Transmission Coefficient as a
Three-Point Retarded Function

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Previously, we have described a formulation for the transmission probability of small interacting systems connected to noninteracting leads. Using the Kubo formula and a Eliashberg theory for the analytic continuation of vertex functions, the dc conductance g has been shown to be written in a Landauer-type form:

\[
g = \frac{(2e^2)}{h} \int d\epsilon \left(-\frac{\partial f}{\partial \epsilon}\right) \mathcal{T}(\epsilon),
\]

where \(f(\epsilon)\) is the Fermi function. In Ref. 1, we have provided the expression of the transmission probability \(\mathcal{T}(\epsilon)\) in terms of a vertex function eq. (2.36). Also, we gave another expression, eq. (3.6) in Ref. 1, which uses a three-point correlation function. Both of the two expressions have been obtained after carrying out the analytic continuation for the Matsubara frequencies.

The purpose of this short note is to show that \(\mathcal{T}(\epsilon)\) can also be expressed in terms of the retarded products of the three-point correlation function, and eq. (8) is the main result of this report. Since the retarded product is defined in the real time, it gives us direct information about the relationship between the transmission probability and dynamic correlation functions.

In the following, we will use the same notation with that in Ref. 1. A schematic picture of the system is illustrated in Fig. 1. The label 1 (N) is assigned to the localized state at the interface on the left (right), and the label 0 and N + 1 are assigned to the site at the reservoir-side of the interface. The inter-electron interaction is switched on only for the electrons inside the central region: the complete Hamiltonian \(H\) is given by eq. (2.1) of Ref. 1. The transmission probability of this system can be written as (see eq. (3.6) of Ref. 1)

\[
\mathcal{T}(\epsilon) = 2\Gamma_L(\epsilon) \Phi_{[2]}^{[2]}(\epsilon, \epsilon),
\]

where \(\Gamma_L(\epsilon) = \pi \rho_L(\epsilon) v_L^2\), \(\rho_L(\epsilon)\) is the local density of states at the site “0” in the left lead, and \(v_L\) is the mixing matrix element which connects the sample and the left lead. The three-point function \(\Phi_{[2]}^{[2]}(\epsilon, \epsilon + \omega)\) has been introduced using the imaginary-time formulation,

\[
\Phi_{R,11}(\tau; \tau_1, \tau_2) = \left\langle T_\tau J_R(\tau) c_{1\sigma}(\tau_1) c_{1\sigma}^+(\tau_2) \right\rangle,
\]

where \(J_R \equiv i \sum_{\nu, \nu'} \left\langle c_{N,1\sigma}^+ c_{N,\sigma} - c_{N,\sigma}^+ c_{N,1\sigma} \right\rangle\) is the current flowing through the right interface, \(J_R(\tau) = e^{\tau \mathcal{H}} J_R e^{-\tau \mathcal{H}}\), and \(c_{1\sigma}^+\) creates an electron with spin \(\sigma\) at the site “1” at the left interface. As a function of complex variables, \(\Phi_{R,11}(z, z + w)\) has singularities along the lines \(\text{Im}(z) = 0\) and \(\text{Im}(z + w) = 0\), which can be seen in eq. (6). These two singularities divide the complex z plane into three regions (see Fig. 2), in each of which \(\Phi_{R,11}(z, z + w)\) corresponds to the analytic function

\[
\begin{align*}
\Phi_{[1]}^{[2]}_{R,11}(\epsilon, \epsilon + \omega) &= \Phi_{R,11}(\epsilon + i0^+, \epsilon + \omega + i0^+), \\
\Phi_{[2]}^{[2]}_{R,11}(\epsilon, \epsilon + \omega) &= \Phi_{R,11}(\epsilon - i0^+, \epsilon + \omega + i0^+), \\
\Phi_{[3]}^{[2]}_{R,11}(\epsilon, \epsilon + \omega) &= \Phi_{R,11}(\epsilon - i0^+, \epsilon + \omega - i0^+).
\end{align*}
\]

Therefore it is the analytic continuation in the region [2], i.e., \(\Phi_{[2]}^{[2]}_{R,11}(\epsilon, \epsilon + \omega)\), that determines the transmission probability through eq. (2). The aim of this report is to present another approach to get this function starting from the real time without carrying out the analytic continuation. To this end, we consider the Lehmann representation for \(\Phi_{R,11}(i\epsilon, i\epsilon + iv)\). Inserting a complete set of the eigenstates satisfying \(\mathcal{H}\langle n \rangle = E_n \langle n \rangle\) into eq. (3), we have

