix} \psi_{0,A} \\ \psi_{1,A} \\ \psi_{0,B} \\ \psi_{1,B} \end{pmatrix}. \tag{46}$$

The transfer matrix for $x \neq 0$ is given as

$$\begin{pmatrix} \psi_{x-1,A} \\ \psi_{x,A} \\ \psi_{x-1,B} \\ \psi_{x,B} \end{pmatrix} = \begin{pmatrix} E & -1 & -1 & 0 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & E & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_{x,A} \\ \psi_{x+1,A} \\ \psi_{x,B} \\ \psi_{x+1,B} \end{pmatrix} \equiv T \begin{pmatrix} \psi_{x,A} \\ \psi_{x+1,A} \\ \psi_{x,B} \\ \psi_{x+1,B} \end{pmatrix}. \tag{47}$$

3.2.1 Dispersion relation for $x \neq 0$

In order to obtain the dispersion relation, we diagonalize the transfer matrix T in Eq. (47). From the argument in Eqs. (23)–(26), the eigenvalues of the transfer matrix T appears as complex-conjugate pairs. Hence we can express the eigenvalues λ as

$$\lambda = \begin{cases} e^{\pm ik_1}, \\ e^{\pm ik_2}. \end{cases} \tag{48}$$

In a way similar to the argument in Eqs. (28)–(30) we obtain

$$\begin{pmatrix} \psi^{(\pm)}_{x,A} \\ \psi^{(\pm)}_{x+1,A} \\ \psi^{(\pm)}_{x,B} \\ \psi^{(\pm)}_{x+1,B} \end{pmatrix} \propto \begin{pmatrix} e^{\pm ik_1 x} \\ e^{\pm ik_1 (x+1)} \\ e^{\pm ik_1 x} \\ e^{\pm ik_1 (x+1)} \end{pmatrix}, \begin{pmatrix} e^{\pm ik_2 x} \\ e^{\pm ik_2 (x+1)} \\ -e^{\pm ik_2 x} \\ -e^{\pm ik_2 (x+1)} \end{pmatrix}. \tag{49}$$

By substituting Eq. (49) for the Schrödinger equation

$$\begin{aligned} |\psi^{(\pm)}_{x+1,A}\rangle + |\psi^{(\pm)}_{x-1,A}\rangle + |\psi^{(\pm)}_{x,B}\rangle &= E|\psi^{(\pm)}_{x,A}\rangle, \\ |\psi^{(\pm)}_{x+1,B}\rangle + |\psi^{(\pm)}_{x-1,B}\rangle + |\psi^{(\pm)}_{x,A}\rangle &= E|\psi^{(\pm)}_{x,B}\rangle, \end{aligned} \tag{50}$$

we arrive at

$$E = \begin{cases} 2\cos k_1 + 1, \\ 2\cos k_2 - 1. \end{cases} \tag{51}$$

We show the dispersion relation in Fig. 7(a). We notice that the ladder lattice has two channels. We define the state of the wave number k_1 as the channel 1 and that of the number k_2 as the channel 2.

3.2.2 Scattering at $x = 0$

In the scattering problem in this case, each of the incident, reflection and transmission waves consists of the two channels. Consequently, we must consider the following situation (Fig. 8). When the wave $\Psi_{1\mathrm{R}}$ of the channel 1 incidents from the left, we have

$$\Psi_{1\mathrm{R}} + r_{11}\Psi_{1\mathrm{L}} + r_{12}\Psi_{2\mathrm{L}} = t_{11}\Phi_{1\mathrm{R}} + t_{12}\Phi_{2\mathrm{R}}, \tag{52}$$

where the factor $t(r)$ is the transmission (reflection) coefficient and the index (ij) represents the scattering from the ith channel to the jth channel. In the same way we obtain the other three relations as follows:

$$\begin{aligned} \Psi_{2\mathrm{R}} + r_{21}\Psi_{1\mathrm{L}} + r_{22}\Psi_{2\mathrm{L}} &= t_{21}\Phi_{1\mathrm{R}} + t_{22}\Phi_{2\mathrm{R}}, \\ \Phi_{1\mathrm{L}} + r'_{11}\Phi_{1\mathrm{R}} + r'_{12}\Phi_{2\mathrm{R}} &= t'_{11}\Psi_{1\mathrm{L}} + t'_{12}\Psi_{2\mathrm{L}}, \\ \Phi_{2\mathrm{L}} + r'_{21}\Phi_{1\mathrm{R}} + r'_{22}\Phi_{2\mathrm{R}} &= t'_{21}\Psi_{1\mathrm{L}} + t'_{22}\Psi_{2\mathrm{L}}, \end{aligned} \tag{53}$$

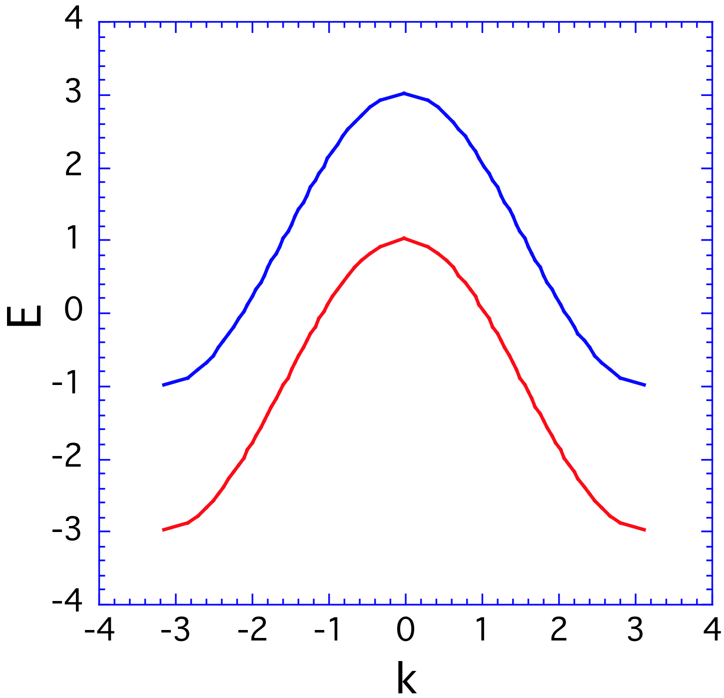


Figure 7: The dispersion relation for $x \neq 0$. The upper line is the channel 1 and the lower line is the channel 2.

