MODELLING OF QUANTUM MECHANICAL DEVICES BY GREEN'S FUNCTION TECHNIQUE*

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In the paper we show that for detailed treatment of small devices by the Green's function technique the self-energies due to the leads should be considered for both extended and localized states.

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1. Introduction: the Green's function technique

It is known that the quantity which describes well transport properties of the quantum mechanical device is the Green's function corresponding to device Hamiltonian. In the notation of Tight-Binding Hamiltonian (TBH)

$$H = \sum_i |i\rangle \varepsilon_i \langle i| - \sum_{i,j} |i\rangle t \langle j| \ , \tag{1}$$

where the second sum runs only over nearest neighbor (n.n.) sites i, j. The Green's function becomes a matrix

$$[G] = (z[I] - [H])^{-1} \tag{2}$$

with elements $[G]_{ij}(z)$ which describe response at site i due to excitation in site j. In the above, $z = E + i\eta$ is the complex variable and $[I]$ is the identity matrix. The matrix $[G]$ has poles at the positions of discrete (real) eigenvalues E_{p} of the Hamiltonian [1]. The residua at these poles provide information about corresponding localized eigenstates, $\mathrm{res}[G]_{ij}(z = E_n) = \sum_k \phi_k(i)\, \phi_k^*(j)$, where the summation is over all degenerate eigenfunctions

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ϕ_k with energy E_p. The situation is quite different for energies from the continuous spectrum of H. In this case the Green's function is not well defined. For such energies the retarded Green's function is defined by the limiting procedure $[G^\mathrm{R}]_{ij}(E) = \lim_{\eta\to 0^+}[G]_{ij}(z)$, and the quantity

$$-\frac{1}{\pi}\mathrm{Im}\left\{\left[G^\mathrm{R}\right]_{ii}(E)\right\} = [\rho]_i(E) \tag{3}$$

is the local density of (extended) states (DOS) per unit volume.

When making use of Eq. (2) the problem of infinite-dimensional matrices emerges. This is because of the leads which should be considered as stretching out to infinity. Otherwise we would deal with closed system with no transport at all. The solution of this "infinite dimensional" problem is described in the book of Datta [2]. It is that

$$[G] = (z[I] - [H_\mathrm{D}] - [\Sigma_\mathrm{DL1}] - [\Sigma_\mathrm{DL2}])^{-1}\,, \tag{4}$$

where $[H_\mathrm{D}]$ is the Hamiltonian of isolated device whereas $[\Sigma_\mathrm{DL1}]$ and $[\Sigma_\mathrm{DL2}]$ describe the interactions between device and leads 1 and 2 respectively. They are called the self-energies due to the leads. Their elements can be expressed in terms of the Green's function of isolated semi-infinite lead $[G_\mathrm{L}]$. What is important, the only matrix elements of $[G_\mathrm{L}]$ involved in the calculation of $[\Sigma_\mathrm{DL}]$ are those between sites l_i, l_j in the lead which are adjacent to the sites i, j in the device

$$[\Sigma_\mathrm{DL}]_{i,j} \equiv t^2[G_\mathrm{L}]_{l_i,l_j}\,, \quad \text{where } l_i, l_j \text{ are n.n. of } i, j\,. \tag{5}$$

This makes calculations of self-energy possible because all the matrices in Eq. (4) are of size $M \times L$ for a device which is M sites wide and L sites long.

2. Self-energy due to the leads

To calculate the self-energy $[\Sigma_\mathrm{DL}]$ one needs the Green's function of the lead. These leads usually take the form of multi-moded quasi one dimensional semi-infinite wires. In 2-D such a wire stretches from $x = -\infty$ to $x = 0$ and is M sites wide. If we assume $\varepsilon_i = 0$ for all site energies in the lead then the transverse components of the wave functions χ_m and corresponding eigenenergies E_m, $m = 1, 2, ...M$ can be found easily. The retarded Green's function is then [2,3].

$$\left[G^\mathrm{R}\right]_{l_i,l_j}(E) = -\frac{1}{t}\sum_m \chi_m(l_i)\,\chi_m(l_j)\exp(ik_m a)\,, \tag{6}$$

where $\cos(k_m a) = q \equiv -(E - E_m)/2t$, a is the site separation. The above relation holds only for modes m with eigenenergies E_m that lie within the

range $E - 2t < E_m < E + 2t$. For each such a mode the longitudinal component of the energy $E - E_m$ lies within the band of extended states. Thus Eq. (6) describes the propagation of extended states in the lead. For energies from outside the band of extended states of mode m *i.e.* for $|E - E_m| > 2t$ we have [1]

$$[G]_{l_i,l_j}(E) = -\frac{1}{t}\sum_m \chi_m(l_i)\,\chi_m(l_j)\left(q \pm \sqrt{q^2-1}\right), \tag{7}$$

where the signs $+/-$ correspond to $E < E_m - 2t$ or $E > E_m + 2t$, respectively. Eq. (7) describes the "propagation" of localized states in the lead.

