

Time-Dependent Real-Space Renormalization Group Method

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Abstract

In this paper, using the tight-binding model, we extend the real-space renormalization group method to time-dependent Hamiltonians. We derive the time-dependent recursion relations for the renormalized tight-binding Hamiltonian by decimating selective sites of lattice iteratively. The formalism is then used for the calculation of the local density of electronic states for a one dimensional quantum wire with time-dependent random potential. Specifically, we study the electronic densities of states of a single and chains of quantum dots connected to two noisy leads.

Keywords: Renormalization group; Time-dependent; Quantum dot

1. Introduction

Nowadays, nanostructures are commonly employed in electronic and optoelectronic devices [1,2] especially, devices based on one-dimensional (1D) systems have received considerable attentions [3]. Within the theoretical methods for studying 1D systems, the technique of the real space renormalization group, due to its simplicity, has been used extensively, both for ordered and disordered time-independent systems [4]. Many nanostructures, such as quantum dot, in connection to leads experience time dependent random potentials, either through their interactions with the environment or the inherent noise present in the system[5-7]. So, it is vital to determine their effects on the electronic properties of the nanostructures. In this paper, we extend the real-space renormalization group method (decimation method) to time dependent problems. Firstly, we derive the time-dependent recursion relations for the renormalized 1D tight-

binding (TB) Hamiltonian. Then, regarding reference [8], we extend the formalism to TB Hamiltonians with time-dependent random potentials. At the end, we apply the developed formalism to study the densities of electronic states of a single and chains of quantum dots in contact with two noisy leads.

2. Theory

The real-space renormalization group method is a technique for calculating the Green's function and the density of states of an ordered (disordered) system. The method consists of an iterative procedure for obtaining the local Green's function of a given Hamiltonian by decimating selective sites [8,9]. It is, particularly, a simple approach for the study of TB Hamiltonian with nearest-neighbor hopping in one dimension. In this section, we extend the method to the time-dependent one dimensional systems. We use TB Hamiltonian with time-dependent on site potential and nearest-neighbor

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hopping of the form

$$\begin{aligned}
 H(t) = & \sum_n [V_n(t) + v_n] a_n^\dagger(t) a_n(t) + \\
 & \sum_n \int dt_1 [T_{n,n-1}^o(t, t_1) a_n^\dagger(t_1) a_{n-1}(t_1) + \\
 & T_{n,n+1}^o(t, t_1) a_n^\dagger(t_1) a_{n+1}(t_1)]
 \end{aligned} \quad (1)$$

where v_n is the on-site static potential and $V_n(t)$ and $T_{n,n\pm 1}(t, t_1)$, are respectively, time-dependent on-site potential and nearest neighbor hoppings.

The time-dependent Green's function associated with the above Hamiltonian satisfies the following time evolution equation

$$\begin{aligned}
 i \hbar \frac{\partial}{\partial t} G_{m,n}(t, t') - [V_m(t) + v_m] G_{m,n}(t, t') + \\
 \int dt_1 [T_{m,m+1}^o(t, t_1) G_{m+1,n}(t, t') + \\
 T_{m,m-1}^o(t, t_1) G_{m-1,n}(t, t')] = \delta(t - t') \delta_{n,m}
 \end{aligned} \quad (2)$$

Defining the on-site Green's function, $g_n^0(t, t')$, as the inverse of the operator $[i \hbar \frac{\partial}{\partial t} - V_n(t) - v_n]$, we can rewrite Equation (2) as

$$\begin{aligned}
 G_{m,n}(t, t') = g_m^o(t, t') \delta_{m,n} - \\
 \int dt_1 \int dt_2 g_m^o(t, t_1) [T_{m,m+1}^o(t_1, t_2) G_{m+1,n}(t_2, t') + \\
 T_{m,m-1}^o(t_1, t_2) G_{m-1,n}(t_2, t')]
 \end{aligned} \quad (3)$$

An iterative procedure can now be used to solve for $G_{00}(t, t')$ by eliminating the equations containing odd sites and re-numbering the sites, at each iteration step. After each iteration the resulting equation has a structure similar to Equation (3) but with renormalized on-site Green's function and hopping terms. After j th decimation the renormalized quantities, are given by the recursion relations

$$\begin{aligned}
 T_{m,m+2^j}^{(j)}(t, t') = \\
 - \int dt_1 \int dt_2 T_{m,m+2^{j-1}}^{(j-1)}(t, t_1) \\
 g_{m+2^{j-1}}^{(j-1)}(t_1, t_2) T_{m+2^{j-1}, m+2^j}^{(j-1)}(t_2, t')
 \end{aligned} \quad (4)$$