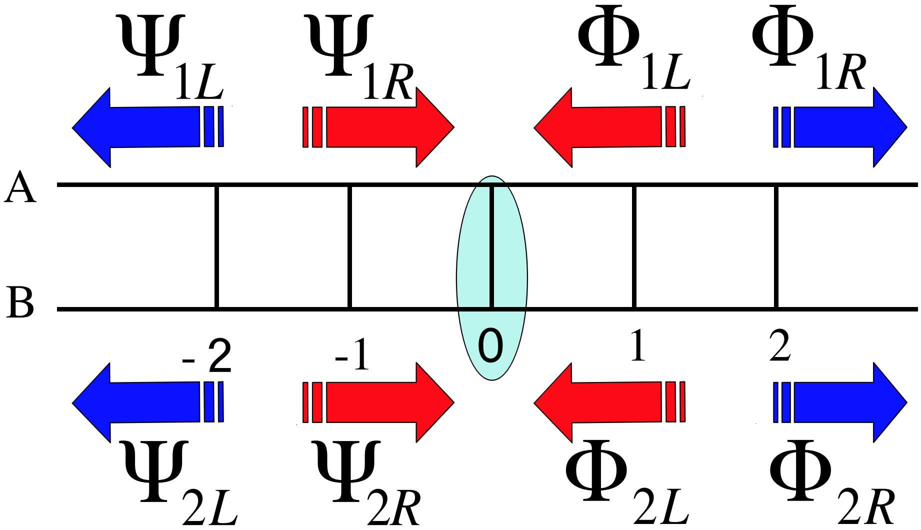


Figure 8: We represent the state for $x \leq 0$ with four waves; the right and left-going waves of the channel 1 and the channel 2, $\Psi_{1\mathrm{R}}, \Psi_{1\mathrm{L}}, \Psi_{2\mathrm{R}}, \Psi_{2\mathrm{L}}$, respectively. In the same way, we represent the state for $x \geq 0$ with four waves $\Phi_{1\mathrm{R}}, \Phi_{1\mathrm{L}}, \Phi_{2\mathrm{R}}, \Phi_{2\mathrm{L}}$.

where

$$\begin{aligned}
\Psi_{1\mathrm{R}} &\equiv \begin{pmatrix} \psi_{x,A} \\ \psi_{x,B} \end{pmatrix} \propto \begin{pmatrix} e^{ik_1x} \\ e^{ik_1x} \end{pmatrix}, \quad \Psi_{1\mathrm{L}} \propto \begin{pmatrix} e^{-ik_1x} \\ e^{-ik_1x} \end{pmatrix}, \\
\Psi_{2\mathrm{R}} &\propto \begin{pmatrix} e^{ik_2x} \\ -e^{ik_2x} \end{pmatrix}, \quad \Psi_{2\mathrm{L}} \propto \begin{pmatrix} e^{-ik_2x} \\ -e^{-ik_2x} \end{pmatrix}, \quad (x \leq 0),
\end{aligned} \tag{54}$$

$$\begin{aligned}
\Phi_{1\mathrm{R}} &\equiv \begin{pmatrix} \psi_{x,A} \\ \psi_{x,B} \end{pmatrix} \propto \begin{pmatrix} e^{ik_1x} \\ e^{ik_1x} \end{pmatrix}, \quad \Phi_{1\mathrm{L}} \propto \begin{pmatrix} e^{-ik_1x} \\ e^{-ik_1x} \end{pmatrix}, \\
\Phi_{2\mathrm{R}} &\propto \begin{pmatrix} e^{ik_2x} \\ -e^{ik_2x} \end{pmatrix}, \quad \Phi_{2\mathrm{L}} \propto \begin{pmatrix} e^{-ik_2x} \\ -e^{-ik_2x} \end{pmatrix}, \quad (x \geq 0).
\end{aligned} \tag{55}$$

We summarize Eqs. (52) and (53) to obtain

$$\begin{pmatrix} -\mathbf{r} & \mathbf{t} \\ \mathbf{t}' & -\mathbf{r}' \end{pmatrix} \begin{pmatrix} \Psi_{1\mathrm{L}} \\ \Psi_{2\mathrm{L}} \\ \Phi_{1\mathrm{R}} \\ \Phi_{2\mathrm{R}} \end{pmatrix} = \begin{pmatrix} \Psi_{1\mathrm{R}} \\ \Psi_{2\mathrm{R}} \\ \Phi_{1\mathrm{L}} \\ \Phi_{2\mathrm{L}} \end{pmatrix}, \tag{56}$$

where

$$\begin{aligned}
\mathbf{t} \equiv \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix}, \quad \mathbf{r} \equiv \begin{pmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{pmatrix}, \\
\mathbf{t}' \equiv \begin{pmatrix} t'_{11} & t'_{12} \\ t'_{21} & t'_{22} \end{pmatrix}, \quad \mathbf{r}' \equiv \begin{pmatrix} r'_{11} & r'_{12} \\ r'_{21} & r'_{22} \end{pmatrix}.
\end{aligned} \tag{57}$$

In order to calculate the transmission and reflection coefficients correctly, we normalize the flux of each wave function to unity. Let us first define the flux in the present case. Consider the waves $\psi_{x,A} = e^{ikx}$ and $\psi_{x,B} = e^{ikx}$. We define the flux operator in the form

$$\hat{P}\psi_x \equiv \frac{\hbar}{i}\frac{\psi_{x+1} - \psi_{x-1}}{2}, \tag{58}$$

which is a discretized version of the momentum operator $\frac{\hbar}{i}\frac{\partial}{\partial x}$. The expectation value of the flux is given by

$$\begin{aligned}
\begin{pmatrix} \psi^*_{x,A}\hat{P}\psi_{x,A} \\ \psi^*_{x,B}\hat{P}\psi_{x,B} \end{pmatrix} &= \begin{pmatrix} e^{-ikx} & e^{-ikx} \end{pmatrix} \frac{\hbar}{i} \begin{pmatrix} \frac{\psi_{x+1,A}-\psi_{x-1,A}}{2} \\ \frac{\psi_{x+1,B}-\psi_{x-1,B}}{2} \end{pmatrix} \\
&= \hbar e^{-ikx} \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} \frac{e^{ikx}\left(e^{ik}-e^{-ik}\right)}{2i} \\ \frac{e^{ikx}\left(e^{ik}-e^{-ik}\right)}{2i} \end{pmatrix} \\
&= \hbar \begin{pmatrix} 1 & 1 \end{pmatrix} \sin k \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 2\hbar \sin k. \qquad (59)
\end{aligned}$$

