Self-similarity of single-channel transmission for electron transport in nanowires

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We demonstrate that the single-channel transmission in the resonance tunneling regime exhibits self-similarity as a function of the nanowire length and the energy of incident electrons. The self-similarity is used to design the nonlinear transformation of the nanowire length and energy which, on the basis of known values of transmission for a certain region on the energy-length plane, yields transmissions for other regions on this plane. Test calculations with a one-dimensional tight-binding model illustrate the described transformations. Density function theory based transport calculations of Na atomic wires confirm the existence of the self-similarity in the transmission.

I. INTRODUCTION

When a nanowire is attached to two electron reservoirs with different chemical potentials, the electric current flows through it. Studies of the electrical conductance at the nanoscale have resulted in discoveries of interesting physical effects, which include conductance quantization, molecular rectification, negative differential resistance, hysteresis, oscillatory length-dependence of the conductance. These and other unusual and potentially useful properties make nanowires promising candidates for creating various electronic nanodevices.

Electrical conduction in nanowires can be approximated under certain conditions as a ballistic scattering of electrons along the one-dimensional quasiperiodic superlattice of finite length. Since the first fabrication of quasiperiodic GaAs-AlAs multilayer structure propagation of elementary excitations (electrons, photons, polaritons, spin waves) through one-dimensional fractal structures has been extensively studied. It has been demonstrated, in particular, that the quasi-periodic structure of the medium manifests itself in the self-similarity of the transmission. The Landauer conductance of the generalized Thue-Morse and Fibonacci one-dimensional lattices has also been investigated. In addition, the fractal conductance fluctuations have been predicted and measured in two-dimensional electronic billiards in magnetic fields. If the system has a quasiperiodic structure and consists of a number of identical or similar scattering blocks, the transmission through a single block can be mapped into the transmission through the entire system. This is the central idea behind several powerful approaches to the calculation of transmission through quasiperiodic structures, those like transfer matrix and Dyson-equation. The aim of our paper is to explore the possibility of the self-similarity for single-channel transmission for electron transport in nanowires.

We demonstrate that a single-channel transmission in the resonance scattering regime exhibits self-similarity as a function of the incident electron energy and the nanowire length. We use one-dimensional tight-binding model with nearest-neighbor hopping and Landauer theory to explain the self-similarity of the transmission coefficient for electron transport in nanowires. Based upon

II. SELF-SIMILARITY OF TRANSMISSION

To describe a nanowire of length \( N \), we adopt the standard tight-binding model with the nearest neighbor constant hopping rate \( V \) and the site energy \( E_0 \). The system Hamiltonian is thus described by the three-diagonal \( N \times N \) matrix:

\[
H = \begin{bmatrix}
E_0 & V & 0 & 0 & 0 & 0 \\
V & E_0 & V & 0 & 0 & 0 \\
0 & V & E_0 & V & 0 & 0 \\
0 & 0 & . & . & . & 0 \\
0 & 0 & 0 & . & . & 0 \\
0 & 0 & 0 & 0 & V & E_0 \\
0 & 0 & 0 & 0 & 0 & V & E_0
\end{bmatrix}.
\]

The interaction between the wire and the leads is not considered explicitly and is accounted for by the introduction of the self-energy matrix, \( \Sigma(E) \), into the wire Green’s function,

\[
G(E) = [E - H - \Sigma(E)]^{-1}.
\]

Assuming that the molecule is connected to the left (right) lead through its 1(\( N \))th sites, the transmission is determined by the 1\( \times N \) element of the Green’s function

\[
T(E) = 4\Delta^2(E)|G_{1N}(E)|^2,
\]

where \( \Delta(E) \) is the imaginary part of the self-energy function

\[
\Sigma(E) = \Lambda(E) - i\Delta(E).
\]
The conductance at low temperature and small voltage is given (in units of $e^2/\pi \hbar$) by the Landauer formula

$$g = T(E_F),$$

(5)

$E_F$ being the Fermi-energy of the electrodes.

