Direct calculation of the nonequilibrium current by a recursive method

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The spatial distribution of the nonequilibrium current in a series of two point contacts under a finite bias voltage is investigated numerically making use of a recursive Green-function method based on the Keldysh formalism. The results of the current distribution show an interesting behavior such as the existence of vortices in between the two barriers. The temperature dependence of the nonlinear current-voltage characteristic is also studied. [S0163-1829(98)02216-4]

With advanced technology for the fabrication and the growth of high-mobility heterostructures, it becomes possible to create various structures on a nanometer scale, and nonlinear transport in mesoscopic systems becomes one of the problems of current interest. However, in spite of the importance of studying the nonlinear response, theoretical approaches seem still to be in a developmental stage because of the difficulty in treating the nonequilibrium quantum systems. Therefore, in order to obtain information about the underlying physics of the nonequilibrium systems, it seems quite important to examine and develop efficient numerical approaches. So far, we have studied the effects of Coulomb interaction on transport in the linear-response regime, making use of the recursive Green-function method. The purpose of this paper is to extend it for obtaining the spatial distribution of the nonequilibrium current based on the Keldysh formalism and show the numerical results. To this end, we apply the method to a series of two point contacts modeled on a two-dimensional tight-binding lattice, and examine the spatial distribution of the current and temperature dependence of the nonlinear current-voltage (I-V) characteristics. Specifically, in the present study we concentrate on a noninteracting case for simplicity. The effects of interaction within a mean-field level can be included in a straightforward way, as in the linear-response case.

We consider a quantum wire described by a two-dimensional tight-binding model the lattice sites of which are labeled with \((i,j)\). The wire is assumed to be infinitely long in the \(x\) direction, and finite in the \(y\) direction. Specifically, the system consists of three parts along the \(x\) direction: a finite central region at \(1 \leq i \leq N\), and two semi-infinite leads at \(-\infty < i \leq 0\) and \(N+1 \leq i < +\infty\). Along the \(y\) direction the system consists of \(M\) lattice sites, and we assume free boundary condition, i.e., the transfer integral which connects the sites at \(j=1\) and \(j=M\) is set to zero. The Hamiltonian is given by

\[
\mathcal{H} = -t \sum_{i} \sum_{j} (C_{i,j+1}^\dagger C_{i,j} + C_{i+1,j}^\dagger C_{i,j}) + \text{H.c.}
\]

\[
+ \sum_{i=1}^{N} \sum_{j=1}^{M} v_{i,j} C_{i,j}^\dagger C_{i,j} + \sum_{j=1}^{M} \Phi_{j} C_{i,j}^\dagger C_{i,j},
\]

where \(C_{i,j}^\dagger\) is the creation operator for an electron at the lattice site \((i,j)\), \(t\) is the nearest-neighbor transfer integral, and \(v_{i,j}\) is the on-site energy due to the impurities in the sample region. The last term appears when the bias voltage \(eV\) along the \(x\) direction is applied to the central region, and we assume the electrostatic potential to be \(\Phi_{j} = eV\) in the left lead, and \(\Phi_{j} = 0\) in the right lead. In the central region, for \(1 \leq i \leq N\), it is assumed to be \(\Phi_{j} = eV (N+1-i) / (N+1)\) if the electric field is uniform.

We now introduce three \(M \times M\) matrices \(G^+(i,i')\), \(G^-(i,i')\), and \(F(i,i')\) the elements of which are given by

\[
F_{j,j'}(i,i') = -i \int_{-\infty}^{\infty} dt' \langle \{C_{i,j}(t'), C_{i,j'}^\dagger(0)\} \rangle e^{i\omega t'},
\]

\[
G^+_{j,j'}(i,i') = -i \int_{-\infty}^{\infty} dt' \theta(t') \langle \{C_{i,j}(t'), C_{i,j'}^\dagger(0)\} \rangle e^{i\omega t'},
\]

\[
G^-_{j,j'}(i,i') = i \int_{-\infty}^{\infty} dt' \theta(-t') \langle \{C_{i,j}(t'), C_{i,j'}^\dagger(0)\} \rangle e^{i\omega t'}.
\]