We put $\hbar = 1$ hereafter. Thus we can normalize the wave function as

$$\psi_x = \frac{1}{\sqrt{2\sin k}} e^{ikx}, \qquad (60)$$

so that the flux is unity. We hence re-define the waves in Eqs. (54) and (55) as

$$\begin{aligned}
\Psi_{1\mathrm{R}} &= \frac{1}{\sqrt{2\sin k_1}} \begin{pmatrix} e^{ik_1x} \\ e^{ik_1x} \end{pmatrix}, \quad \Psi_{1\mathrm{L}} = \frac{1}{\sqrt{2\sin k_1}} \begin{pmatrix} e^{-ik_1x} \\ e^{-ik_1x} \end{pmatrix}, \\
\Psi_{2\mathrm{R}} &= \frac{1}{\sqrt{2\sin k_2}} \begin{pmatrix} e^{ik_2x} \\ -e^{ik_2x} \end{pmatrix}, \\
\Psi_{2\mathrm{L}} &= \frac{1}{\sqrt{2\sin k_2}} \begin{pmatrix} e^{-ik_2x} \\ -e^{-ik_2x} \end{pmatrix}, \quad (x \le 0), \qquad (61)
\end{aligned}$$

$$\begin{aligned}
\Phi_{1\mathrm{R}} &= \frac{1}{\sqrt{2\sin k_1}} \begin{pmatrix} e^{ik_1x} \\ e^{ik_1x} \end{pmatrix}, \quad \Phi_{1\mathrm{L}} = \frac{1}{\sqrt{2\sin k_1}} \begin{pmatrix} e^{-ik_1x} \\ e^{-ik_1x} \end{pmatrix}, \\
\Phi_{2\mathrm{R}} &= \frac{1}{\sqrt{2\sin k_2}} \begin{pmatrix} e^{ik_2x} \\ -e^{ik_2x} \end{pmatrix}, \\
\Phi_{2\mathrm{L}} &= \frac{1}{\sqrt{2\sin k_2}} \begin{pmatrix} e^{-ik_2x} \\ -e^{-ik_2x} \end{pmatrix}, \quad (x \ge 0). \qquad (62)
\end{aligned}$$

Let us make a comment here. We notice in Eqs. (61) and (62) the relations

$$\langle \Psi_{1\mathrm{R}} | \Psi_{2\mathrm{R}} \rangle = \langle \Psi_{1\mathrm{L}} | \Psi_{2\mathrm{L}} \rangle = 0, \qquad (63)$$

$$\langle \Phi_{1\mathrm{R}} | \Phi_{2\mathrm{R}} \rangle = \langle \Phi_{1\mathrm{L}} | \Phi_{2\mathrm{L}} \rangle = 0. \qquad (64)$$

In other words, the channels are orthogonal to each other.

To relate the transfer matrix in Eq. (46) to Eq. (56), we transfer the transmission wave $\Phi_{1\mathrm{R}}$ on the right to the waves on the left. Thus we have

$$\Phi_{1\mathrm{R}} = x_{11\mathrm{R}}\Psi_{1\mathrm{R}} + x_{12\mathrm{R}}\Psi_{2\mathrm{R}} + y_{11\mathrm{L}}\Psi_{1\mathrm{L}} + y_{12\mathrm{L}}\Psi_{2\mathrm{L}}, \tag{65}$$

where the factor $x(y)$ is the incident (reflection) coefficient while the index (ijK) represents that ij is the scattering from the ith channel to the jth channel and $K = \mathrm{L}$ or R. In the same way we have the following relations:

$$\begin{aligned}
\Phi_{2\mathrm{R}} &= x_{21\mathrm{R}}\Psi_{1\mathrm{R}} + x_{22\mathrm{R}}\Psi_{2\mathrm{R}} + y_{21\mathrm{L}}\Psi_{1\mathrm{L}} + y_{22\mathrm{L}}\Psi_{2\mathrm{L}},\\
\Psi_{1\mathrm{L}} &= x'_{11\mathrm{L}}\Phi_{1\mathrm{L}} + x'_{12\mathrm{L}}\Phi_{2\mathrm{L}} + y'_{11\mathrm{R}}\Phi_{1\mathrm{R}} + y'_{12\mathrm{R}}\Phi_{2\mathrm{R}},\\
\Psi_{2\mathrm{L}} &= x'_{21\mathrm{L}}\Phi_{1\mathrm{L}} + x'_{22\mathrm{L}}\Phi_{2\mathrm{L}} + y'_{21\mathrm{R}}\Phi_{1\mathrm{R}} + y'_{22\mathrm{R}}\Phi_{2\mathrm{R}},
\end{aligned} \tag{66}$$

To relate Eqs. (65) and (66) to Eq. (56), we rewrite them in the form:

$$\begin{pmatrix} \Psi_{1\mathrm{L}} \\ \Psi_{2\mathrm{L}} \\ \Phi_{1\mathrm{R}} \\ \Phi_{2\mathrm{R}} \end{pmatrix} = \begin{pmatrix} \emptyset & \mathbf{y}' \\ \mathbf{y} & \emptyset \end{pmatrix} \begin{pmatrix} \Psi_{1\mathrm{L}} \\ \Psi_{2\mathrm{L}} \\ \Phi_{1\mathrm{R}} \\ \Phi_{2\mathrm{R}} \end{pmatrix} + \begin{pmatrix} \emptyset & \mathbf{x}' \\ \mathbf{x} & \emptyset \end{pmatrix} \begin{pmatrix} \Psi_{1\mathrm{R}} \\ \Psi_{2\mathrm{R}} \\ \Phi_{1\mathrm{L}} \\ \Phi_{2\mathrm{L}} \end{pmatrix}, \tag{67}$$

where

$$\begin{aligned}
\mathbf{x} &= \begin{pmatrix} x_{11\mathrm{R}} & x_{12\mathrm{R}} \\ x_{21\mathrm{R}} & x_{22\mathrm{R}} \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} y_{11\mathrm{L}} & y_{12\mathrm{L}} \\ y_{21\mathrm{L}} & y_{22\mathrm{L}} \end{pmatrix},\\
\mathbf{x}' &= \begin{pmatrix} x_{11\mathrm{L}} & x_{12\mathrm{L}} \\ x_{21\mathrm{L}} & x_{22\mathrm{L}} \end{pmatrix}, \quad \mathbf{y}' = \begin{pmatrix} y_{11\mathrm{R}} & y_{12\mathrm{R}} \\ y_{21\mathrm{L}} & y_{22\mathrm{R}} \end{pmatrix},\\
\emptyset &= \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.
\end{aligned} \tag{68}$$