The matrix element of the molecular Green’s function $G_{1N}(E)$ can be analytically computed for our model Hamiltonian. To simplify the presentation, we define the self-energy within the broadband approximation assuming that $\Lambda = 0$ in eq. (4) and considering $\Delta$ as an energy-independent constant. The assumption can be relaxed and its consequences are discussed later.

The analytical calculations yield the following expression for the transmission:

$$T(E) = 4\xi^2 \left| \frac{\sin \theta}{\sin((N + 1)\theta) + 2i\xi \sin(N\theta) - \xi^2 \sin((N - 1)\theta)} \right|^2.$$  

(6)

where we have introduced the dimensionless quantities

$$\cos \theta = \frac{E - E_0}{2V}, \quad \xi = \frac{\Delta}{V}.  \tag{7}$$

If $|E - E_0| > 1$, then the trigonometric function in eq. (7) are transformed into the corresponding hyperbolic functions. This results in the exponential scaling of the transmission with the nanowire length $N$. If $|E - E_0| \leq 1$, then eq. (7) describes the resonance tunneling regime where the transmission oscillates as a function of the nanowire length $N$. Oscillatory regime is the intrinsic property of the single channel atomic nanowires such as Au and Na, to which the one-dimensional tight-binding Hamiltonian is applicable. Therefore we restrict our consideration to this regime and demonstrate that the transmission exhibits scaling and self-similarity.

Suppose that the coupling between the wire and the lead is weak, i.e. $\xi < 1$. The transmission $T(E) \sim \xi^2 + O(\xi^4)$ is very small for $\xi \ll 1$ unless $\sin((N + 1)\theta)$ in the denominator of eq. (7) tends to zero. If we put $\sin((N + 1)\theta) = 0$, which is equivalent to assuming that

$$\theta_k = \frac{\pi k}{N + 1}, \quad E_k = E_0 + 2V \cos \theta_k, \quad k = 1, 2, ..., N$$

then the transmission achieves its maximum

$$T(E_k) = \frac{1}{1 + \xi^2 \cos^2 \theta_k}.$$  

(9)

For any given length of the wire there are $N$ different resonances in the transmission. The resonance label $k$ in eqs. (8) can be interpreted as the number of the transmission maxima achieved for the given molecular length $N$ within the energy interval $[E_k, E_0 + 2V]$.

The resonance condition suggests the existence of the self-similarity of the transmission $T(E)$ as we vary the nanowire length $N$ and energy $E$ of transmitted electrons. Indeed, the following simple linear transformation

$$\tilde{N} = j(N + 1) - 1,$$  

(10)

leaves the resonance condition unaffected, thereby preserving the number of resonances of the transmission by deforming the energy interval. The mapping parameter $j = (N + 1)/(N + 1)$ is not, in general, an integral but a rational number. If the angles $\theta$ and $\tilde{\theta}$ are expressed explicitly in terms of the corresponding energies $E$ and $\tilde{E}$ via eq. (7), then the transformation becomes nonlinear:

$$\tilde{E} = E_0 + 2V \cos(\arccos \left( \frac{E - E_0}{2V} \right)/j), \quad j > 1.$$  

(12)

The transformation leads to the self-similarity of transmission at $[\tilde{E}, E_0 + 2V]$ and $[E, E_0 + 2V]$ energy intervals: the wire of the length $\tilde{N}$ within the interval $[\tilde{E}, E_0 + 2V]$ has exactly the same number $k$ of the transmission maxima as the wire of the length $N$ within the interval $[E, E_0 + 2V]$. Furthermore, consider the transmission $T(E)$ of a wire of the length $N$ when the energy of incident electrons varies within the range $[E_1, E_2]$. Then $T(E)$ can be mapped into $\tilde{T}(E)$ for any $\tilde{N} > N$ within the window $[\tilde{E}_1, \tilde{E}_2]$, provided that $j$ is defined via eq. (11). The number and positions of the conductance peaks for $T(E)$ within $[E_1, E_2]$ will be exactly the same as that of $\tilde{T}(E)$ within $[\tilde{E}_1, \tilde{E}_2]$.