Here \(C_{i,j}(t') = e^{i\omega t'} C_{i,j} e^{-i\omega t'}\), and the brackets and curly brackets denote the commutator and anticommutator, respectively. In the nonequilibrium Keldysh formalism, \(\langle \cdots \rangle\) denotes an average with respect to the density matrix at \(t' = 0\). Initially, at \(t' = -\infty\), the two leads and the sample at the center are not connected, and the left and right leads are in their own thermal equilibrium with the chemical potentials \(\mu_L\) and \(\mu_R\), respectively, with \(\mu_L = \mu_R + eV\). The time evolution of the density matrix is described by the adiabatic switching on of the hopping matrix element which connects the leads and the sample. The perturbation expansion for this type of the adiabatic switching-on can be written in a simplified form by using a matrix formulation. Specifically, in the present case, it is convenient to introduce \(2M \times 2M\) matrices \(\tilde{G}(i,i')\) and \(\tilde{T}\):

\[
\tilde{G}(i,i') = \begin{bmatrix} G^+(i,i') & G^-(i,i') \\ F(i,i') & \end{bmatrix}, \quad \tilde{T} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.
\]

In this representation the Dyson equation can be written as
\[ G(i,i') = G_0(i) \delta_{i,i'} - G_0(i) \mathcal{T} G(i+1,i') - G_0(i) \times \mathcal{T} G(i-1,i'). \] (6)

Here \( 1 \leq i, i' \leq N \), and \( G_0(i) \) is the Green function for the isolated column at \( x = i \). Thus, for instance, the intracolumn Green function \( G(i,i) \) can be obtained from a set of recursion formulas analogous to those for equilibrium systems,\(^6\)

\[ G(i,i) = [G_0(i)^{-1} - \mathcal{T} G_L(i-1) \mathcal{T} - \mathcal{T} G_R(i+1) \mathcal{T}]^{-1}, \] (7)

\[ G_L(i) = [G_0(i)^{-1} - \mathcal{T} G_L(i-1) \mathcal{T}]^{-1}, \] (8)

\[ G_R(i) = [G_0(i)^{-1} - \mathcal{T} G_R(i+1) \mathcal{T}]^{-1}. \] (9)

Here \( 1 \leq i \leq N \), and the boundary condition for the recursive relations Eqs. (8) and (9) are given at \( i = 1 \) and \( N \), respectively. At the boundary, \( G_L(0) \) and \( G_R(N+1) \) are given by the Green functions for the edge of the unconnected leads on the left and right, respectively, and those are written in the form of a partitioned matrix as Eq. (5). The off-diagonal \( M \times M \) parts, which correspond to \( G^{\pm} \) in Eq. (5), of \( G_L(0) \) and \( G_R(N+1) \), are given by the usual retarded (+) and advanced (-) Green functions, denoted hereafter by \( G^{\pm}_{L}(0) \) for the left lead and \( G^{\pm}_{R}(N+1) \) for the right lead. The remaining diagonal \( M \times M \) part for the left and right are given by \( F_L(0) = (1-2f_L)[G^+(0) - G^-(0)] \) and \( F_R(N+1) = (1-2f_R)[G^+(N+1) - G^-(N+1)] \), respectively. Here \( f_L = [e^{\beta v_H - \mu_H R}]^{-1} + 1 \), with \( \beta \) being the inverse temperature \( 1/T \), and thus it is this diagonal part that describes the initial condition of the density matrix for an unconnected lead. In contrast to these Green functions at the boundary, the diagonal part of the matrix for the isolated column \( G_0(i)^{-1} \) becomes zero, as in the case of the single-impurity Anderson model.\(^3\) Therefore, the distribution function which describes the initial condition for the sample disappears, and the averages of physical quantities are independent of it.\(^5\)

