A Numerical Method to Calculate the Conductance of Mesoscopic Conductors
Using Singular Value Decomposition

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We present a new method to calculate electric conductance of a mesoscopic conductor by utilizing singular value decomposition, which is a mathematical technique to manipulate matrices. Our method is useful in treating conductors with rather complicated atomic structures, for which naive recursion formula is cumbersome. It also has an advantage in scaling up the calculation by using parallel computation, which potentially allows us real-scale calculations at the atomic level. In this paper, we treat graphene nanoribbons with external leads, for an example.

KEYWORDS: Transport, Conductance, Landauer Formula, Graphene, Nano-constrictions

1. Introduction

Numerical methods has been developed as one of the most powerful tool to study mesoscopic systems. Especially, the effects of impurities and randomness on electric conduction have been intensively studied in relation to the Anderson localization. Among these studies the recursive calculation of the scattering states of electrons within tight-binding approximation has been developed. The numerical approach is strengthened with the help of the well-known Landauer formula, which is established as a standard to calculate mesoscopic conductance. Especially, the approximation has been developed.

In this literature, a method called singular value decomposition (SVD) is utilized. Using this we can decompose arbitrary real (or complex) \( m \times n \) matrix \( A \) as

\[
A = U W V^\dagger
\]

where \( U \) and \( V \) are \( m \times m \) and \( n \times n \) orthogonal (or unitary) matrices, respectively, and \( U, \tilde{U}, \tilde{V} \) and \( V \) are block matrices obtained by partitioning \( U \) and \( V \). \( (X^\dagger) \) is the Hermite conjugate of the matrix or vector \( X \). The integer \( r \) is the matrix rank of \( A \), i.e., \( r = \text{rank}(A) \), and \( \sigma_j \)'s are positive numbers called singular values of \( A \). Here we write \( \tilde{U} = (\tilde{u}_1, \ldots, \tilde{u}_r) \), \( \hat{U} = (\hat{u}_{r+1}, \ldots, \hat{u}_m) \), \( \hat{V} = (\hat{v}_1, \ldots, \hat{v}_r) \) and \( \tilde{V} = (\tilde{v}_{r+1}, \ldots, \tilde{v}_n) \), where \( \tilde{u}_j \)'s and \( \tilde{v}_j \)'s, respectively, are \( m \) and \( n \) dimensional columnar vectors.

The following mathematical features are easily confirmed: We define the range of \( A \), \( \text{Ran}(A) \), and the null space of \( A \), \( \text{Null}(A) \), as

\[
\text{Ran}(A) = \{ \tilde{y} \in \mathbb{C}^m : \tilde{y} = Ax \text{ for some } x \in \mathbb{C}^n \},
\]

\[
\text{Null}(A) = \{ \tilde{y} \in \mathbb{C}^m : A\tilde{y} = 0 \}.
\]

where \( \mathbb{C} \) is the set of complex numbers. Then \( \text{Ran}(A) \) is spanned by \( \{ \hat{u}_1, \ldots, \hat{u}_r \} \) and \( \text{Null}(A) \) is spanned by \( \{ \hat{v}_{r+1}, \ldots, \hat{v}_n \} \). It is also useful to see that the left null space of \( A \), namely a set of vectors \( \tilde{u} \) satisfying \( \tilde{u}^\dagger A = 0 \), is spanned by \( \{ \hat{u}_{r+1}, \ldots, \hat{u}_m \} \). Equivalently we obtain the relation \( \hat{U}^\dagger A = 0 \).

For convenience we define an operator, which extract \( \hat{U} \) from

\[\]
SVD of the matrix $A$, Eq. (1), as,

$$\tilde{U} = \mathcal{N}_L[A].$$

(2)

The most widely known application of the SVD may be so-called Moore-Penrose quasi-inverse. The Moore-Penrose quasi-inverse matrix of $A$, which we denote by $A^{MP}$ in this paper, is given as

$$A^{MP} = \hat{\Psi} \begin{pmatrix} \sigma_1^{-1} & O \\ O & \sigma_r^{-1} \end{pmatrix} \hat{\Psi}^\dagger.$$

(3)

Using this, we can obtain an approximate solution of the equation $Ax = y$ as $x = A^{MP}y$. If $y \in \text{Ran}(A)$, this solution is exact (but not unique since we have freedom to add arbitrary superposition of $v_{+1}, \ldots, v_n$ to $x$). Useful numerical algorithm to calculate SVD is described in Ref. 37.

This paper is organized as follows: In Sec. 2, we describe the basic formalism of our method. In Sec. 3, we study the conduction through ideal wires, which is used as external leads. In Sec. 4, we discuss how the Landauer formula is expressed within our formalism. In Sec. 5, we apply our formalism to the calculation of electric conductance of graphene nanoribbons with external leads. Although the system size of the calculation is not large enough, this is the first result obtained by treating the contact to realistic leads. Since the calculation is not large enough, this is the first result obtained by treating the contact to realistic external leads, as far as we know. In Sec. 6, some prospect for the application of our formalism to the calculation of electric conductance of graphene is discussed. Some remaining problems and possible future studies are discussed. Some supplemental issues are discussed in Appendices.

2. Basic Formalism

2.1 Schrödinger equation in a recurrence form

We divide the system into several blocks which are serially connected side by side in a row to form a conductor. Both ends of the conductor is connected to electron bath of left and right leads.

We start from the tight-binding model described by the following Hamiltonian,

$$H = \sum_{(m,n) \in N} t_{mn} c_m^\dagger c_n + \text{H.c.},$$

(4)

where $c_m$ is the annihilation operator of an electron at the $m$-th site and the summation $\langle m,n \rangle$ is over all the bonds. We suppress the spin index for simplicity throughout this paper. From the Heisenberg form,

$$i\hbar \frac{\partial c_m}{\partial t} = [H, c_m],$$

(5)

we obtain the probability conservation relation as,

$$\frac{\partial p_m}{\partial t} = \frac{\partial}{\partial t} c_m^\dagger c_m = \sum_{n \in N(m)} \frac{i}{\hbar} (t_{mn} c_n^\dagger c_m - t_{nm} c_m^\dagger c_n)$$

$$= \sum_{n \in N(m)} J_{nm},$$

(6)

where $N(m)$ is the set of sites connected to the $m$-th site and $J_{nm}$ stands for the probability current flowing from the site $n$ to $m$. We write the wave function as

$$\Psi = \sum_m \psi_m c_m,$$

(7)

and, then, $\psi_m$ satisfies the Schrödinger equation in the matrix form.

An example of the conductor is depicted in Fig. 1. Each circle corresponds to an atomic site of tight binding model. The whole system is decomposed into several blocks, numbered by $j$ in the figure. We divide the wave function $\psi_n$ of the $j$-th block into three components, $\tilde{L}_j$, $\tilde{R}_j$ and $\tilde{\psi}_j$, each of which is defined in the columnar vector form. The vector $\tilde{L}_j$ ($\tilde{R}_j$) represents the wave functions of sites shown by gray (black) circles in Fig. 1, which are located at the left (right) edge of the $j$-th block and are connected to the sites in the $(j-1)$-th ($(j+1)$-th) block. The vector $\tilde{\psi}_j$ represents the wave functions of the sites in the $j$-th block, which are not included in $\tilde{L}_j$ or $\tilde{R}_j$. Here we assume that there is no overlap in the elements of $\tilde{R}_j$ and $\tilde{L}_j$. If some elements are overlapped, we can extend the area of the $j$-th block until the overlap is dissolved. Such extension is always possible without long range hopping.