From Eq. (67), we obtain

$$\begin{pmatrix} \mathbf{I} & -\mathbf{y}' \\ -\mathbf{y} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \Psi_{1\mathrm{L}} \\ \Psi_{2\mathrm{L}} \\ \Phi_{1\mathrm{R}} \\ \Phi_{2\mathrm{R}} \end{pmatrix} = \begin{pmatrix} \emptyset & \mathbf{x}' \\ \mathbf{x} & \emptyset \end{pmatrix} \begin{pmatrix} \Psi_{1\mathrm{R}} \\ \Psi_{2\mathrm{R}} \\ \Phi_{1\mathrm{L}} \\ \Phi_{2\mathrm{L}} \end{pmatrix}, \tag{69}$$

where

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{70}$$

Equation (69) is followed by

$$
\begin{aligned}
\begin{pmatrix} \Psi_{1\mathrm{R}} \\ \Psi_{2\mathrm{R}} \\ \Phi_{1\mathrm{L}} \\ \Phi_{2\mathrm{L}} \end{pmatrix}
&= \begin{pmatrix} \emptyset & \mathbf{x}' \\ \mathbf{x} & \emptyset \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{I} & -\mathbf{y}' \\ -\mathbf{y} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \Psi_{1\mathrm{L}} \\ \Psi_{2\mathrm{L}} \\ \Phi_{1\mathrm{R}} \\ \Phi_{2\mathrm{R}} \end{pmatrix} \\
&= \begin{pmatrix} \emptyset & \mathbf{x}^{-1} \\ \mathbf{x}'^{-1} & \emptyset \end{pmatrix} \begin{pmatrix} \mathbf{I} & -\mathbf{y}' \\ -\mathbf{y} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \Psi_{1\mathrm{L}} \\ \Psi_{2\mathrm{L}} \\ \Phi_{1\mathrm{R}} \\ \Phi_{2\mathrm{R}} \end{pmatrix} \\
&= \begin{pmatrix} -\mathbf{x}^{-1}\mathbf{y} & \mathbf{x}^{-1} \\ \mathbf{x}'^{-1} & -\mathbf{x}'^{-1}\mathbf{y}' \end{pmatrix} \begin{pmatrix} \Psi_{1\mathrm{L}} \\ \Psi_{2\mathrm{L}} \\ \Phi_{1\mathrm{R}} \\ \Phi_{2\mathrm{R}} \end{pmatrix}. \qquad (71)
\end{aligned}
$$

Comparing Eq. (71) to Eq. (56), we notice the following relation:

$$
\begin{aligned}
\mathbf{t} &= \mathbf{x}^{-1} \\
\mathbf{t}' &= \mathbf{y}^{-1} \qquad (72)
\end{aligned}
$$

Thus we need to calculate the inverse of $\mathbf{x}$ and $\mathbf{x}'$ in Eqs. (65) and (66) to obtain $\mathbf{t}$ and $\mathbf{t}'$.

3.2.3 Solution for $E = 0$

We now compute the coefficients in Eqs. (65) and (66). We here solve the problem for $E = 0$, $V_A \neq 0$ and $V_B = 0$, for example. From Eq. (51), we obtain

$$
k_1 = \frac{2\pi}{3}, \qquad k_2 = \frac{\pi}{3} \quad \text{for } E = 0. \qquad (73)
$$

Thus the normalization constants in Eqs. (61) and (62) are

$$
\begin{aligned}
\frac{1}{\sqrt{2\sin k_1}} &= \frac{1}{\sqrt{2\cdot\sqrt{3}/2}} = 3^{\frac{1}{4}}, \\
\frac{1}{\sqrt{2\sin k_2}} &= \frac{1}{\sqrt{2\cdot\sqrt{3}/2}} = 3^{\frac{1}{4}} \quad \text{for } E = 0. \qquad (74)
\end{aligned}
$$

We first consider the situation that the transmission wave $\Phi_{1\mathrm{R}}$, which is the channel 1, is on the right. From Eqs. (61) and (62) we obtain the wave function on the both sides by the superposition of the wave function:

$$3^{\frac{1}{4}}\begin{pmatrix} x_{11\mathrm{R}}e^{-\frac{2\pi}{3}i}+y_{11\mathrm{L}}e^{\frac{2\pi}{3}i}+x_{12\mathrm{R}}e^{-\frac{\pi}{3}i}+y_{12\mathrm{L}}e^{\frac{\pi}{3}i} \\ x_{11\mathrm{R}}+y_{11\mathrm{L}}+x_{12\mathrm{R}}+y_{12\mathrm{L}} \\ x_{11\mathrm{R}}e^{-\frac{2\pi}{3}i}+y_{11\mathrm{L}}e^{\frac{2\pi}{3}i}-x_{12\mathrm{R}}e^{-\frac{2\pi}{3}i}-y_{12\mathrm{L}}e^{\frac{2\pi}{3}i} \\ x_{11\mathrm{R}}+y_{11\mathrm{L}}-x_{12\mathrm{R}}-y_{12\mathrm{L}} \end{pmatrix} = 3^{\frac{1}{4}}T_0\begin{pmatrix} 1 \\ e^{\frac{2\pi}{3}i} \\ 1 \\ e^{\frac{2\pi}{3}i} \end{pmatrix}$$
$$= 3^{\frac{1}{4}}\begin{pmatrix} -V_A & -1 & -1 & 0 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ e^{\frac{2\pi}{3}i} \\ 1 \\ e^{\frac{2\pi}{3}i} \end{pmatrix} \tag{75}$$

We now use the relations (63) and (64) to calculate the coefficients. By taking the inner product of Eq. (75) and the complex conjugate of the channel 1,

$$\begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix}^{\dagger} = 3^{\frac{1}{4}}\begin{pmatrix} e^{\mp\frac{2\pi}{3}i} \\ 1 \\ e^{\mp\frac{2\pi}{3}i} \\ 1 \end{pmatrix}^{\dagger} = 3^{\frac{1}{4}}\left(e^{\pm\frac{2\pi}{3}i} \quad 1 \quad e^{\pm\frac{2\pi}{3}i} \quad 1 \right), \tag{76}$$

we can cancel out the components of the channel 2 and obtain the coefficients of the channel 1, $x_{11\mathrm{R}}$ and $y_{11\mathrm{L}}$. In fact, by calculating the inner products of Eqs. (75) and (76), we obtain

$$\begin{aligned} x_{11\mathrm{R}}+\frac{e^{-\frac{\pi}{3}i}}{2}y_{11\mathrm{L}} &= 1-\frac{e^{\frac{2\pi}{3}i}}{4}V_A, \\ x_{11\mathrm{R}}+\frac{e^{\frac{\pi}{3}i}}{2}y_{11\mathrm{L}} &= \frac{e^{\frac{\pi}{3}i}}{2}-\frac{e^{-\frac{2\pi}{3}i}}{4}V_A, \end{aligned} \tag{77}$$

or

$$\begin{pmatrix} 1 & \frac{e^{-\frac{\pi}{3}i}}{2} \\ \frac{e^{\frac{\pi}{3}i}}{2} & 1 \end{pmatrix}\begin{pmatrix} x_{11\mathrm{R}} \\ y_{11\mathrm{L}} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{e^{\frac{\pi}{3}i}}{2} \end{pmatrix} - \frac{V_A}{4}\begin{pmatrix} e^{\frac{2\pi}{3}i} \\ e^{-\frac{2\pi}{3}i} \end{pmatrix}. \tag{78}$$