In the above the recursive relations are written in terms of the partitioned matrices in Eqs. (7)-(9) explicitly:

\[ G^+(i) = [G_0(i)^{-1} - \int^2 G^+_R(i-1)]^{-1}, \] (10)

\[ G^-(i) = [G_0(i)^{-1} - \int^2 G^+_R(i+1)]^{-1}, \] (11)

\[ F_L(i) = \int^2 G_L^+(i) F_L(i-1) G_L^-(i), \] (12)

\[ F_R(i) = \int^2 G_R^+(i) F_R(i+1) G_R^-(i). \] (13)

\[ G^\pm(i,i) = [G_0(i)^{-1} - \int^2 G^+_R(i-1) - \int^2 G^+_R(i+1)]^{-1}, \] (14)

\[ F(i,i) = \int^2 G^+(i,i)[F_L(i-1) + F_R(i+1)] G^-(i,i). \] (15)

Here \( G_0(i)^{-1} \) is the off-diagonal part of \( G_0(i)^{-1} \), with \( H_0(i) \) being the Hamiltonian for the isolated \( i \)-th column. Similarly, the intercolumn Green functions can be obtained through the relations \( \hat{G}(i,i+1) = -\hat{G}(i,i) \mathcal{T} G_R(i+1) \) and \( \hat{G}(i,i-1) = -\hat{G}(i,i) \mathcal{T} G_L(i-1) \):

\[ G^+(i,i+1) = -\int^2 G^+(i,i) G^+_R(i+1), \] (16)

\[ G^-(i,i-1) = -\int^2 G^+(i,i) G^+_L(i-1), \] (17)

\[ F(i,i+1) = -\int^2 \{G^+(i,i) F_R(i+1) + F(i,i) G_R(i+1)\}, \] (18)

\[ F(i,i-1) = -\int^2 \{G^+(i,i) F_L(i-1) + F(i,i) G_L(i-1)\}. \] (19)

The local current in the sample can be written in terms of the intercolumn Green functions\(^8\)

\[ I_{ij} = e \int \frac{d\omega}{2\pi} \frac{1}{2} \{F_{j,j}(i,i+1) - F_{j,j}(i+1,i)\}, \] (20)

\[ I'_{ij} = e \int \frac{d\omega}{2\pi} \frac{1}{2} \{F_{j,j+1}(i,i) - F_{j,j+1}(i+1,i)\}. \] (21)

In particular, the total current flowing along the direction of the applied field, \( I_{tot} = \sum_{j} I'_{ij} \), can be expressed only in terms of the retarded and advanced Green functions\(^1,2,8,9\)

\[ I_{tot} = e \int d\omega \langle f_L - f_R \rangle \text{Tr}[\Gamma_L G^+(1,N) \Gamma_R G^-(N,1)], \] (22)

where \( \text{Tr} \) denotes the trace for \( M \times M \) matrices, \( \Gamma_L = i\tau [G^{-}\Gamma(0) - G^{+}\Gamma(0)] \), and \( \Gamma_R = i\tau [G^{-}\Gamma(N+1) - G^{+}\Gamma(N+1)] \). Therefore, the total current can be obtained without a knowledge of \( F(i,i') \). Note that at \( T = 0 \) the integration region of Eq. (22) is restricted to be \( \mu_R < \omega < \mu_R + eV \).