Our aim is to re-express the Schrödinger equation of the whole system into a set of equations, which relates $(\tilde{L}_j, \tilde{R}_{j-1})$ to $(\tilde{L}_{j+1}, \tilde{R}_j)$. In order to carry this out, the vectors, $\tilde{\psi}_j$, should be truncated (or integrated out) by some means. We will show that this process can be readily performed by employing SVD and Moore-Penrose quasi-inverse matrices.36

Let us denote the number of components of $\tilde{L}_j$, $\tilde{R}_j$ and $\tilde{\psi}_j$ by $n^R_j$, $n^L_j$ and $n^\psi_j$, respectively. We also define the total site number of the $j$-th block as $n_j = n^R_j + n^L_j + n^\psi_j$.

![Fig. 1. The $(j - 1)$-th, $\cdots$, $(j + 2)$-th block of the conductor are shown. Gray, black and white circles correspond to $\tilde{R}_j$, $\tilde{L}_j$ and $\tilde{\psi}_j$, respectively.](image)

First we start with the Schrödinger equation of the $j$-th block given by

$$(EI_{n_j} - H_j) \begin{pmatrix} \tilde{L}_j \\ \tilde{R}_j \\ \tilde{\psi}_j \end{pmatrix} = \begin{pmatrix} \Lambda_j^{LR} \cdot \tilde{R}_{j-1} \\ \Lambda_j^{RL} \cdot \tilde{L}_{j+1} \\ \tilde{\Omega}_j \end{pmatrix},$$

(8)

where $E$ is the energy, $I_n$ is the identity matrix of order $n$, $\tilde{\Omega}_j$ is a zero vector whose dimension is $n^\psi_j$, $H_j$ is the Hamiltonian of sites within the $j$-th block, and $\Lambda_j^{RL}$ is the hopping
matrix elements between the \((j - 1)\)-th and the \(j\)-th block. Since the Hamiltonian is Hermitian, we have the relation, 
\[
\Lambda_{j}^{LR} = \Lambda_{j}^{RL} \dagger. 
\]
(Not that the matrix \(\Lambda_{j}^{RL}\) is not necessarily square.) The current flowing from \((j - 1)\)-th block to \(j\)-th block is given by
\[
J = \frac{i}{\hbar} (\vec{R}_{j-1} \cdot \vec{L}_{j}) \begin{pmatrix} O & -\Lambda_{j}^{RL} \cr \Lambda_{j}^{LR} & 0 \end{pmatrix} \begin{pmatrix} \vec{R}_{j-1} \cr \vec{L}_{j} \end{pmatrix},
\]
where we have introduced the matrix \(\Lambda_{j}\). Since in the equilibrium the probability current conserves at all the blocks, this quantity does not depend on \(j\).

Here we rewrite the Eq. (8) as follows,
\[
K_{j}^{\psi} \tilde{\psi}_{j} = -K_{j}^{L} \tilde{L}_{j} - K_{j}^{R} \tilde{R}_{j} + \begin{pmatrix} \Lambda_{j}^{LR} \cdot \tilde{R}_{j-1} \\ \Lambda_{j}^{RL} \cdot \tilde{L}_{j+1} \end{pmatrix} \equiv \tilde{\Gamma},
\]
where \(K_{j}^{L}, K_{j}^{R}\) and \(K_{j}^{\psi}\) are block matrices composing the matrix \(E I_{n_{j}} - H_{j} = (K_{j}^{L} | K_{j}^{R} | K_{j}^{\psi})\), whose dimensions are \(n_{j} \times n_{j}^{L}\), \(n_{j} \times n_{j}^{R}\) and \(n_{j} \times n_{j}^{\psi}\), respectively.

We note that the conditions to be satisfied by \((\tilde{R}_{j-1}, \tilde{L}_{j})\) and \((\tilde{R}_{j}, \tilde{L}_{j+1})\) are obtained in the following way: first, we introduce the SVD of \(K_{j}^{\psi}\) as follows,
\[
K_{j}^{\psi} = U_{j} W_{j} V_{j}^{\dagger}
\]
\[
= \begin{pmatrix} \tilde{U}_{j} & \tilde{V}_{j} \end{pmatrix} \begin{pmatrix} O & \sigma_{j,1} & \cdots & O \\ \sigma_{j,1} & \ddots & \cdots & \sigma_{j,1}^{*} \\ \vdots & \ddots & \ddots & \vdots \\ O & \cdots & \sigma_{j,1}^{*} & O \end{pmatrix} \begin{pmatrix} \tilde{V}_{j}^{\dagger} \cr \tilde{U}_{j}^{\dagger} \end{pmatrix},
\]
(11)
where \(r_{j} = \text{rank}(K_{j}^{\psi})\). Here \(U_{j} = N_{j}[K_{j}^{\psi}]\) using the definition Eq. (2). From this we obtain the condition that Eq. (10) is solvable as
\[
\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} = U_{j} \begin{pmatrix} \Lambda_{j}^{LR} \cdot \tilde{R}_{j-1} \\ \Lambda_{j}^{RL} \cdot \tilde{L}_{j+1} \end{pmatrix} \equiv \tilde{\Gamma},
\]
(12)

Conversely, if this holds, we can solve \(\tilde{\psi}_{j}\) by \(\tilde{\psi}_{j} = V_{j} \tilde{W}_{j}^{-1} U_{j}^{\dagger} \tilde{\Gamma}\) or \(\tilde{\psi}_{j} = (K_{j}^{\psi})^{\dagger,MP} \tilde{\Gamma}\), where \((K_{j}^{\psi})^{\dagger,MP}\) is the Moore-Penrose inverse of the matrix \(K_{j}^{\psi}\) (see Eq. 3) and Appendix A for details).

Introducing the partitioning of \(\tilde{U}_{j}, K_{j}^{L}\) and \(K_{j}^{R}\) (into upper \(n_{j}^{L}\) rows, middle \(n_{j}^{R}\) rows, and lower \(n_{j}^{\psi}\) rows) as
\[
\tilde{U}_{j} = \begin{pmatrix} U_{j}^{L} \cr U_{j}^{R} \cr U_{j}^{\psi} \end{pmatrix}, \quad K_{j}^{L} = \begin{pmatrix} K_{j}^{LL} & K_{j}^{LR} \\ K_{j}^{RL} & K_{j}^{RR} \end{pmatrix}, \quad K_{j}^{R} = \begin{pmatrix} K_{j}^{LR} \\ K_{j}^{RR} \end{pmatrix},
\]
(13)
the Eq. (12) is rewritten as
\[
-A_{j} \tilde{L}_{j} - B_{j} \tilde{R}_{j} + \check{U}_{j}^{L} \Lambda_{j}^{LR} \tilde{R}_{j-1} + \check{U}_{j}^{R} \Lambda_{j}^{RL} \tilde{L}_{j+1} = 0,
\]
(14)
where
\[
A_{j} = \check{U}_{j}^{L} K_{j}^{LL} + \check{U}_{j}^{R} K_{j}^{RL} \check{U}_{j}^{L} K_{j}^{LR} + \check{U}_{j}^{R} K_{j}^{RR},
\]
\[
B_{j} = \check{U}_{j}^{L} K_{j}^{RL} + \check{U}_{j}^{R} K_{j}^{RR} + \check{U}_{j}^{R} K_{j}^{LR}. \]