III. EXAMPLE CALCULATIONS

A. Numerical calculations with one-dimensional tight-binding model

We confirm the existence of the self-similarity of a single-channel transmission by numerical calculations via eq. (12). The computations are performed for $E_0 = 0$ eV, $V = 2.5$ eV and $\xi = 0.04$. Several illustrative results are presented in Fig. 1 for rational mapping parameters $j$. The transmission $T(E)$ is computed within the energy intervals...
Thus, the higher is $N$ the nearest-neighbor basis functions overlap significantly, and the definition of the Green’s function (2) remains valid, but the definition of the non-equilibrium Green’s function (12) in the energy domain should be modified to account for the basis nonorthogonality:

$$E = \frac{E_0 + 2V \cos(\arccos \left( \frac{E - E_0}{2(V - E\lambda)} \right)}{1 + 2\lambda \cos(\arccos \left( \frac{E - E_0}{2(V - E\lambda)} \right))}, \ j > 1. \quad (17)$$

If $\lambda = 0$, then the transformations (12) and (17) coincide, evidently. If $\lambda \neq 0$, the non-orthogonality of the basis functions causes, through the (energy-dependent) scaling factor $(1 + 2\lambda \cos(\theta/j))^{-1}$, an additional stretching (shrinking) in the energy space, depending on whether the product $\lambda \cos(\theta/j)$ is negative (positive). For example, if we assume that the overlap parameter $\lambda = 0.2$ and plot the transmissions analogies to those in Fig. 1, we obtain exactly the same curves. However, according to eqs. (10) and (14), the energy intervals will shrink (we use eV units for energy $E$): $1.34 \leq E \leq 3.31$ for $N = 21$, $2.73 \leq E \leq 3.47$ for $N = 34$, and $3.49 \leq E \leq 3.56$ for $N = 107$. On the contrary, if we put $\lambda = -0.2$ (this is equivalent to the consideration of $T(-E)$ for $\lambda = 0.2$) and plot the same transmissions, the corresponding energy intervals will stretch as compared with those in Fig. 1: $1.70 \leq E \leq 7.03$ for $N = 21$, $4.86 \leq E \leq 7.79$ for $N = 34$, and $7.88 \leq E \leq 8.27$ for $N = 107$.

**B. First principle simulations for sodium nanowires**

In this section, we examine the prediction of transmission self-similarity by performing the first principle simulations of transport properties of Na atomic wires. The calculations were performed using our plane wave/pseudopotential implementation of the density functional based non-equilibrium Green’s function.
Our implementation is based on nonorthogonal Wannier-type atomic orbitals. All systems were treated employing periodic boundary conditions and the Kohn-Sham orbitals were expanded in plane waves (50 Ry cutoff) at the Γ point of the Brillouin zone. We used local density approximation for the exchange-correlation functional and Stumpf, Gonze, and Schettler pseudopotentials for core electrons. The system is treated as a “supermolecule” placed in a large supercell. The size of supercell is chosen in such a way that the distance between the nearest atoms in the neighboring cells is larger than 8.5Å, so that the interaction between supercell images is negligible. The whole system is divided into three parts: left electrode, central wire, and right electrode. The electrode part is obtained by cutting a few atoms from Na (001) surface. The geometry of the electrodes is fixed to the bulk values. The wire part is a single chain of Na atoms, where the distance between the atoms is constrained to the nearest neighbor distance in the bulk system. The distance between the electrode part and the wire part is optimized.

The results of our first principle transport calculations are illustrated by Figs. 2. Figs. 2a and 2b depict the transmission calculated for Na nanowire with \( N = 3 \) and \( N = 5 \), respectively. Figs. 2c and 2d show zoomed portions of Figs. 2a and 2b, which are seen to exhibit quite a good resemblance.