Let us notice that usually the only self-energies included when analyzing transport through a device are those of Eq. (6) which describe propagating states. For detailed treatment of the problem this is, however, not sufficient since the contributions arising from Eq. (7) also influence the Green's function in Eq. (4). In the next section we prove this presenting the results of numerical calculations performed for a simple scattering device.

3. An example: a single site scatterer

To illustrate the statement made in of the previous section we have performed numerical calculations of a simple scattering device. The dimensions were chosen $M = 3$ and $L = 3$ (short device) or $M = 3$ and $L = 11$ (long device). All but one device sites have energies $\varepsilon_i = 0$. The only exception was the impurity site l in the centre of device, which energy was set to $\varepsilon_l = -t$. Note that if we consider the whole "device + leads" system both devices are identical: it is infinite, 3 moded strip with one impurity site in the middle of its width. Thus we expect that calculations give identical results for both short and long device provided the self-energy approach works well.

It is well known that single site impurity works as scattering centre and produce one localized state at some energy E_p below (for $\varepsilon_l < 0$) the band and extended, resonant state at some energy E_r within the band. The state below the band introduces a pole into the Green's function at $z = E_\mathrm{p}$. The squared eigenfunction corresponding to this state can be obtained as the residue at this pole. It is shown in Fig. 1(a) where the results of numerical calculations are presented. We can see that the data for long and short devices coincides well so we conclude that including self-energies due to the leads for both extended and localized states properly describes the interactions between the device and the leads for energies from outside the band.

The next test checks how the self-energy approach works for energies from the band. In Fig. 2(a) a sample DOS calculated at the impurity site l is shown. The state below the band appears as a δ function located at energy E_p. Inside the band one can recognize a typical M-mode quasi 1-D DOS

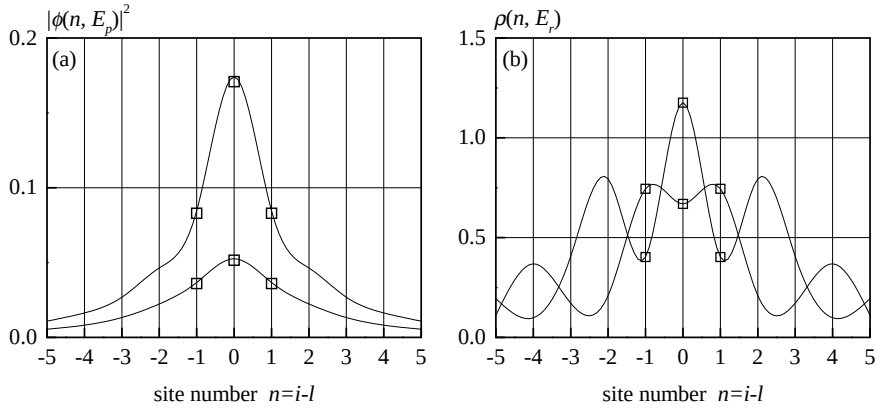

Fig. 1. The shape of (a) localized eigenstate at $E_\mathrm{p} \simeq -3.49t$ (b) DOS at resonant state at $E_\mathrm{r} \simeq -0.65t$ along the x direction of the scattering device. In both figures lines refer to the long device of $L = 11$ sites and squares are for the short device of $L = 3$ sites. The width of the devices in the y direction was $M = 3$ sites. Upper line is the cross-section in the plane $y = 0$. The lower one is for $y = \pm a$. The impurity site was at $x = 0$, $y = 0$.

perturbed by the resonant state at E_r. The excellent agreement between the results of calculations for long and short devices is evident. Now we conclude that when both types of self-energies are taken into account the interaction between device and the lead is well described for extended states from the band. This conclusion can be also derived from Fig. 1(b) where DOS at $E = E_\mathrm{r}$ is shown. Again excellent agreement between the calculations for long and short devices is observed.