Rearranging this equation, we obtain the relation between \((\tilde{R}_{j-1}, \tilde{L}_{j})\) and \((\tilde{R}_{j}, \tilde{L}_{j+1})\) as
\[
P_{j} \begin{pmatrix} \tilde{R}_{j-1} \\ \tilde{L}_{j} \end{pmatrix} = Q_{j} \begin{pmatrix} \tilde{R}_{j} \\ \tilde{L}_{j+1} \end{pmatrix},
\]
(16)
where
\[
P_{j} = \begin{pmatrix} \check{U}_{j}^{L} A_{j}^{LR} & -A_{j} \cr B_{j} & -\check{U}_{j}^{R} A_{j}^{RL} \end{pmatrix},
\]
\[
Q_{j} = \begin{pmatrix} \check{U}_{j}^{L} \Lambda_{j}^{LR} & -A_{j} \cr B_{j} & -\check{U}_{j}^{R} \Lambda_{j}^{RL} \end{pmatrix}. \]

In case of \(n_{j}^{\psi} = 0\), we should put \(U_{j} = I_{n_{j}^{L}+n_{j}^{R}}\) and omit all the terms with \(\psi\) symbol.

2.2 Boundary condition and transfer matrix

Let us define \(\tilde{\Phi}_{j} = \begin{pmatrix} \tilde{R}_{j} \\ \tilde{L}_{j} \end{pmatrix}\). When the whole system is composed of \(M\) blocks, the equation is described by \(\tilde{\Phi}_{1}, \tilde{\Phi}_{2}, \cdots, \tilde{\Phi}_{M+1}\). Then, \(\tilde{R}_{0}\) and \(\tilde{L}_{M+1}\), included respectively in \(\tilde{\Phi}_{1}\) and \(\tilde{\Phi}_{M+1}\), give the boundary condition for the equation. It is convenient to derive an equation which relates the components, \(\tilde{\Phi}_{1}\) and \(\tilde{\Phi}_{M+1}\). We rewrite whole equation into the form \(A \tilde{\Phi} = \tilde{\Theta}\) where
\[
A = \begin{pmatrix} Q_{1} & P_{2} & Q_{2} & \cdots & O \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ P_{M-1} & Q_{M-1} & \cdots & \cdots & O \\ O & \cdots & \cdots & \cdots & P_{M} \end{pmatrix},
\]
\[
\tilde{\Phi} = \begin{pmatrix} \tilde{\Phi}_{2} \\ \vdots \\ \tilde{\Phi}_{M-1} \\ \tilde{\Phi}_{M} \end{pmatrix}, \quad \tilde{\Theta} = \begin{pmatrix} -P_{1} \tilde{\Phi}_{1} \\ \vdots \\ \vdots \\ -Q_{M} \tilde{\Phi}_{M+1} \end{pmatrix}. \]
(18)

Introducing \(\check{U} = N_{j}[A]\) using the definition, Eq. (2), we can see that \(\tilde{\Theta}\) satisfies the condition \(\check{U}^{\dagger} \tilde{\Theta} = 0\). By partitioning \(\check{U}^{\dagger} = (\check{U}_{1}^{\dagger} | \cdots | \check{U}_{M+1}^{\dagger})\), where \(\check{U}_{1}^{\dagger}\) and \(\check{U}_{M+1}^{\dagger}\) are block matrices whose columns corresponds to \(\tilde{\Phi}_{1}\) and \(\tilde{\Phi}_{M+1}\), respectively, we obtain the relation between \(\tilde{\Phi}_{1}\) and \(\tilde{\Phi}_{M+1}\) as
\[
\check{U}_{1}^{\dagger} P_{1} \tilde{\Phi}_{1} = -\check{U}_{M+1}^{\dagger} Q_{M} \tilde{\Phi}_{M+1}.
\]
(19)

Denoting \(\check{U}_{1}^{\dagger} P_{1}\) and \(-\check{U}_{M+1}^{\dagger} Q_{M}\) by \(P^{1}\) and \(Q^{1}\), respectively, and introducing the wave function of the left lead \(\tilde{\Phi}^{\dagger} = \tilde{\Phi}_{1}\) and right lead \(\tilde{\Phi}^{\ast} = \tilde{\Phi}_{M+1}\) we obtain the transfer matrices
which connect the left and right leads as
\[ P^A \tilde{\Phi} = Q^A \tilde{\Phi}. \] (20)

3. A Generalized Ideal wire: Wave Function in a Periodic System

Here we study the completely periodic ideal wire, which is the model for lead electrodes. For easy examples, we will examine zigzag and armchair graphene nano-ribbons in Appendix C.

In an ideal wire where periodicity is complete, all the matrices \( P_j (Q_j) \) are \( j \)-independent and we denote it by \( P \) (\( Q \)).

We assume that the eigenstates satisfy the relation\(\text{Eq. (12)}\)
\[
\tilde{\Phi}_j = z \tilde{\Phi}_{j-1},
\] (21)
where \( z \) is a complex number. From the Eq. (16), the equation determining \( z \) and the eigenvector is given by
\[
P \tilde{\Phi}_j = z Q \tilde{\Phi}_j.
\] (22)

We should note that \( P \) and \( Q \) are not necessarily square matrices. In that sense this is a generalized eigenvalue problem. The method to obtain the eigenvalues and corresponding eigenvectors are given in the Appendix B. Here we discuss only the basic properties of the eigenmodes.

There are several types of eigenmodes: the mode with \(|z| = 1 \) corresponds to a propagating mode (or channel), and that with \(|z| \neq 1 \) to an evanescent mode. When \(|z| > 1 \) (\(|z| < 1 \)) the wave function grows (decays) as \( j \) increases. We found that some evanescent modes have complex \( z \)'s and they oscillates as well as grows or decays.

Here we argue the following mathematical statements.

1) Definition: we call \( z \) the \text{transfer eigenvalue} of the wire and corresponding vector, \( \text{Ev}(\tilde{R}_{j-1}, \tilde{L}_j) \equiv \tilde{\Phi}_z \), the \text{transfer eigenvector} or \text{eigenstate}.

2) If \( z \) is a transfer eigenvalue, \( 1/z \) also is. In case of \(|z| = 1 \), \( 1/z = z^* \).

3) The current matrix \( \Lambda_j \) (see Eq. (9)) is diagonalized as
\[
\tilde{\Phi}_{1j}: \Lambda_j \tilde{\Phi}_z = 0 \quad \text{(if } z \neq z' \text{)}
\] (23)
by the transfer eigenvectors.

Here we note that 2) seems clear if the system has a time-reversal symmetry. However, similar feature may also exist even without time-reversal symmetry. The rigorous proof of this is not yet obtained and is left for future studies.

In the preceding works, it has sometimes been assumed that the direction parallel and perpendicular to the wire are separable\(\text{,[12]}\) such as in the case of a wire made of a square lattice. In that case, we can define the transverse modes rather easily and property expressed in 3) is clearly satisfied. Our statement is the generalization of such cases. The rigorous proof of this seems a little more difficult than that of 2). We give only a numerical evidence in the Appendix C and the proof is left open.

Some attentions are required when some of the transfer eigenvalues are degenerate. This point is argued in Appendix D.