We thus arrive at

$$\begin{aligned} \begin{pmatrix} x_{11\mathrm{R}} \\ y_{11\mathrm{L}} \end{pmatrix} &= \begin{pmatrix} 1 & \frac{e^{-\frac{\pi}{3}i}}{2} \\ \frac{e^{\frac{\pi}{3}i}}{2} & 1 \end{pmatrix}^{-1}\left[\begin{pmatrix} 1 \\ \frac{e^{\frac{\pi}{3}i}}{2} \end{pmatrix} - \frac{V_A}{4}\begin{pmatrix} e^{\frac{2\pi}{3}i} \\ e^{-\frac{2\pi}{3}i} \end{pmatrix}\right] \\ &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{\sqrt{3}}{6}V_A\begin{pmatrix} 1 \\ -1 \end{pmatrix}. \end{aligned} \tag{79}$$

In the same way, by calculating the inner product of Eq. (75) and the complex conjugate of the channel 2 ($k_2 = \pi/3$),

$$\begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix}^\dagger = 3^{\frac{1}{4}} \begin{pmatrix} e^{\mp\frac{\pi}{3}i} \\ 1 \\ -e^{\mp\frac{\pi}{3}i} \\ -1 \end{pmatrix}^\dagger = 3^{\frac{1}{4}} \begin{pmatrix} e^{\pm\frac{\pi}{3}i} & 1 & -e^{\pm\frac{\pi}{3}i} & -1 \end{pmatrix}, \tag{80}$$

we obtain

$$\begin{pmatrix} 1 & \frac{e^{\frac{\pi}{3}i}}{2} \\ \frac{e^{-\frac{\pi}{3}i}}{2} & 1 \end{pmatrix} \begin{pmatrix} x_{12\mathrm{R}} \\ y_{12\mathrm{L}} \end{pmatrix} = -\frac{V_A}{4} \begin{pmatrix} e^{\frac{\pi}{3}i} \\ e^{-\frac{\pi}{3}i} \end{pmatrix}. \tag{81}$$

We arrive at

$$\begin{aligned} \begin{pmatrix} x_{12\mathrm{R}} \\ y_{12\mathrm{L}} \end{pmatrix} &= \begin{pmatrix} 1 & \frac{e^{\frac{\pi}{3}i}}{2} \\ \frac{e^{-\frac{\pi}{3}i}}{2} & 1 \end{pmatrix}^{-1} \left[-\frac{V_A}{4} \begin{pmatrix} e^{\frac{\pi}{3}i} \\ e^{-\frac{\pi}{3}i} \end{pmatrix} \right] \\ &= -\frac{\sqrt{3}}{6} i V_A \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \end{aligned} \tag{82}$$

We next consider the situation where the transmission wave $\Phi_{2\mathrm{R}}$, which is the channel 2, is on the right. From Eqs. (61) and (62) we obtain the wave function on the both sides by the superposition of the wave function:

$$3^{\frac{1}{4}} \begin{pmatrix} x_{21\mathrm{R}} e^{-\frac{2\pi}{3}i} + y_{21\mathrm{L}} e^{\frac{2\pi}{3}i} + x_{22\mathrm{R}} e^{-\frac{\pi}{3}i} + y_{22\mathrm{L}} e^{\frac{\pi}{3}i} \\ x_{21\mathrm{R}} + y_{21\mathrm{L}} + x_{22\mathrm{R}} + y_{22\mathrm{L}} \\ x_{21\mathrm{R}} e^{-\frac{2\pi}{3}i} + y_{21\mathrm{L}} e^{\frac{2\pi}{3}i} - x_{22\mathrm{R}} e^{-\frac{\pi}{3}i} - y_{22\mathrm{L}} e^{\frac{\pi}{3}i} \\ x_{21\mathrm{R}} + y_{21\mathrm{L}} - x_{22\mathrm{R}} - y_{22\mathrm{L}} \end{pmatrix} = 3^{\frac{1}{4}} T_0 \begin{pmatrix} 1 \\ e^{\frac{\pi}{3}i} \\ -1 \\ -e^{\frac{\pi}{3}i} \end{pmatrix}. \tag{83}$$

We obtain the following relations by calculating the inner products of Eq. (83) and Eqs. (76) and (80):

$$\begin{aligned} \begin{pmatrix} 1 & \frac{e^{-\frac{\pi}{3}i}}{2} \\ \frac{e^{\frac{\pi}{3}i}}{2} & 1 \end{pmatrix} \begin{pmatrix} x_{21\mathrm{R}} \\ y_{21\mathrm{L}} \end{pmatrix} &= -\frac{V_A}{4} \begin{pmatrix} e^{\frac{2\pi}{3}i} \\ e^{-\frac{2\pi}{3}i} \end{pmatrix}, \\ \begin{pmatrix} 1 & \frac{e^{\frac{\pi}{3}i}}{2} \\ \frac{e^{-\frac{\pi}{3}i}}{2} & 1 \end{pmatrix} \begin{pmatrix} x_{22\mathrm{R}} \\ y_{22\mathrm{L}} \end{pmatrix} &= \begin{pmatrix} 1 \\ \frac{e^{-\frac{\pi}{3}i}}{2} \end{pmatrix} - \frac{V_A}{4} \begin{pmatrix} \frac{e^{\frac{\pi}{3}i}}{2} \\ \frac{e^{-\frac{\pi}{3}i}}{2} \end{pmatrix}. \end{aligned} \tag{84}$$

We arrive at

$$
\begin{aligned}
\begin{pmatrix} x_{21\mathrm{R}} \\ y_{21\mathrm{L}} \end{pmatrix} &= -\frac{\sqrt{3}}{6} i V_A \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \\
\begin{pmatrix} x_{22\mathrm{R}} \\ y_{22\mathrm{L}} \end{pmatrix} &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{\sqrt{3}}{6} i V_A \begin{pmatrix} 1 \\ -1 \end{pmatrix}.
\end{aligned} \tag{85}
$$

Equations (79), (83) and (85) yield

$$
\mathbf{x} = \begin{pmatrix} x_{11\mathrm{R}} & x_{12\mathrm{R}} \\ x_{21\mathrm{R}} & x_{22\mathrm{R}} \end{pmatrix} = \begin{pmatrix} 1 - \frac{\sqrt{3}}{6} i V_A & -\frac{\sqrt{3}}{6} i V_A \\ -\frac{\sqrt{3}}{6} i V_A & 1 - \frac{\sqrt{3}}{6} i V_A \end{pmatrix}, \tag{86}
$$

from which we finally obtain

$$
\begin{aligned}
\mathbf{t} &= \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} = \mathbf{x}^{-1} \\
&= \frac{1}{1 - \frac{\sqrt{3}}{3} i V_A} \begin{pmatrix} 1 - \frac{\sqrt{3}}{6} i V_A & \frac{\sqrt{3}}{6} i V_A \\ \frac{\sqrt{3}}{6} i V_A & 1 - \frac{\sqrt{3}}{6} i V_A \end{pmatrix}.
\end{aligned} \tag{87}
$$

In the same way, we obtain the transmission coefficient $\mathbf{t}'$ from the right side to the left side by assuming the transmission wave on the left. We show $\sum_{i,j} |t_{ij}|^2$ in Fig. 9 for $V_A = 0.0, 1.0, 2.0, 3.0$ with $V_B = 0.0$.