For TBH it is required for every site n that

$$a^2 \int_{-\infty}^{+\infty} [\rho]_n(E)dE = 1\,. \tag{8}$$

The scattering device we are dealing with contains one discrete eigenstate below the band and so the above equation could be rewritten as

$$a^2 \left(\mathrm{res}\,[G]_{n,n}\,(z = E_\mathrm{p}) + \int_{E_\mathrm{L}}^{E_\mathrm{U}} -\frac{1}{\pi}\mathrm{Im}\left[G^\mathrm{R}\right]_{n,n}(E)dE \right) = 1\,, \tag{9}$$

where E_L and E_U are the lower and upper band edges. The first term in this sum has been calculated already in our first test, where the squared wave function for energy E_p below the band has been found (see Fig. 1(a)).

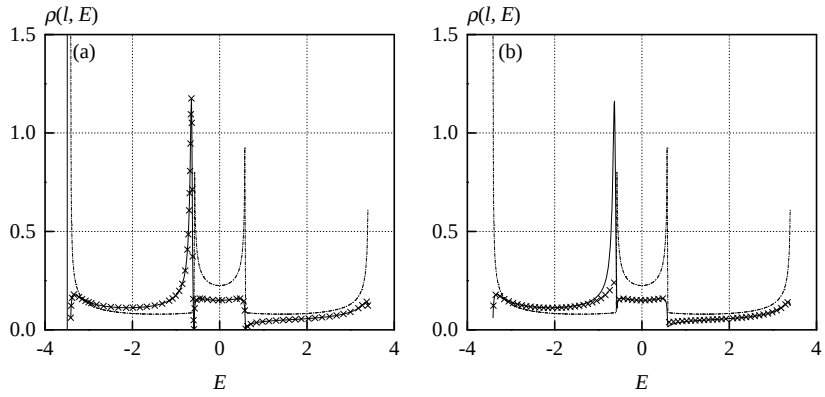

Fig. 2. The local DOS at impurity site l of the scattering device (see text) calculated with self-energies due to the leads for (a) both extended and localized states of Eqs. (6) and (7) (b) only extended states of Eq. (6). Solid line/crosses refer to long/short device. The sharp peak at low energies is δ function located at energy $E_{\rm p}$ of the localized state. The peak in the middle of the band corresponds to resonant state of energy $E_{\rm r}$. For comparison DOS of the system with no impurities (*i.e.* for perfect 3 moded 1-D strip) is shown as the dashed line.

To complete the balance we have integrated the local DOS (such as those in Fig. 2(a)) over all energies at every point n of the device. For each site the integration gives the value 1 ± 0.001 in excellent agreement with Eq. (9). We may conclude that including both types of self-energy does not violate the balance of Eq. (8).

Let us notice, however, that if the (real) self-energies of Eq. (7) were not included the contribution $\mathrm{res}[G]_{n,n}\,(z = E_{\rm p})$ in Eq. (9) coming from the localized state at $E_{\rm p}$ would have been omitted and the balance of Eq. (8) would have been violated! In Table I we summarize the integrated DOS of the short device for which the interaction with the leads was introduced only by the complex self-energies given by Eq. (6). Indeed, one can see from Table I that in this case the balance of Eq. (8) is broken for all sites of the device.

TABLE I

The integrated DOS at sites in the position $x = ia$, $y = ja$. In the calculations of the Green's function in Eq. (4) only complex self-energies given by Eq. (6) were included.

	$j=-1$	$j=0$	$j=1$
$i=-1$	0.908	0.891	0.908
$i=0$	0.888	0.752	0.888
$i=1$	0.908	0.891	0.908

This is even better noticeable in Fig. 2(b) where the DOS calculated with only complex self-energy terms of Eq. (6) included in the calculations of Green's function are shown. Large discrepancies between DOS for long and short devices are observed in some range of energies especially near the resonant state. We conclude that omitting the real terms of self-energy due to the leads given by Eq. (7) not only neglects the (localized) states below the band but also gives incorrect DOS. This is important for example in the case when Coulomb interactions must be included in the analysis. In this case the charge of electrons is calculated by integrating DOS up to the Fermi level.

4. Conclusions

The interactions between device and leads can be formulated in terms of self-energies included into Green's function. These self-energies are complex valued if the energy lies within the band $\pm 2t$ around the energy E_m of transverse mode m. In this case they describe the lead-device interaction for extended states. For energies from outside the band of mode m, *i.e.* for $|E - E_m| > 2t$ the self-energies are real. In this case they describe the lead-device interaction for localized (non-propagating) states. For the correct treatment of the problem the contributions from both extended and localized states should be taken into account. This is especially important when the charge of electrons captured in the states below the Fermi level is involved in the analysis, for example in the self-consistent Schrödinger/Poisson calculations.

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