4. Landauer Formula and Conductance

We consider the situation depicted in Fig. 2. The scatterer is connected to left and right leads. Two leads are not necessarily identical to each other. However they should be made of periodic repetition of a set of atoms, and channels are well-defined. We assume the lengths of the two leads are infinite.

As depicted in Fig.2, we consider right- and left-going channels and the evanescent modes decaying in left (right) direction in the left (right) lead. We assume that there are \( n'_l \) (\( n'_r \)) channels and \( n''_l \) (\( n''_r \)) evanescent modes in the left (right) lead. (Note that one channel corresponds to a pair of right- and left-going mode.) For the evanescent modes we take only the wave functions which grow towards the scatterer based on the physical consideration.

Now we calculate the conductance of this conductor. To do this, we utilize the so-called Landauer formula. First we introduce \((n'_l + n''_l) \times (n'_r + n''_r)\) matrix \( S \) of the transmission coefficients, which relates the probability currents of incoming waves to that of outgoing waves, as
\[
\tilde{J}_{\text{out}} = \begin{pmatrix} \tilde{J}_{l+}^r & \tilde{J}_{l-}^r \\ \tilde{J}_{r+}^l & \tilde{J}_{r-}^l \end{pmatrix} = \begin{pmatrix} R & T' \\ T & R' \end{pmatrix} \begin{pmatrix} \tilde{J}_{l+}^r & \tilde{J}_{l-}^r \\ \tilde{J}_{r+}^l & \tilde{J}_{r-}^l \end{pmatrix} \equiv S \tilde{J}_{\text{in}},
\] (24)
where \( \tilde{J}_{l+r}^i \) and \( \tilde{J}_{l+r}^f \) respectively are \( n'_l \) (\( n'_r \)) component vectors, representing the probability currents carried by the right-moving (+) and left-moving (−) channels in the left (right) lead.

We denote the wave functions at the left and right lead by \( \tilde{\Phi}_l \) and \( \tilde{\Phi}_r \), respectively. Each function is given as a superposition of right-moving, left-moving and evanescent modes:
\[
\tilde{\Phi}_l = \sum_{j=1}^{n'_l} \left( \alpha_{j+}^l \tilde{\phi}_{j+}^l + \alpha_{j-}^l \tilde{\phi}_{j-}^l \right) + \alpha_{j+}^{l'c} \tilde{\phi}_{j+}^{l'c}, \]
\[
\tilde{\Phi}_r = \sum_{j=1}^{n'_r} \left( \alpha_{j+}^r \tilde{\phi}_{j+}^r + \alpha_{j-}^r \tilde{\phi}_{j-}^r \right) + \alpha_{j+}^{r'c} \tilde{\phi}_{j+}^{r'c},
\] (25)
where \( \alpha_{j+}^{l+r} \), \( \alpha_{j+}^{l'r} \) and \( \alpha_{j+}^{r=c} \) are constants. The vectors \( \tilde{\phi}_{j+}^{l+r} \) and
represent the wave functions of right-moving and left-moving modes (propagating modes) in the left (l) and right (r) lead. The vectors $\tilde{\phi}_j$ and $\tilde{\phi}_j^r$ represent the wave functions of evanescent modes in the left and right lead, respectively. These vectors, $\tilde{\phi}_j$, are obtained by the procedure described in the preceding section in each lead.

Here we introduce matrix representation of wave-function bases such as $\Theta^f = (\phi^{li}_1, \cdots, \phi^{li}_n)$. Then the Eqs. (25) are rewritten as

$$
\begin{align*}
\tilde{\phi}_j^l &= \Theta^l \phi^{li} + \Theta^l \phi^{ri} + \Theta^l \phi^{lc} \\
\tilde{\phi}_j &= \Theta^r \phi^{ri} + \Theta^r \phi^{rr} + \Theta^r \phi^{rc},
\end{align*}
$$

where $\phi^{li} = (\phi^{li}_1, \cdots, \phi^{li}_m)$, $\cdots$, are columnar vectors. From the Eq. (20), we obtain

$$
P^A \left( \Theta^l \phi^{li} + \Theta^l \phi^{ri} + \Theta^l \phi^{lc} \right) = Q^A \left( \Theta^r \phi^{ri} + \Theta^r \phi^{rr} + \Theta^r \phi^{rc} \right).
$$

This is rewritten in a matrix form as

$$
F \begin{pmatrix}
\phi^{li} \\
\phi^{ri} \\
\phi^{lc}
\end{pmatrix} = G \begin{pmatrix}
\phi^{li} \\
\phi^{ri} \\
\phi^{rc}
\end{pmatrix},
$$

where

$$
F = \begin{pmatrix}
P^A \Theta^l & -Q^A \Theta^r & P^A \Theta^l \\
0 & Q^A \Theta^r & 0 \\
-P^A \Theta^l & Q^A \Theta^r & 0
\end{pmatrix},
$$

$$
G = \begin{pmatrix}
-P^A \Theta^l & Q^A \Theta^r & P^A \Theta^l \\
0 & Q^A \Theta^r & 0 \\
P^A \Theta^l & -Q^A \Theta^r & 0
\end{pmatrix}.
$$

We calculate $\bar{U}_G = N_L[G]$ along the definition Eq. (2). Then we obtain,

$$
\bar{U}_G^T F \begin{pmatrix}
\phi^{li} \\
\phi^{ri} \\
\phi^{lc}
\end{pmatrix} = 0
$$

(30)

gives the condition, which relates the amplitudes of incoming and outgoing waves. Note that, if there are no evanescent modes, $\bar{U}_G$ should be the identity matrix of order $2(n^l_c + n^r_c)$.

Writing $\bar{U}_G^T F \equiv (D^{in} | D^{out})$, where $D^{in(out)}$ is the left (right) $n^l_c + n^r_c$ columns of $\bar{U}_G^T F$, and $\tilde{\alpha} \equiv \begin{pmatrix}
\alpha^{li} \\
\alpha^{ri} \\
\alpha^{lc}
\end{pmatrix}$, $\tilde{D} \equiv \begin{pmatrix}
D^{in} \\
D^{out}
\end{pmatrix}$, we reach the expression

$$
\tilde{\alpha}^{out} = -D^{out} \tilde{\alpha}^{in}.
$$

(31)

From the argument of the Sec. 3, the total probability current is given by a sum of the independent contributions of the channels. Let us denote the contribution of the $j$-th “in (out)” channel by $J^{in}_j$, the probability currents carried by incoming and outgoing channels are given by

$$
\{ J^{in} \} = \eta^l_j |\alpha^{in}_j|^2, \{ J^{out} \} = \eta^r_j |\alpha^{out}_j|^2.
$$

Using Eq. (31), the probability current carried by the $j$-th outgoing channel is given by

$$
J^{out}_j = \sum_{k,k=1}^{n^l_c+n^r_c} D^{out}_{jk} \eta^r_j |\alpha^{out}_j|^2 + \sum_{k,k=1}^{n^l_c+n^r_c} D^{out}_{jk} \eta^l_j |\alpha^{in}_j|^2.
$$

(32)

Here we separated the summation into diagonal and off-diagonal terms with respect to $k$ and $k'$. We assume that electrons are injected to the modes $\alpha^{k}_c$ from the reservoir incoherently, and then the cross term (the last line of Eq. (32)) may vanish after time averaging. This seems to be an intuitively correct assumption, however microscopic justification may be desirable.