3.3 Chain connected to ladder

3.3.1 Virtual-site method

Now we consider a problem where the channel numbers are different on the left and on the right. We should now pay attention to two points. One is the normalization of the flux. The eigenstates on the both sides differ when the channel number of the right side is one and the left are two. We need to normalize the flux to calculate the transmission coefficient correctly. We use the procedure similar to the one in Sec. 3.2. The other point is the difference of the matrix dimension. The transfer matrix T is not a square matrix when the channel number of the right side is one and the left are two. We cannot obtain the coefficients in the same way as above.

We here propose the virtual-site method, by which we can compute the coefficients in a much similar way. Tamura and Tsukada previously proposed

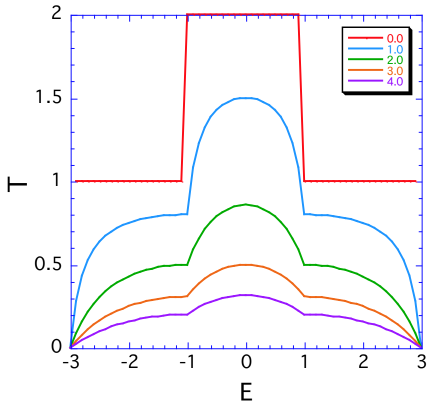


Figure 9: The energy dependence of the transmission probability T for $V_A = 0.0, 1.0, 2.0, 3.0$ with $V_B = 0.0$.

the conditioned transfer-matrix method [4]. An advantage of our new method is that we can use the same transfer matrix as before.

We consider the situation that the channel number of the right side is one and the left are two (Fig. 10(a)). We can write down the following transfer matrix T_0 at $x = 0$ for the tight-binding model:

$$\begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix} = \begin{pmatrix} E & -1 & -1 \\ 1 & 0 & 0 \\ -1 & 0 & E \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \psi_{0,A} \\ \psi_{1,A} \\ \psi_{0,B} \end{pmatrix} = T_0 \begin{pmatrix} \psi_{0,A} \\ \psi_{1,A} \\ \psi_{0,B} \end{pmatrix} \tag{88}$$

We notice that the transfer matrix T_0 is not a square matrix. We hence introduce virtual sites (Fig. 10(b)). That is, we temporarily add sites (x, B) for $x \geq 1$, and later make the wave amplitudes on these sites zero. Taking account of the virtual sites, we write the transfer matrix similar to Eq. (46)

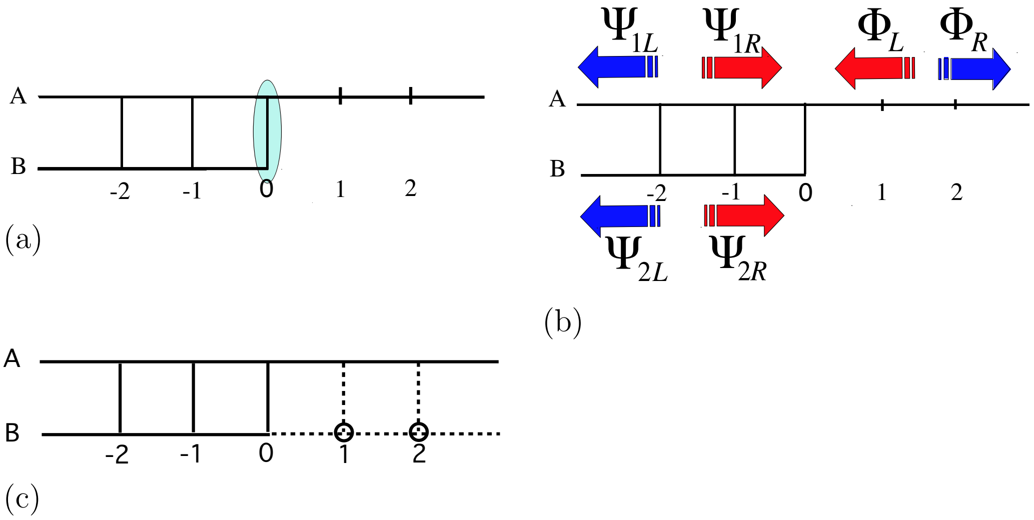


Figure 10: (a) The lattice where a chain is connected to a ladder. (b) The channel number of the right side is one and the left are two. (c) The open circles indicate the virtual sites at (x, B) for $x > 0$.

as

$$\begin{aligned} \begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix} &= \begin{pmatrix} E - V_A & -1 & -1 & 0 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & E - V_B & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_{0,A} \\ \psi_{1,A} \\ \psi_{0,B} \\ \psi_{1,B} \end{pmatrix} \\ &\equiv T_0 \begin{pmatrix} \psi_{0,A} \\ \psi_{1,A} \\ \psi_{0,B} \\ 0 \end{pmatrix}. \end{aligned} \tag{89}$$

Thus we obtain a square transfer matrix T_0. We calculate the coefficients in the same way as in Sec. 3.2.

3.3.2 Comparison with a previous method

We here show that our new method is mathematically equivalent to a previous method by Tamura and Tsukada [4], called the conditioned transfer-matrix method. We emphasize that their method is numerically less accurate and time-consuming since it involves the numerical matrix inversion.

Let us first briefly review the conditioned transfer-matrix method. Tamura and Tsukada used the generalized inverse matrix of the rectangular transfer matrix T_0 in Eq. (88). The generalized inverse (or "pseudo-inverse" as Tamura and Tsukada called it) of the rectangular matrix T_0 is defined by

$$T_0^{-1} = \left(T_0^\dagger T_0\right)^{-1} T_0^\dagger, \tag{90}$$

which satisfies

$$T_0^{-1} T_0 \equiv I \quad \text{but} \quad T_0 T_0^{-1} \neq I. \tag{91}$$

We can hence rewrite Eq. (88) as follows:

$$\begin{pmatrix} \psi_{0,A} \\ \psi_{1,A} \\ \psi_{0,B} \end{pmatrix} = T_0^{-1} \begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix}. \tag{92}$$

We then need the condition that Eq. (88) is derived from Eq. (92) again by multiplying T_0 on the both sides. The condition reads

$$\begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix} = T_0 T_0^{-1} \begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix}. \tag{93}$$

Note that this not an identity. On the contrary, this gives an equation involving $\psi_{-1,A}, \psi_{0,A}, \psi_{-1,B}$ and $\psi_{0,B}$.