We now present numerical results. In what follows, we take the transfer integral \( t \) as a unit of energy. For computing the nonequilibrium current, the integral in Eqs. (20)-(22) is replaced by Simpson’s sum, and the mesh is taken to be typically \( \Delta \omega = 10^{-5} \). As an example, we consider the current through a series of two point contacts, which is modeled by arranging the values of \( \sigma_{ij} \). To be specific, we introduce a system with \( N = 28 \) and \( M = 20 \), and choose the on-site potential to be finite, \( \sigma_{ij} = 1.0 \), for the sites which constitute the two point contacts, i.e., all the sites on the column \( i = 6, 7, 22, \) and 23, except those on the row \( j = 9, 10, 11, \) and 12 (see the inset of Figs. 1 and 4). We apply the electric field only to the region in between the two point contacts, choosing the electrostatic potential as \( \Phi_s = eV \) for \( i = 5, \Phi_s = 0 \) for \( i \geq 24 \), and \( \Phi_s = eV (24 - i)/19 \) for \( 6 \leq i < 23 \). Note that the two leads and the central region are connected at \( i = 0 \) and 29. This choice enable us to compute the current distribution outside the potential barriers in a simple way, and the total current is independent of the choice of the position of the connections.

In Fig. 1, the total current in the case of \( eV = 0.001 \) is shown as a function of \( \mu_R \) for several temperatures. Here \( \mu_R \) is measured from \( -4t \), i.e., the energy corresponding to the bottom of the conduction band for an infinitely large square lattice is taken to be the origin. In this case, the applied voltage is small, so that the number of electrons contributing
to the current increases linearly. At $T=0$ there are many peaks of the resonant tunneling. These peaks are broadened with increasing temperatures. In order to examine the effect of the bias voltage, we have also plotted the total current at $T=0$ for several values of $eV$ in Fig. 2. As the bias voltage is increased, the total current increases and peaks become broader. This is because many resonant states exist in the energy spectrum between $\mu_R$ and $\mu_R + eV$, and thus the current becomes less sensitive to the change of $\mu_R$. This feature somewhat resembles the temperature dependence shown in Fig. 1. However, a characteristic behavior is seen in the bias dependence, typically, around $\mu_R = 0.05$ in Fig. 1. A peak seen in the curve for $eV = 0.001$ becomes broader with a trapezoidal shape when $eV$ is increased slightly (see the case $eV = 0.05$). This type of behavior is seen when a single resonant level exists in the region $\mu_R < \omega < \mu_R + eV$, and the shape disappears gradually when $eV$ is increased sufficiently that a number of resonant levels can contribute to the current (see the case $eV = 0.5$). We have also plotted the temperature dependence of the nonlinear $I$-$V$ characteristic in Fig. 3, setting $\mu_R = 0.05$. At $T=0$, many peaks which reflect local levels are seen, and these peaks become broader as temperature increases. Note that the total current remains finite even for $eV \approx 4.0$, owing to the intersubband scattering by the barriers.

We next examine the current distribution. Specifically, we set $\mu_R$ to be 0.055. The corresponding wavelength is estimated about 35 in units of the lattice constant, and the resonance occurs for small $eV$ (see Fig. 2). Figure 4(a) shows the...
results in a linear-response regime \((eV = 0.001)\). In this case, the current flowing through the point contact on the left is spread gradually till the center of the sample, and then focused at the point contact on the right. This feature may be determined by a standing wave due to the resonance, and the half-wavelength agrees with the distance of the two contacts, which is about 17 in units of the lattice constant. We have also examined the case \(eV = 0.5\) where the \(I-V\) characteristic is nonlinear, and the results are shown in Fig. 4(b). The current distribution becomes complicated compared to Fig. 4(a). In particular, there are vortices near the potential barrier on the right. The complicated structure of the current distribution in the nonlinear regime is realized as a result of the contributions of a large number of resonant levels.

In summary, we have studied the nonequilibrium current distribution and the temperature dependence of the nonlinear \(I-V\) characteristics in a series of two point contacts, and have found an interesting behavior such as the existence of vortices. To obtain the numerical results, we have used the recursive method for the Keldysh Green function. This method can be used for investigating the effects of a magnetic field, a disorder, etc., and may also be used for computing the current noise. The behavior of the vortices under a finite magnetic field is currently being studied and will be discussed elsewhere.

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9. We note, as for the total current, the similar method was examined by P. Lake, G. Klimeck, R. C. Bowen, and D. Jovanovic, J. Appl. Phys. 81, 7845 (1997).