As a result we obtain the following relation,

$$
\{ J^{out} \} = \sum_{k=1}^{n^l_c+n^r_c} \eta^r_j |D^{out}_{jk}|^2 |\alpha^{out}_j|^2 = \sum_{k=1}^{n^l_c+n^r_c} S_{jk} J^{in}_k.
$$

(33)

Then the scattering matrix $S$ is given by

$$
S_{jk} = \frac{\eta^{out}_j}{\eta^{in}_j} |D^{out}_{jk}|^2.
$$

(34)

Using the Landauer formula we can calculate the conductance as

$$
G = \frac{2e^2}{h} \sum_{j=n^l_c+1}^{n^l_c+n^r_c} \sum_{k=1}^{n^l_c+n^r_c} S_{jk}.
$$

(35)

In actual calculation, the wave functions should be normalized appropriately. However, such normalization is not relevant to the present result. Therefore we can adopt any normalization for our convenience.

In the preceding theories, the Landauer formula is argued using the so-called “transmission matrix”, which is obtained by connecting the probability amplitudes of the wave functions in left and right leads. In this case we should pay attention to the normalization of the wave functions, so that each channel carries unit flux. In our treatment, the currents in the left and right leads are directly related and we do not need transmission matrix in a conventional sense.

5. Application to Graphene Constrictions

We apply the present method to graphene constrictions of several forms. The nature of the graphene is taken into account only by considering the honeycomb lattice structure, and the hopping is restricted to nearest neighbors. (Extension to more realistic structure is easy.)

We consider graphene wires with (I) a short, (II) a middle, and (III) a long constriction as depicted in Fig. 3. The narrowest part of the wire is composed of $N = 4$ armchair nanoribbon. The leads are assumed to be two-dimensional square lat-
Fig. 3. The geometries of the graphene nanoribbons studied in this paper. I, II and III have constrictions in the middle of the conductor, though the lengths of the constricted regions differ. The constricted region is $N = 4$ armchair nanoribbon in all cases as one can see from the magnification. Both leads are modeled by square lattice conductors, and the direction of the lattice is intentionally rotated from the wire axis.

The lattice parallel to the graphene surface, whose lattice spacing is $0.55 \times a$ ($a$: minimum C-C spacing in graphene). The transfer integral within leads, $t$, are taken to be same as that in graphene, and the transfer integral between graphene and leads, $t'$, is taken as $t' = 0.3 \times t$. It is assumed that the hopping between sites in leads and graphene is present only when the horizontal distance (parallel to graphene surface) is smaller than $2 \times a$.

The conductance of the wires at zero temperature are calculated as a function of the energy and the results are shown in Fig. 4 (a) ~ (c). The apparent step like function (indicated in blue) is the conductance of an ideal $N = 4$ wire, where contributions of the four channels are clearly seen.

As one can see, all the curves of constrictions consist of spiky peaks, which may appear as a result of the various resonances of conduction electrons. The resemblance to the blue steps are not obvious in all cases. However at some energies the conductance approaches the perfect transmission especially in the lowest step $G = 2e^2/h$.

Near zero energy, some peaks are seen in (a) and (b), which is more distinct in the magnified plot (d). These may come from the transmission through the evanescent states in the wider part of the graphene wire, which decay in the constricted region. This explanation is plausible since such peaks are not significant in the case of the longest constriction (c), though a small peak exists even in this case.

The conductance at finite temperatures are calculated from the equation,

$$G(E, T) = \int_{-\infty}^{\infty} G(E', 0)f(E')dE'$$

where $f(E)$ is the Fermi distribution function and $G(E, T)$ is the conductance at bias $E$ and temperature $T$. The finite temperature result is shown for the constriction I. In Fig. 5,
we have shown the results for $T = 0, 0.05 \times t, 0.1 \times t$. At $T = 0.05 \times t$, several steps can be seen. At this stage, it is no clear whether they correspond to the steps of $N = 4$ wire or not. More intensive study is required to clarify the conductance quantization in graphene constrictions.

![Graphene Conductance](image)

**Fig. 5.** Conductance of Fig. 3 (a) after thermal average. The result of $T = 0$ is shown by thin green curve, $T = 0.05 \times t$ by thick red curve, and $T = 0.1 \times t$ by dashed purple curve.

6. Reduction of the Matrix Dimensions and Parallelization

We argue that the dimension of the large matrix appearing in Eq. (18) can be reduced by the following methods. Let us take a part of the equation,

$$P_j \Phi_j = Q_j \Phi_{j+1}$$

(37)

and

$$P_{j+1} \Phi_{j+1} = Q_{j+1} \Phi_{j+2}.$$  

(38)

Here we show that we can truncate $\Phi_{j+1}$ without obtaining $\Phi_j$ and $\Phi_{j+2}$.

We rewrite the equation by introducing block matrices as,

$$
\begin{pmatrix}
P_j \\
O
\end{pmatrix}
\begin{pmatrix}
Q_j \\
O_{j+1}
\end{pmatrix}
\begin{pmatrix}
\Phi_j \\
\Phi_{j+2}
\end{pmatrix}
= 
\begin{pmatrix}
P_j \\
O
\end{pmatrix}
\begin{pmatrix}
Q_j \\
O_{j+1}
\end{pmatrix}
\begin{pmatrix}
\Phi_j \\
\Phi_{j+2}
\end{pmatrix}.
$$

(39)

Then we obtain the condition relating $\Phi_j$ and $\Phi_{j+2}$ as

$$N_t \left( \begin{pmatrix}
Q_j \\
P_{j+1}
\end{pmatrix} \right)^\dagger 
\begin{pmatrix}
P_j \\
O
\end{pmatrix}
\begin{pmatrix}
Q_j \\
O_{j+1}
\end{pmatrix}
\begin{pmatrix}
\Phi_j \\
\Phi_{j+2}
\end{pmatrix}
= 0.$$  

(40)

Rewiring the blocks of the matrix by

$$P'_j \equiv N_t \left( \begin{pmatrix}
Q_j \\
P_{j+1}
\end{pmatrix} \right)^\dagger 
\begin{pmatrix}
P_j \\
O
\end{pmatrix},$$

$$Q'_j \equiv -N_t \left( \begin{pmatrix}
Q_j \\
P_{j+1}
\end{pmatrix} \right)^\dagger 
\begin{pmatrix}
O \\
Q_{j+1}
\end{pmatrix},$$

(41)

we obtain

$$P'_j \Phi_j = Q'_{j+1} \Phi_{j+2}.$$  

(42)

If we need the wave function $\Phi_{j+1}$, we can obtain it by using Moore-Penrose inverse as

$$\tilde{\Phi}_{j+1} = \left( \frac{Q_j}{P_{j+1}} \right)^{\text{MP}} 
\begin{pmatrix}
P_j \\
O
\end{pmatrix}
\begin{pmatrix}
Q_j \\
O_{j+1}
\end{pmatrix}
\begin{pmatrix}
\Phi_j \\
\Phi_{j+2}
\end{pmatrix}.$$  

(43)

By using the above transformation we can reduce the number of blocks in the large matrix in Eq. (18) by one. Applying this method repeatedly, the matrix dimension is remarkably reduced.

Furthermore, this process can be carried out for several different $j$'s simultaneously. Therefore the calculation process can be parallelized. These features may allow us a calculation in a huge system. Appropriate truncation procedure is required for the actual application, which we left for future problem.