Tamura and Tsukada obtain an expanded square transfer matrix $\tilde{T}_0$ by adding a condition in Eq. (93) to Eq. (92). The condition from our method, on the other hand, is to substitue zero for the virtual site. We show that these two conditions are equivalent for $V_A = V_B = 0$, for example. The generalized inverse of T_0 is given by

$$\begin{aligned} T_0^{-1} &= \left(T_0^\dagger T_0\right)^{-1} T_0^\dagger \\ &= \left\{ \begin{pmatrix} E & 1 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ -1 & 0 & E & 1 \end{pmatrix} \begin{pmatrix} E & -1 & -1 \\ 1 & 0 & 0 \\ -1 & 0 & E \\ 0 & 0 & 1 \end{pmatrix} \right\}^{-1} \begin{pmatrix} E & 1 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ -1 & 0 & E & 1 \end{pmatrix} \\ &= \frac{1}{E^2+2} \begin{pmatrix} 0 & E^2+1 & -1 & E \\ -E^2-2 & E^3 & -2E & E^2-2 \\ 0 & E & E & 2 \end{pmatrix}. \end{aligned} \tag{94}$$

Equation (94) satisfies the relation (91). We obtain from Eq. (93) the following condition:

$$\emptyset = \left(T_0 T_0^{-1} - I\right) \begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix} = \frac{1}{E^2+2} \begin{pmatrix} 0 & 0 & 2E & 0 \\ 0 & -1 & -1 & E \\ 0 & -1 & -1 & E \\ 0 & E & E & -E^2 \end{pmatrix} \begin{pmatrix} \psi_{-1,A} \\ \psi_{0,A} \\ \psi_{-1,B} \\ \psi_{0,B} \end{pmatrix} . \tag{95}$$

One of the equations give

$$\psi_{0,A} + \psi_{-1,B} - E\psi_{0,B} = 0. \tag{96}$$

This is the condition for the wave function on the ladder to survive on the chain. The wave function that does not satisfy this condition cannot transmit into the chain.

On the other hand, we obtain the following equation from the third row of Eq. (89):

$$\psi_{-1,B} = -\psi_{0,A} + E\psi_{0,B} - \psi_{1,B}, \tag{97}$$

or

$$\psi_{0,A} + \psi_{-1,B} - E\psi_{0,B} = -\psi_{1,B}. \tag{98}$$

By substituting zero for the virtual site $\psi_{1,B}$ in Eq. (98), we notice that the condition of the virtual-site method is equivalent to the condition (97) of the conditioned transfer-matrix method. We expect that the numerical calculation becomes extremely precise in the former method because the matrix inversion in the latter method is not necessary.

3.3.3 Solution for $E = 0$

We here solve the problem for $E = 0$ and $V_A = V_B = 0$, for example. The lattice is a chain for $x > 0$ and a ladder for $x \le 0$. The eigenvectors for $x > 0$ are given by Eq. (30) with $k = \pi/2$ because of Eq. (33). We normalize the flux of the wave function in the same way as Eq. (60), obtaining

$$\begin{aligned} \Phi_{\mathrm{R}} &= \psi_{x,A} = \frac{1}{\sqrt{\sin k}} e^{ikx} = \frac{1}{\sqrt{\sin \pi/2}} e^{\frac{\pi}{2} ix} = e^{\frac{\pi}{2} ix}, \\ \Phi_{\mathrm{L}} &= \frac{1}{\sqrt{\sin k}} e^{-ikx} = \frac{1}{\sqrt{\sin \pi/2}} e^{-\frac{\pi}{2} ix} = e^{-\frac{\pi}{2} ix}, \end{aligned} \tag{99}$$

with

$$\psi_{x,B} \equiv 0. \qquad (x > 0) \tag{100}$$

Next, the eigenvectors for $x \leq 0$ are given by Eq. (61) with Eq. (74):

$$\begin{aligned}
\Psi_{1\mathrm{R}} &= 3^{\frac{1}{4}} \begin{pmatrix} e^{\frac{2\pi}{3}ix} \\ e^{\frac{2\pi}{3}ix} \end{pmatrix}, \quad \Psi_{1\mathrm{L}} = 3^{-\frac{1}{4}} \begin{pmatrix} e^{\frac{2\pi}{3}ix} \\ e^{\frac{2\pi}{3}ix} \end{pmatrix}, \\
\Psi_{2\mathrm{R}} &= 3^{\frac{1}{4}} \begin{pmatrix} e^{\frac{\pi}{3}ix} \\ -e^{\frac{\pi}{3}ix} \end{pmatrix}, \quad \Psi_{2\mathrm{L}} = 3^{\frac{1}{4}} \begin{pmatrix} e^{-\frac{2\pi}{3}ix} \\ -e^{-\frac{2\pi}{3}ix} \end{pmatrix}
\end{aligned} \tag{101}$$

We now consider the situation that the transmission wave Φ_{R} is on the right:

$$\Phi_{\mathrm{R}} = x_1\Psi_{1\mathrm{R}} + y_1\Psi_{2\mathrm{L}} + x_2\Psi_{2\mathrm{R}} + y_2\Psi_{2\mathrm{L}}, \tag{102}$$

from which we obtain

$$3^{\frac{1}{4}} \begin{pmatrix} x_1 e^{-\frac{2\pi}{3}i} + y_1 e^{\frac{2\pi}{3}i} + x_2 e^{-\frac{\pi}{3}i} + y_2 e^{\frac{\pi}{3}i} \\ x_1 + y_1 + x_2 + y_2 \\ x_1 e^{-\frac{2\pi}{3}i} + y_1 e^{\frac{2\pi}{3}i} - x_2 e^{-\frac{\pi}{3}i} - y_2 e^{\frac{\pi}{3}i} \\ x_1 + y_1 - x_2 - y_2 \end{pmatrix} = \begin{pmatrix} 0 & -1 & -1 & 0 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ e^{\frac{\pi}{2}i} \\ 1 \\ 0 \end{pmatrix} \tag{103}$$

By calculating the inner products of Eq. (103) and Eqs. (76) and (80), we have

$$\begin{aligned}
\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} &= \frac{1}{8 \cdot 3^{\frac{3}{4}}} \begin{pmatrix} 12 + 4\sqrt{3} - 4\sqrt{3}i \\ 12 - 4\sqrt{3} + 4\sqrt{3}i \end{pmatrix}, \\
\begin{pmatrix} x_2 \\ y_2 \end{pmatrix} &= \frac{1}{8 \cdot 3^{\frac{3}{4}}} \begin{pmatrix} 4\sqrt{3} \\ -4\sqrt{3} \end{pmatrix}.
\end{aligned} \tag{104}$$

The factors x and y represent the incident and the reflection amplitudes. Thus the flux amplitudes of the incident waves are

$$\begin{aligned}
|x_1|^2 &= \frac{1}{4} + \frac{5}{4\sqrt{3}}, \\
|x_2|^2 &= \frac{1}{4\sqrt{3}}.
\end{aligned} \tag{105}$$

The transmission probability is given by

$$\begin{aligned} T &= \frac{1}{|x_1|^2 + |x_2|^2} \\ &= \frac{1}{\frac{1}{4} + \frac{6}{4\sqrt{3}}} = \frac{4}{6+\sqrt{3}} = 0.517327\cdots \end{aligned} \tag{106}$$

We followed the same procedure as above for general E and obtain Fig. 11. We notice that the wave function of the wave number k_2 does not transmit to the right side.

