Calculation of the Self-energy of Open Quantum Systems

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The electronic conduction in mesoscopic systems has been studied extensively in recent years. A theoretically interesting feature of the problem is the fact that the system in question is an open quantum system with semi-infinite leads. The open quantum system intrinsically has resonant states, which can strongly affect the electronic conduction.$^1$

A popular way of treating the semi-infinite leads is to contract the leads to the self-energy. The self-energy of leads is a useful way of computing the conductance as well as obtaining resonant states. In this note, we propose a new method of calculating the self-energy of the leads. The self-energy $\Sigma(E)$ was originally defined in$^2$

$$\langle x|\frac{1}{E-H+i\delta}|x'\rangle = \langle x|\frac{1}{E-(H_c+\Sigma(E))}|x'\rangle$$

(1)

for sites $x$ and $x'$ inside the central conductor, where $H_c$ is the Hamiltonian of the central conductor and $H$ is the total Hamiltonian including semi-infinite leads attached to the conductor. The self-energy has been calculated by various methods. The method that we present here is much easier than previous methods. The main claim of this note is that the self-energy is equivalent to the boundary conditions for resonant states.

We consider the Hamiltonian of a conductor with semi-infinite leads attached to it: $H = H_c + \sum_\alpha H_\alpha$, where $H_c$ is a one-body Hamiltonian of a finite-size conductor, while $H_\alpha$ describes a semi-infinite lead given by the tight-binding model

$$H_\alpha \equiv -t \sum_{x_\alpha=0}^\infty (|x_\alpha+1\rangle\langle x_\alpha| + |x_\alpha\rangle\langle x_\alpha+1|).$$

(2)

This includes the hopping between a site $x_\alpha = 0$ on the conductor and the lead $\alpha$. (Note that, if we have hopping between the conductor and a lead with the amplitude different from $-t$, we include it in $H_c$.)

Equation (1) suggests that the eigenvalues of the effective Hamiltonian $H_{\text{eff}}(E) \equiv H_c + \Sigma(E)$ are the poles (bound states and resonant states) of the total Hamiltonian $H$ on the complex $E$ plane. Therefore, we seek discrete and generally complex eigenvalues $E_n$ of resonant
states and bound states of the whole system:

\[ H|\psi_n\rangle = E_n|\psi_n\rangle \quad \text{and} \quad \langle \tilde{\psi}_n|H = E_n\langle \tilde{\psi}_n| \tag{3} \]

The eigenfunctions are bi-orthogonal: \( \langle \tilde{\psi}_n|\psi_m\rangle = \delta_{nm} \). The eigenvalues \( E_n \) are related to the corresponding eigen-wave-number \( k_n \), which is also generally complex, through the dispersion relation \( E_n = -2t \cos k_n \). The eigen-wave-number \( k_n \) is on the upper-half plane for the bound states and on the lower-half plane for the resonant states.

It is known that the resonant states as well as the bound states can be found by requiring the boundary conditions \( \langle x_\alpha|\psi_n\rangle \propto e^{i k_n x_\alpha} \) for \( x_\alpha \geq 0 \) in the leads. \(^3\) In other words, the discrete states satisfy the boundary conditions

\[ \langle x_\alpha + 1|\psi_n\rangle = e^{i k_n} \langle x_\alpha|\psi_n\rangle \quad \text{for} \quad x_\alpha \geq 0, \tag{4} \]

where \( \Re k_n \geq 0 \). The boundary conditions (4) transform the Schrödinger equation

\[ \langle x_\alpha = 0|H_c|\psi_n\rangle - t\langle x_\alpha = 1|\psi_n\rangle = E_n \langle x_\alpha = 0|\psi_n\rangle \tag{5} \]

to

\[ \langle x_\alpha = 0|H_c|\psi_n\rangle + V_{\alpha}^{(\alpha)}(E_n) \langle x_\alpha = 0|\psi_n\rangle = E_n \langle x_\alpha = 0|\psi_n\rangle, \tag{6} \]

where

\[ V_{\alpha}^{(\alpha)}(E) \equiv -te^{ik} \tag{7} \]

is the energy-dependent effective potential.

We claim that the self-energy of the lead \( \alpha \) is nothing but the effective potential:

\[ \Sigma^{(\alpha)}(E) = V_{\alpha}^{(\alpha)}(E)|x_\alpha = 0\rangle\langle x_\alpha = 0|. \tag{8} \]

The total self-energy is the sum over the leads: \( \Sigma(E) = \sum_\alpha \Sigma^{(\alpha)}(E) \). The effective potential \( V_{\alpha}^{(\alpha)} \) is rewritten in terms of \( E \) as

\[ V_{\alpha}^{(\alpha)}(E) = \frac{E - i\sqrt{4t^2 - E^2}}{2} \tag{9} \]

by using the dispersion relation \( E = -2t \cos k \). Note that we choose the branch \( \Im V_{\alpha}^{(\alpha)} < 0 \) for the retarded Green function. Equation (9) is indeed equivalent to the expression obtained by other methods.\(^2\)

Let us now demonstrate that the present method is easily generalized to other types of leads such as \( N \)-leg ladder and carbon nanotube. Hereafter, we drop the lead index \( \alpha \) for simplicity. First, we calculate the self-energy of a lead of \( N \)-leg ladder (Fig.1):

\[ H_{\text{ladder}} = -t \sum_{x=0}^{\infty} \sum_{y=1}^{N} (|x + 1, y\rangle\langle x, y| + |x, y + 1\rangle\langle x, y| + \text{c.c.}) \tag{10} \]
We first diagonalize $H_{\text{ladder}}$ in the $y$ direction and obtain the conduction channels $\{\phi_j(y) | j = 1, 2, \ldots, N\}$, where

$$\phi_j(y) = \sin \frac{j\pi y}{N+1} \sqrt{\sum_{y''=1}^{N} \sin^2 \frac{j\pi y''}{N+1}}. \quad (11)$$

Each channel has the dispersion relation $E = -2t \cos k_j + \omega_j$, where $\omega_j \equiv -2t \cos(2\pi j/N)$.