\[
\Phi_{R,11}(i\epsilon, i\epsilon + iv) = \frac{1}{Z} \sum_{l,m} \langle l|c_{1\sigma}^\dagger|\epsilon\rangle \langle m|J_R|n\rangle \langle n|c_{1\sigma}|l\rangle \times \left[ e^{-\beta E_m} \left( e^{i\epsilon + iv + E_m - E_l} (i\epsilon + iv + E_m - E_l) \right) - \left( e^{i\epsilon + E_m - E_l} (i\epsilon + iv + E_m - E_l) \right) - \left( e^{i\epsilon + E_m - E_l} (i\epsilon + iv + E_m - E_l) \right) \right],
\]

where \(Z\) is the partition function.
where $Z = \text{Tr} e^{-\beta \mathcal{H}}$. From eq. (6), we can also obtain the Lehmann representation of $\Phi^{[k]}_{R;11}(\epsilon, \epsilon + \omega)$ for $k = 1, 2, 3$ by replacing the imaginary frequencies $\xi$ and $\imath \nu$ with the real ones $\epsilon$ and $\omega$, respectively, taking the infinitesimal imaginary parts summarized in the right-hand side of eq. (5) into account. Then, it is straightforward to show that the same analytic functions can be derived form the real-time functions defined by

$$
\Phi^{[1]}_{R;11}(t; t_1, t_2) = \theta(t - t_1) \theta(t_1 - t_2) \left\langle \left[ \left\{ c_{1\sigma}(t_1), c_{1\sigma}^\dagger(t_2) \right\}, J_R(t) \right] \right\rangle
+ \theta(t_1 - t) \theta(t_2 - t_2) \left\langle \left\{ c_{1\sigma}(t_1), \left\{ c_{1\sigma}(t_2), J_R(t) \right\} \right\rangle,
\right.
$$

$$
\Phi^{[2]}_{R;11}(t; t_1, t_2) = \theta(t - t_1) \theta(t_1 - t_2) \left\langle \left\{ c_{1\sigma}^\dagger(t_2), \left\{ c_{1\sigma}(t_1), J_R(t) \right\} \right\rangle
- \theta(t - t_2) \theta(t_2 - t_1) \left\langle \left\{ c_{1\sigma}(t_1), \left\{ c_{1\sigma}(t_2), J_R(t) \right\} \right\rangle,
\right.
$$

$$
\Phi^{[3]}_{R;11}(t; t_1, t_2) = -\theta(t - t_2) \theta(t_2 - t_1) \left\langle \left\{ c_{1\sigma}(t_1), c_{1\sigma}^\dagger(t_2) \right\}, J_R(t) \right\rangle
- \theta(t_2 - t) \theta(t - t_1) \left\langle \left\{ c_{1\sigma}^\dagger(t_2), \left\{ c_{1\sigma}(t_1), J_R(t) \right\} \right\rangle,
$$

through the Fourier transform

$$
\int_{-\infty}^{\infty} dt_1 dt_2 e^{i\omega t_1} e^{i\epsilon t_2} \Phi^{[k]}_{R;11}(t; t_1, t_2)
= 2\pi \delta(\epsilon + \omega - \epsilon') \Phi^{[k]}_{R;11}(\epsilon, \epsilon + \omega).
$$

Here $J_R(t) \equiv e^{i\mathcal{H}t} J_R e^{-i\mathcal{H}t}$ and $\theta(t)$ is the step function. The two types of the brackets denote the commutator $[A, B] \equiv AB - BA$, and the anticommutator $\{A, B\} \equiv AB + BA$. One can confirm the above statement about eqs. (7)–(9) by carrying out the integration in eq. (10) explicitly. For instance, the Fourier transform of a function

$$
F(t; t_1, t_2) = \theta(t - t_1) \theta(t_1 - t_2) \left\langle J_R(t) c_{1\sigma}(t_1) c_{1\sigma}^\dagger(t_2) \right\rangle
$$

can be calculated as

$$
F(\epsilon, \epsilon + \omega) = \frac{-1}{Z} \sum_{lmn} e^{-\beta E_m} \langle l|c_{1\sigma}^\dagger|m\rangle \langle m|J_R|n\rangle \langle n|c_{1\sigma}|l\rangle
\left(\omega + E_m - E_n + i0^+\right).
$$

Among the three real-time functions eqs. (7)–(9), only $\Phi^{[2]}_{R;11}(t; t_1, t_2)$ in eq. (8) is relating to the transmission probability: eqs. (7) and (9) are provided for comparison. Note that, in both of the two averages in the right-hand side of eq. (8), the commutator for one fermion operator and current $J_R$ is situated inside the anticommutator for another fermion operator.

In conclusion the three-point function $\Phi^{[2]}_{R;11}(\epsilon, \epsilon + \omega)$, which determines the transmission probability eq. (2), can be described as the Fourier transform of the real-time correlation function $\Phi^{[2]}_{R;11}(t; t_1, t_2)$ introduced in eq. (8). This real-time formulation seems to be applicable to non-perturbative approaches to the transmission probability $T(\epsilon)$ of correlated electron systems.

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Fig. 2. Three analytic regions of $\Phi_{R;11}(z, z + w)$.

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