To link these calculations to the theory developed in the paper, the parameters of the tight-binding molecular Hamiltonian \( \mathbf{H} \), the self-energy matrix \( \Sigma(E) \) and the overlap matrix \( \mathbf{S} \) were extracted from the first principle transport calculations. Since we use nonorthogonal basis set, the Green’s function should be taken in the form \( \langle \mathbf{1} \rangle \) which accounts for the overlap matrix \( \mathbf{S} \) between Wannier type atomic orbitals. The calculated molecular Hamiltonian and overlap matrix are described fairly well by the three-diagonal matrices \( \langle \mathbf{11} \rangle \) and \( \langle \mathbf{15} \rangle \), respectively, with the parameters \( E_0 = -2.88 \text{ eV}, V = 1.25 \text{ eV}, \) and \( \lambda = -0.28 \). If we insert these parameters into eqs. \( \langle \mathbf{10} \rangle \) and \( \langle \mathbf{17} \rangle \), then the energy window \([ -0.56, 0] \) for \( N = 3 \) will be mapped into \([ -0.57, -0.35] \) for \( N = 5 \). This correlates reasonably well with the actual window \([ -0.64, -0.35] \). Of course, the calculated \( \mathbf{H} \) and \( \mathbf{S} \) matrices comply with simple three-diagonal formulas \( \langle \mathbf{11} \rangle \) and \( \langle \mathbf{15} \rangle \) only approximately, and the actual self-energy function \( \Sigma(E) = \Lambda(E) - i\Delta(E) \) is neither purely imaginary, nor energy independent. Evidently, the presence of \( \Lambda(E) \neq 0 \) causes an additional shift of transmission maxima, and \( \Sigma(E) \) brings an additional energy dependence of \( T(E) \) which has not been taken into account within the present theoretical analyses. If, however, \( \Sigma(E) \) does not change significantly within the interval \([ E_1 < E < E_2 ] \), then the self-similarity in \( T(E) \) should be preserved, as is proven by Figs. 2c and 2d.

FIG. 2: First principle simulations for Na nanowire. Transmissions calculated for \( N = 3 \) and \( N = 5 \) are presented in Figs. (a) and (b), respectively. Fig. (c) depicts a portion of Fig. (a) at the energy interval \([ -0.56, 0] \), and Fig. (d) shows a part of Fig. (b) at the interval \([ -0.64, -0.35] \). The Fermi energy is set to zero.

### IV. DISCUSSION AND OUTLOOK

In this paper, we have demonstrated that a single-channel transmission for electron transport in nanowires exhibits the self-similarity in resonance tunneling regime. Starting from the resonance condition, we proposed the transformation of the wire length and the incident electron energy, which preserves the number of maxima in the transmission. A sample calculations on one-dimensional tight binding model produces exact agreement with analytical results. The density functional based transport calculations of Na atomic wires confirm the existence of self-similarity in the transmission for realistic system.

The existence of scaling properties and self-similarity of the molecular transmission is also supported by a possibility to define it via the Friedel sum rule. It is not necessary to have a detailed information on a large variety of the parameters describing the molecule and the leads to predict transport properties of a single channel conductor. To compute the single-channel conductance by the Friedel sum rule, it is sufficient to know only the difference between the number of electrons occupying the even and the odd eigensates of the molecule.

It is thus not very unrealistic to suggest that the self-similarity in molecular transmission and conductance may be a rather general phenomenon. In terms of possible applications, our results suggest that the transmission, computed within a certain energy and length window, can be transferred to other windows via the transformation \( \langle \mathbf{10} \rangle, \langle \mathbf{12} \rangle, \langle \mathbf{17} \rangle \). For example, the transmission of a short wire within a relatively wide energy window can be mapped into the transmission of a longer wire.
within a narrower energy window. If we assume, additionally, that the site energy \( E_0 \) can be purposefully modified\(^{34,35}\), then the molecular conductance \( g \), eq. (5), becomes a function of the (modified) site energy \( E_0 \) and molecular length \( N \) and also exhibits the self-similarity.

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