Each channel yields its effective potential of the form Eq. (7), or

$$V_{\text{eff}}^{(j)}(E) = -te^{ik_j} = \frac{E - \omega_j - i\sqrt{4t^2 - (E - \omega_j)^2}}{2}. \quad (12)$$

The self-energy of $N$-leg ladder is given in the $N \times N$ matrix form

$$(\Sigma_{\text{ladder}}(E))_{y,y'} = \sum_{j=1}^{N} \phi_j(y)V_{\text{eff}}^{(j)}(E)\phi_j(y')^*. \quad (13)$$

The result is equivalent to the one obtained in Ref. 4.

Second, we calculate the self-energy of a lead of $(n,0)$ zigzag carbon nanotube attached to the conductor as in Fig. 2, where $n$ is the chiral number. The Schrödinger equation of the zigzag carbon nanotube $H_{\text{zigzag}}|\psi_{A/B}^{\pm}(k_j)\rangle = E|\psi_{A/B}^{\pm}(k_j)\rangle$ yields the dispersion relation of the $j$th channel as

$$E = \pm t |h_{k_j}| = \pm t \sqrt{1 + 4\cos \frac{\sqrt{3}k_j}{2} \cos \frac{\pi j}{n} + 4\cos^2 \frac{\pi j}{n}}, \quad (14)$$

with

$$h_{k_j} \equiv e^{ik_j} + 2 \cos \frac{\pi j}{n} e^{-ik_j} \quad (15)$$

where the first Brillouin zone is $|k_j| < \pi/\sqrt{3}$, and its wavefunction on the A and B sub-lattices as

$$\begin{align*}
\langle x, y | \psi_{A}^{\pm} (k_j) \rangle &= \pm \frac{h_{k_j}^*}{|h_{k_j}|} e^{ik_j x} \phi_j(y), \\
\langle x, y | \psi_{B}^{\pm} (k_j) \rangle &= e^{ik_j x} \phi_j(y),
\end{align*} \quad (16)$$

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\end{align*} \quad (16)$$
where \( \phi_j(y) \equiv e^{i \frac{2\pi j}{n} y / \sqrt{n}} \). The boundary conditions (16) transform the Schrödinger equation of the whole system

\[
\langle x = 0, y | H_c | \psi_B^\pm (k_j) \rangle - t \langle x = 1 / \sqrt{3}, y | \psi_A^\pm (k_j) \rangle = E \langle x = 0, y | \psi_B^\pm (k_j) \rangle
\]

(17)
to

\[
\langle x = 0, y | H_c | \psi_B^\pm (k_j) \rangle + V_{\text{zigzag}}^{(j;B)}(E) \langle x = 0, y | \psi_B^\pm (k_j) \rangle = E \langle x = 0, y | \psi_B^\pm (k_j) \rangle,
\]

(18)
where the effective potential of the \( j \)th channel is given by

\[
V_{\text{zigzag}}^{(j;B)}(E) \equiv \pm t e^{i \frac{\hbar k_j}{n}} \sqrt{3} \lambda_j \pm i \sqrt{2t \lambda_j} \left[ E^2 - t^2 - \lambda_j^2 \right] / 2E
\]

(19)
with \( \lambda_j \equiv 2t \cos \pi j / n \). Hence we obtain the self-energy of an \((n,0)\) carbon nanotube in the \( n \times n \) matrix form

\[
(\Sigma_{\text{zigzag}}(E))_{y_B,y'_B} = \sum_{j=1}^{n} \phi_j(y_B) V_{\text{zigzag}}^{(j;B)}(E) \phi_j(y'_B)^*,
\]

(21)
where \( y_A \) and \( y_B \) are coordinates on the A and B sub-lattices, respectively, which are indicated in Fig. 2. The result (21) is indeed equivalent to the one obtained in Ref. 6.

When the A sub-lattice, instead of the B sub-lattice, is in contact with the conductor, we obtain the self-energy in the form

\[
(\Sigma_{\text{zigzag}}(E))_{y_A,y'_A} = \sum_{j=1}^{n} \phi_j(y_A) V_{\text{zigzag}}^{(j;A)}(E) \phi_j(y'_A)^*,
\]

(22)
with

\[
V_{\text{zigzag}}^{(j;A)}(E) = \frac{E^2 - t^2 + \lambda_j^2 \pm i \sqrt{2t \lambda_j} \left[ E^2 - t^2 - \lambda_j^2 \right] / 2E}.
\]

(23)

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Fig. 2. A lead of the zigzag carbon nanotube. The upper and lower edges satisfy the periodic boundary conditions.
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