7. Discussion

In this paper we have introduced a new formulation to calculate the transmission coefficients and the conductance of wires in mesoscopic scales. The key point of our method is to omit the degrees of freedom in the scatterer irrelevant for the transport phenomena, using SVD. This procedure may be available in other scattering problems. Until now, SVD does not seem to be used so often in the studies of physics. However, it may be much more useful in various field of physics including solid state physics.

In the present study we have not treated the following features:

- random potential,
- magnetic field,
- spin orbit coupling,
- lattice distortion.

Inclusion of these into our formalism may be straight forward. They will provide useful information in the various fields, such as spintronics or topological insulators.

In order to treat the multi-terminal experiments, such as Hall conductance, we need to extend the present approach to multi-terminal geometry. Although it requires a little ingenuity, especially when we divide the sample in to blocks, we think that the present treatment can be extended in the way shown by Baranger et. al.5

Since in nanoscale systems, interaction effects such as Coulomb blockade become important in many situations, developments to cover electron-electron interactions is strongly required. At this stage, it is not clear that our method is useful or not in such direction. We need to incorporate more sophisticated methods, such as one proposed by Darancet et. al., which however is not a simple task.

As for the numerical calculation presented in this paper, we have to say that it is at a primitive stage. The scales of the systems are not large enough to be compared to real experiments. However, we stress that this is the first calculation assuming the contact to realistic leads. We can speculate several features from our results. It can be said that the conductance of $N = 4$
nanoribbons are modified largely from the ideal step-like patterns when the leads are attached. Similar results are also obtained for the case of nanoribbons with disordered edges. In our calculation no disorder has been introduced, however the shapes of the graphene and leads are not uniform. From Fig. 5, it seems that various interferences and resonances in the electrodes may determine the overall shape of the conductance curve. Microscopic study of the current flow in the whole system is strongly required, and in that case the parallelization scheme shown in Sec. 6 may be useful, although the actual implementation may require an elaborate program design.

8. Summary

We have proposed a new method to calculate the conductance through mesoscopic conductors, which has a potential advantage in treating huge systems using parallel computation. A simple example of calculation is shown for graphene nanoribbons with external leads.

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Appendix A: Calculation of $\psi_j$

If one needs $\psi_j$ in order to obtain some information about the inside of the conductor, one can calculate it in the following way. First we operate $U_j$, obtained by Eq. (11), from the left side of Eq. (10) and obtain

$$
\begin{pmatrix}
\sigma_{j,1}\tilde{\psi}_{j,1} \\
\sigma_{j,2}\tilde{\psi}_{j,2} \\
\vdots \\
\sigma_{j,\beta_j}\tilde{\psi}_{j,\beta_j} \\
0 \\
0
\end{pmatrix}
= 
\begin{pmatrix}
\tilde{U}_{j,1} \\
\tilde{U}_{j,2} \\
\vdots \\
\tilde{U}_{j,\beta_j} \\
0 \\
0
\end{pmatrix}
\tilde{\Gamma}_j, \quad (A-1)
$$

or equivalently,

$$
\begin{pmatrix}
\tilde{W}_j \tilde{v}_{j}^\dagger \\
\tilde{O}
\end{pmatrix}
\tilde{\psi}_j = 
\begin{pmatrix}
\tilde{U}_{j}^\dagger \\
\tilde{O}_j
\end{pmatrix}
\tilde{\Gamma}_j, \quad (A-2)
$$

where $\tilde{W}_j = \text{diag}(\sigma_{j,1}, \ldots, \sigma_{j,\beta_j})$. From the upper $\beta_j$ rows of this equation we obtain

$$
\tilde{\psi}_j = \tilde{v}_j \frac{\alpha_1}{\sigma_{j,1}} + \cdots + \tilde{v}_{\beta_j} \frac{\alpha_{\beta_j}}{\sigma_{j,\beta_j}} = \tilde{v}_j \tilde{W}_j^{-1} \tilde{U}_j \tilde{\Gamma}_j, \quad (A-3)
$$

where $\alpha_k = \tilde{U}_{j,k} \tilde{\Gamma}_j$. This solution of $\tilde{\psi}_j$ is not unique, since we can add arbitrary superposition of $\tilde{v}_{\beta_{j+1}}$, $\ldots$, $\tilde{v}_{\beta_j}$ without violating the condition Eq. (A-1). However such indeterminacy is not important for our purpose, namely, to calculate the transport coefficients, since these extra components stand for the wave functions which are not connected to $\tilde{R}_{j-1}$, $\tilde{L}_j$, $\tilde{R}_j$ and $\tilde{L}_{j+1}$, and are irrelevant for transport phenomenon. The solution for $\tilde{\psi}_j$ is more easily obtained by using the Moore-Penrose quasi-inverse matrix (Eq. (3)) of $K_j^\phi$, as $\tilde{\psi}_j = (K_j^\phi)^{\text{MP}} \tilde{\Gamma}_j$. This solution is exactly the same as Eq. (A-3).

Appendix B: A method to solve the generalized eigenvalue problem

We present a simple method to solve the equation of the following type,

$$
P \tilde{x} = zQ \tilde{x} \quad (B-1)
$$

where $P$ and $Q$ are $M \times N$ matrices ($M \neq N$ in general), $z$ and $\tilde{x}$, respectively, are a number and a vector which should be determined. In solving Eq. (B-1), it is advantageous to formulate the problem on the basis of eigenvalue problem. In order to do this, however, we need to manipulate the matrices carefully. The calculation consists of the following two steps.

B.1 Removal of the intersection of the null space of $P$ and $Q$

First we note the case where the intersection of the null space of the matrices $P$ and that of $Q$ is not empty. Suppose a vector $\tilde{v}$ is in the null space of $P$ and $Q$ simultaneously, namely, $P \tilde{v} = 0$ as well as $Q \tilde{v} = 0$, the vector $\tilde{v}$ is a solution of Eq. (B-1) irrespective of the value $z$. In such cases, we cannot determine the other eigenvectors from Eq. (B-1), since even if we can make $P$ and $Q$ square matrices in some way, the characteristic polynomial $\text{det}(P - zQ)$ vanishes for any $z$ and the eigenvalues are not determined. Actually in the case of $N = 2$ graphene analyzed in the next section, we can see that independent solutions exist at energy $E = 1.0 \times t$ (see Fig. C.3).

In order to avoid this situation we need to remove the intersection of the null spaces of $P$ and $Q$ from the basis of the matrices. This process is executed as follows (see Chap. 12.4 of Ref. 36).