4 Application to carbon-based materials

We now show how we can apply the virtual-site method to carbon-based materials. Carbon-based materials have the hexagonal lattice structure. We here demonstrate the way of adding virtual sites to a graphite flake. Consider the situation where there are seven hexagons (Fig. 12(a)). The figures 1, 2 and 3 represent the distance from the center. There are six sites of the number 1 and the number 2, while twelve sites of the number 3. When we transfer waves from inside to outside, the number of the channels increase by six. Hence we add six virtual sites of the number 1 and six of the number 2, as is shown in Fig. 12(b). We thus obtain the situation where the channel number is uniform by superimposing Fig. 12(b) over Fig. 12(a).

5 Summary

In the present thesis, we introduced a new method with virtual sites in order to calculate the conductance of carbon-based materials numerically. In Sec. 2 we introduced the Landauer formula, the scattering matrix and the transfer matrix, which are the basic concepts for obtaining the conductance. In Sec. 3 we show three tutorial examples: a chain lattice, a ladder lattice and a chain connected to ladder. In Sec. 3.1 the channel number was one on the both sides. The conductance decreases as we increase the impurity potential. In Sec. 3.2, the sum of the transmission coefficients is greater than unity since the channel number is two for $-1 < E < 1$. In Sec. 3.3, we use the virtual-site method for the case where the channel number is not uniform. We stress that we can obtain the transmission coefficients in the same way as Secs. 3.1

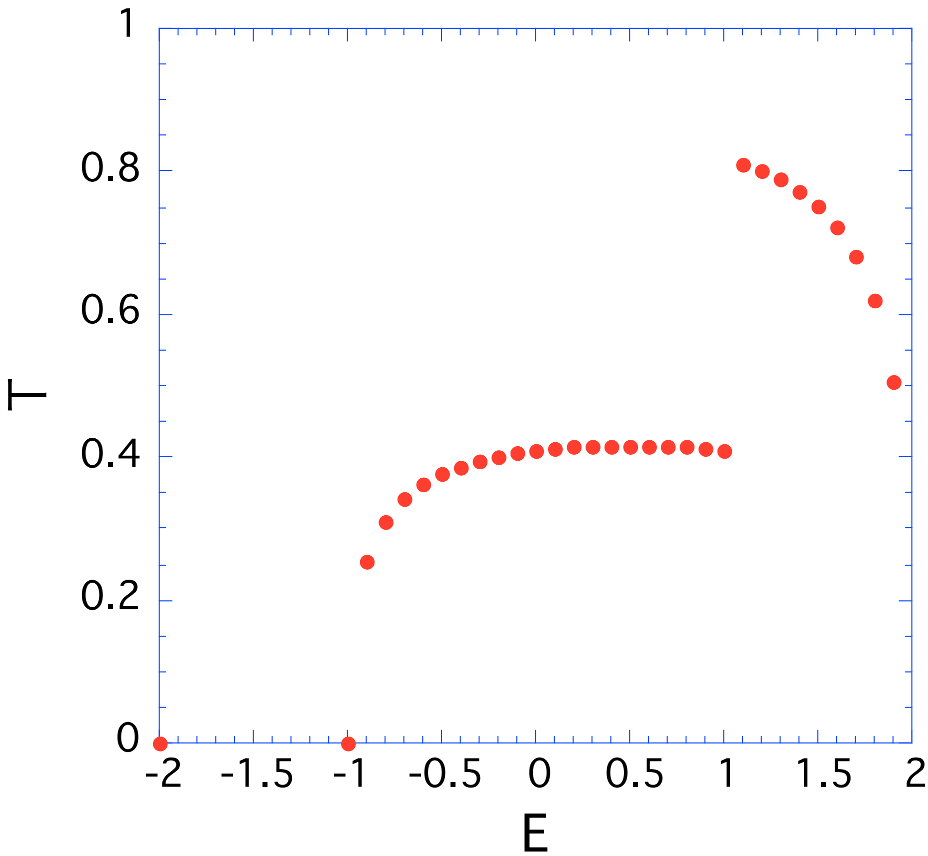
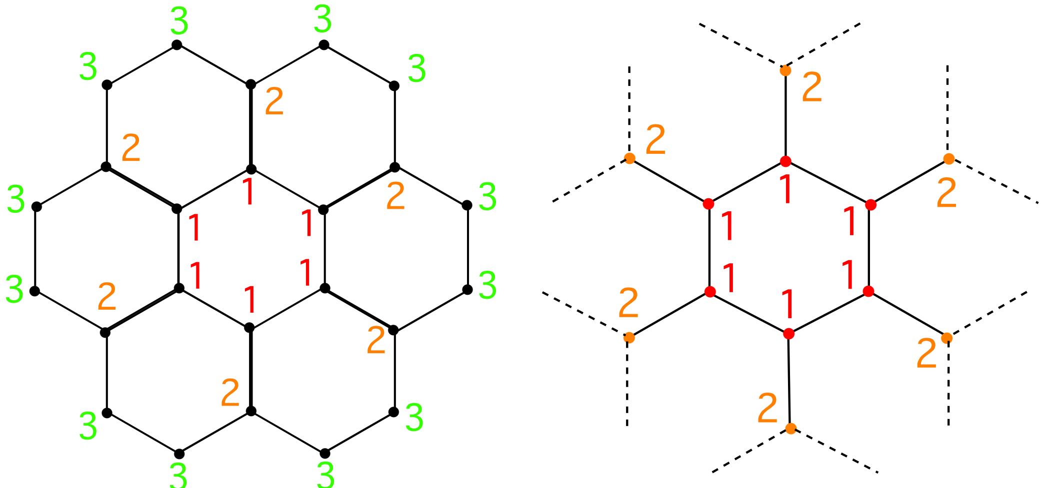


Figure 11: The energy dependence of the transmission probability T of the system in Fig. 10(a) with $V_A = V_B = 0.0$.



(a) (b)

Figure 12: (a) The graphite flake of seven hexagons. The figures 1, 2 and 3 represent the distance from the center. (b) Virtual sites added to the flake in (a).

and 3.2. Finally in Sec. 4 we showed how to apply the virtual-site method to carbon-based materials. The channel number of carbon-based materials can be non-uniform. We can transform by the virtual-site method the problem to the case of a uniform channel number.

Acknowledgments

The author thanks Supervisors Kenn Kubo and Naomichi Hatano for many discussions.

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