First we consider a block matrix $\Omega$ made from $P$ and $Q$ and introduce its SVD as follows,

$$
\Omega \equiv \begin{pmatrix} P \\ Q \end{pmatrix} = U W V^\dagger \equiv \begin{pmatrix} U_P \\ U_Q \end{pmatrix} W V^\dagger. \quad (B-2)
$$

Then we truncate the null space of $\Omega$ in the following way,

$$
\Omega = \begin{pmatrix} U & U \end{pmatrix} \begin{pmatrix} \sigma_1 & \cdots & 0 \\ \cdots & \ddots & \vdots \\ 0 & \cdots & \sigma_r \end{pmatrix} \begin{pmatrix} \tilde{V}_1 \\ \vdots \\ \tilde{V}_r \end{pmatrix},
$$

$$
\equiv \begin{pmatrix} U & U \end{pmatrix} W \begin{pmatrix} \tilde{V}_1 \\ \vdots \\ \tilde{V}_r \end{pmatrix}. \quad (B-3)
$$

where $\sigma_j$ in a singular value of $\Omega$, and $r = \text{rank}(\Omega)$. Here the columns of $V = (\tilde{v}_1, \ldots, \tilde{v}_N)$ form an complete orthonormal basis of the $N$-dimensional space, and the columns of $\tilde{V} = (\tilde{v}_{r+1}, \ldots, \tilde{v}_N)$ form the basis of the null space of $\Omega$. 
which is actually the intersection of the null spaces of $P$ and $Q$. Therefore if we restrict the basis of $\vec{x}$ to $\vec{v}_1, \cdots, \vec{v}_r$, the intersection of the null spaces of $P$ and $Q$ is removed from the space of the solution of $\vec{x}$.

Here we set
\[
\vec{x} = \sum_{j=1}^r \frac{y_j}{\sigma_j} \vec{v}_j = \tilde{V} \tilde{W}^{-1} \vec{y}.
\]  
(B-4)

If we divide $\tilde{U}$ into upper $M$ rows and lower $M$ rows and put
\[
\left( \begin{array}{c} P \\ Q \end{array} \right) = \left( \begin{array}{c} \Pi \\ \Theta \end{array} \right) \tilde{W} \tilde{V},
\]  
(B-5)

the relations $P = \Pi \tilde{W} \tilde{V}$ and $Q = \Theta \tilde{W} \tilde{V}$ hold and the Eq. (B-1) is rewritten as
\[
\Pi \vec{y} = \vec{z} \Theta \vec{y}.
\]  
(B-6)

Note that $\tilde{V}^\dagger \tilde{V} = I_r$ where $I_r$ is the identity matrix of order $r$. At this stage, $\Pi$ and $\Theta$ are not necessarily square matrices.

B.2 Making matrices $\Pi$ and $\Theta$ square

Next we make the matrices $\Pi$ and $\Theta$ square by truncating some of the null spaces of $\Pi$ or $\Theta$. We put the dimensions of $\Pi$ and $\Theta$ to be $m \times n$ and also define $d \equiv \min(m, n)$. The SVD of $\Pi$ and $\Theta$ are given as
\[
\Pi = U^{\Pi} \tilde{W}^{\Pi} V^{\Pi}, \quad \Theta = U^{\Theta} \tilde{W}^{\Theta} V^{\Theta}
\]  
(B-7)

and we truncate these matrices as in the same manner as Eq. (B-3) so that $W^{\Pi}$ and $W^{\Theta}$ become $d \times d$ matrices. 38 The truncated matrices are indicated by tilde signs. Then Eq. (B-6) is rewritten as
\[
\tilde{U}^{\Pi} \tilde{W}^{\Pi} \tilde{V}^{\Pi} \vec{y} = \vec{z} \tilde{U}^{\Theta} \tilde{W}^{\Theta} \tilde{V}^{\Theta} \vec{y}.
\]  
(B-8)

Now we set
\[
\vec{y} = \sum_{j=1}^d \vec{\xi}_j \vec{v}_j^{\Pi} = \tilde{V}^{\Pi} \vec{\xi},
\]  
(B-9)

where $\tilde{V}^{\Pi} = (\vec{v}_1^{\Pi}, \cdots, \vec{v}_d^{\Pi})$ and Eq. (B-8) is rewritten as
\[
\tilde{U}^{\Pi} \vec{\xi} = \vec{z} \tilde{\Theta} \vec{\xi},
\]  
(B-10)

where $\tilde{U}^{\Pi} \equiv \tilde{W}^{\Pi}$ and $\tilde{\Theta} \equiv \tilde{U}^{\Pi} \tilde{U}^{\Theta} \tilde{W}^{\Theta} \tilde{V}^{\Theta} \tilde{V}^{\Pi}$. Here $\Pi$ and $\Theta$ are square matrices of order $d$.

Now the problem is reduced to the ordinary “generalized” eigenvalue problem and we can find the eigenvalues by solving $\det (\tilde{\Pi} - \vec{z} \tilde{\Theta}) = 0$ with respect to $\vec{z}$. Suppose that $\vec{\xi}$ is the eigenvector satisfying Eq. (B-10), that of the original problem, Eq. (B-1), is obtained from $\vec{x} = \tilde{V} \tilde{W}^{-1} \tilde{V}^{\Pi} \vec{\xi}$.

Finally we note that zero or infinite eigenvalues may obtained in solving Eq. (B-10). These eigenvalues originates from the remnant null space of $\Pi$ or $\Theta$. Actually, from Eq. (B-10), the formula $\det (\tilde{\Pi} - \vec{z} \tilde{\Theta})$ is a polynomial of degree $d$. If rank($\tilde{\Pi}$) < $d$, a null vector exists for $\tilde{\Pi}$, which is an eigenvector belonging to eigenvalue zero. In this case, the zero-th order term of $\det (\tilde{\Pi} - \vec{z} \tilde{\Theta})$ vanishes, resulting in zero eigenvalues. If rank($\tilde{\Theta}$) < $d$, a null vector exists for $\tilde{\Theta}$ and the $d$-th order term of $\det (\tilde{\Pi} - \vec{z} \tilde{\Theta})$ vanishes. In this case, we have eigenvalues of infinity, 39 or in other words, $\det (\vec{z} \tilde{\Pi} - \tilde{\Theta}) = 0$ has the solution $\vec{z} = 0$. These eigenvalues are not relevant for the transport phenomena and can be neglected in the present calculations. Actually, they correspond to quantum states localized within a block and isolated from the neighboring blocks.

Appendix C: Transfer eigenstates and current in graphene nanoribbons

We have solved eigenvalues for zigzag and armchair nano ribbons shown in Fig. C-1. In Fig. C-2, the argument of $\vec{z}$ is plotted as a function of $E$: (a) is for the armchair chain and (b) is for the zigzag one. In both figures we can see several propagating modes ($|\vec{z}| = 1$) with dispersion. We can also see some eigenvalues located on the horizontal axis of both (a) and (b), which are evanescent modes with $|\vec{z}| \neq 1$. For these modes, $\text{Im}(\vec{z}) = 0$. In (b), slightly curved horizontal lines are seen near $\arg(\vec{z}) = \pm \pi$. These are also evanescent modes with non-vanishing $\text{Im}(\vec{z})$.

The number of modes for fixed energy gives the number of channels. We have studied several cases, including those shown in Fig. C-1, and found that the number of channels, including propagating and evanescent modes, in an ideal wire is determined by “the minimum number of bond cuttings required to separate the wire”. (We count the set of right-moving (growing) and left-moving (decaying) modes as one channel.) One can see in Fig. C-1 (a), the minimum bond cutting is two, whereas in (b) it is three. Actually, we see two channels for each $E$ in Fig. C-2 (a) and three channels in (b).

It is interesting to see the correspondence of the present results to those obtained by diagonalization of the full Hamiltonian. Fig. C-3 is obtained by solving the non-trivial solution of Eq. (8) under the boundary condition Eq. (21). The energy $E$ for $\vec{z} = e^{i\vec{k}}$ is solved as a usual eigenvalue problem. Fig. C-2 (a) and (b) correspond respectively to Fig. C-3 (a) and (b). In the latter, evanescent modes are not seen, because we have assume $|\vec{z}| = 1$ in solving the equation. On the other hands, completely flat band (vertical line) can be seen in Fig. C-3 (a). The nature of the flat band becomes apparent by examining the the wave function. In the lower figure of Fig. C-3 (a), we have shown the amplitude of wave function in a unit cell corresponding to five points (“a”, “b”, “c”) indicated in the dispersion (upper graph). It can be seen that the flat band
Fig. C.2. Arguments of the transfer eigenvalues, \( \arg z \), is plotted as a function of energy \( E \). (a) and (b) correspond to those in Fig. C.1.

(corresponding to “c”) has a disconnected wave function in the unit cell, whereas other dispersive modes have continuous wave functions through the unit cell. In our calculation, the modes like “c” are neglected, since they belong to the intersection of the null space of matrix \( P \) and \( Q \) of Eq. (22). (see also Appendix B.)

Next we can calculate the probability current carried by a channel using the formula given in Eq. (9). In general, the wave function \( \langle \vec{R}_0, \vec{L}_1 \rangle \) is expressed as a superposition of eigenmodes,

\[
\begin{pmatrix} \vec{R}_0 \\ \vec{L}_1 \end{pmatrix} = \sum_{k=1}^{2n_{\text{modes}}} \alpha_k \phi_k
\]

(C-1)

From Eq. (9), the current can be calculated as follows,

\[
J = \frac{i}{h} \sum_{k,k'} \alpha_k^* \alpha_{k'} \eta_{k,k'} \cdot \eta_{k,k'} = \phi_k^\dagger \Lambda \phi_{k'}.
\]

(C-2)

We have calculated the matrix \( \eta_{k,k'} \) for zigzag and armchair wires. For armchair wire, we obtained

\[
\eta(0.3t) =
\begin{pmatrix}
3.451 & 0 & 0 & 0 \\
0 & 0 & 0.666i & 0 \\
0 & -0.666i & 0 & 0 \\
0 & 0 & 0 & -3.451
\end{pmatrix},
\]

(C-3)

\[
\eta(1.5t) =
\]

Fig. C.3. The energy eigenvalues \( E \) are solved for fixed wave number \( k \), where \( z = e^{ik} \), and \( E \)'s are plotted as function of \( k \). (Vertical and horizontal axes are flipped to correspond to Fig. C.2.) (a) and (b) correspond to those in Fig. C.1. The lower figure of (a) shows the amplitudes of wave function on each sites, corresponding to the eigenstates labelled by “a” ~ “e” in the upper figure.

\[
\eta(2.5t) =
\begin{pmatrix}
-3.528 & 0 & 0 & 0 \\
0 & 1.206 & 0 & 0 \\
0 & 0 & -1.206 & 0 \\
0 & 0 & 0 & 3.528
\end{pmatrix},
\]

(C-4)

\[
\eta(2.5t) =
\begin{pmatrix}
-0.426 & 0 & 0 & 0 \\
0 & 0 & 0.141i & 0 \\
0 & -0.141i & 0 & 0 \\
0 & 0 & 0 & 0.426
\end{pmatrix},
\]

(C-5)

and for the zigzag wire

\[
\eta(0.3t) =
\]
functions by vectors so that the current matrix is diagonal. Let us denote a matrix composed by the degenerate wave functions by $\Phi_D = (\tilde{\phi}_1^D, \cdots, \tilde{\phi}_N^D)$, where $N$ is the degree of the degeneracy. The matrix of current $\tilde{J}$ in the degenerate subspace is given by $\tilde{J} = (i/\hbar)\Phi_D^\dagger \tilde{\rho}_D$. Noting that $\tilde{J}$ is symmetric, we can diagonalize $\tilde{J}$ as $U^\dagger \tilde{J} U = (i/\hbar) U^\dagger \Phi_D^\dagger \tilde{\rho}_D U$ by an orthogonal matrix $U$. Reselecting the eigenvectors in the degenerate subspace as $\Phi_D U = (\tilde{\phi}_1, \cdots, \tilde{\phi}_N)$, we can make the current matrix diagonal.

For evanescent modes the degeneracies are not harmful, since we do not utilize the diagonal properties of current matrix with respect to the evanescent modes in the Landauer formula.

\begin{equation}
\eta(1.5t) =
\begin{pmatrix}
-2.493 & 0 & 0 & 0 & 0 & 0 \\
0 & -0.989 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -0.346i & 0 \\
0 & 0 & 0.346i & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.989 & 0 \\
0 & 0 & 0 & 0 & 0 & 2.493
\end{pmatrix}
\end{equation}

\begin{equation}
\eta(2.5t) =
\begin{pmatrix}
-0.561 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -0.764i & 0 \\
0 & 0 & 0 & 0.527i & 0 & 0 \\
0 & 0 & 0 & -0.527i & 0 & 0 \\
0 & 0.764i & 0 & 0 & 0 & 0.561 \\
0 & 0 & 0 & 0 & 0 & 0.561
\end{pmatrix}
\end{equation}

where the indices of the eigenstates, $k$ and $k'$, are assigned in the order of the arguments of their eigenvalues $-\pi \leq \arg(z) < \pi$.

From these results, with the help of the energy diagram obtained above, we can see that the current is diagonalized within the propagating modes, in the sense of Eq. (23). For evanescent modes, non zero current exists only when the mode with $z$ and $1/z$ (growing and decaying mode) coexist.

We have performed similar calculations in several different systems. However, any counterexamples of Eq. (23) have not been found until now. Therefore, we expect Eq. (23) is a common feature for any wires made by a periodic repetition of a set of atoms.

Appendix D: Degeneracy in the Transfer Eigenvalues

We have to pay attention to the cases, where transfer eigenvalues $z$ are degenerate. In this case we have freedom of mixing eigenvectors of the degenerate modes and then the current matrix $\Lambda^\dagger$ of Eq. (23) can have off-diagonal elements even for propagating modes. In that case, we have to chose the eigenvectors so that the current matrix is diagonal.

Let us denote a matrix composed by the degenerate wave functions by $\Phi_D = (\tilde{\phi}_1^D, \cdots, \tilde{\phi}_N^D)$, where $N$ is the degree of the degeneracy. The matrix of current $\tilde{J}$ in the degenerate subspace is given by $\tilde{J} = (i/\hbar)\Phi_D^\dagger \tilde{\rho}_D$. Noting that $\tilde{J}$ is symmetric, we can diagonalize $\tilde{J}$ as $U^\dagger \tilde{J} U = (i/\hbar) U^\dagger \Phi_D^\dagger \tilde{\rho}_D U$ by an orthogonal matrix $U$. Reselecting the eigenvectors in the degenerate subspace as $\Phi_D U = (\tilde{\phi}_1, \cdots, \tilde{\phi}_N)$, we can make the current matrix diagonal.

For evanescent modes the degeneracies are not harmful, since we do not utilize the diagonal properties of current matrix with respect to the evanescent modes in the Landauer formula.
38) The dimension of the truncated matrices can be for example \( \max(\text{rank}(\Pi), \text{rank}(\Theta)) \). However the final results are essentially unchanged.

39) For example, the solutions of the equation, \( ax^2 + bx + c = 0 \), is \( x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \). In the limit of \( a \to 0 \) the solutions tend to \( x = -c/b \) and \( x = -b/a \). Then the latter one diverges if \( b \neq 0 \).