$$\begin{aligned}
 T_{m,m+2^j}^{(j)}(t, t') = \\
 - \int dt_1 \int dt_2 T_{m,m+2^{j-1}}^{(j-1)}(t, t_1) \\
 g_{m+2^{j-1}}^{(j-1)}(t_1, t_2) T_{m+2^{j-1}, m+2^j}^{(j-1)}(t_2, t')
 \end{aligned} \quad (5)$$

and

$$\begin{aligned}
 i \hbar \left[\frac{\partial}{\partial t} - V_m(t) + v_m \right] g_m^{(j)}(t, t') \\
 - \int dt_1 \sum_m^{(j)}(t, t_1) g_m^{(j)}(t, t') = \delta(t - t') \delta_{n,m}
 \end{aligned} \quad (6)$$

where $\sum_m^{(j)}(t, t')$ is given by

$$\begin{aligned}
 \sum_m^{(j)}(t, t') = - \sum_m^{(j-1)}(t, t') \\
 - \int dt_1 \int dt_2 \left[T_{m,m+2^{j-1}}^{(j-1)}(t, t_1) g_{m+2^{j-1}}^{(j-1)}(t_1, t_2) T_{m+2^{j-1}, m}^{(j-1)}(t_2, t') + \right. \\
 \left. T_{m,m-2^{j-1}}^{(j-1)}(t, t_1) g_{m-2^{j-1}}^{(j-1)}(t_1, t_2) T_{m-2^{j-1}, m}^{(j-1)}(t_2, t') \right]
 \end{aligned} \quad (7)$$

In the above equations $T_{m,m+2^j}^{(j)}(t, t')$, $g_{m+2^j}^{(j)}(t, t')$ and $\sum_m^{(j)}(t, t')$ are, respectively, the renormalized

hopping term, on-site Greens' function and the self-energy after the j th decimation.

To use the above recursion relations, the equation for $g_{(m)}^{(j)}(t, t')$ at each iteration step should be solved. This equation is an integro-differential equation which can be solved iteratively. It should be mentioned that all the Green's function are retarded. The above formalism can also be used for random time-dependent potentials concerning references [8-10]; *i.e.* at each step of decimation the dependence of the renormalized quantities on the readom potentials associated with decimated sites are averaged [11,12].

The quantity of fundamental importance for applying the time-dependent RG method to random time-dependent potentials is the averaged on-site Green's function which we denote it by $\langle g_{(m)}^{(j)}(t, t') \rangle$. The averaged on-site Green's function should be determined at each step of the iteration by solving the averaged form of Equation (6). To obtain the equation for averaged on-sit Green's function, we rewrite Equation (6) as

$$\begin{aligned}
 g_m^{(j)}(t, t') = g_m^{(o)}(t, t') + \\
 \int dt_1 \int dt_2 g_m^{(o)}(t, t_1) \sum_m^{(j)}(t_1, t_2) g_m^{(o)}(t_2, t') +
 \end{aligned}$$

$$\int dt_1 \int dt_2 \int dt_3 \int dt_4 g_m^{(o)}(t, t_1) \sum_m^{(j)}(t_1, t_2) g_m^{(o)}(t_2, t_3) \sum_m^{(j)}(t_3, t_4) g_m^{(o)}(t_4, t') + \dots + \int dt_1 \dots \int dt_{2n} g_m^{(o)}(t, t_1) \sum_m^{(j)}(t_1, t_2) g_m^{(o)}(t_2, t_3) \dots \sum_m^{(j)}(t_{2n-1}, t_{2n}) g_m^{(o)}(t_{2n}, t') + \dots \tag{8}$$

Denoting the averaging over the random potentials by $\langle \dots \rangle$, we have to determine the average of products of $g_m^{(o)}$'s and $\sum_m^{(j)}$'s. But, since they are retarded all the time variables used in the integrals are time ordered, so averaging process for various terms in the product is carried out at different times, therefore, we have

$$\langle g_m^{(o)}(t, t_1) \sum_m^{(j)}(t_1, t_2) \dots \sum_m^{(j)}(t_{2n-1}, t_{2n}) g_m^{(o)}(t_{2n}, t') \rangle = \langle g_m^{(o)}(t, t_1) \rangle \langle \sum_m^{(j)}(t_1, t_2) \rangle \dots \langle \sum_m^{(j)}(t_{2n-1}, t_{2n}) \rangle \langle g_m^{(o)}(t_{2n}, t') \rangle \tag{9}$$

Thus, the equation that determines the averaged on-site Green's function is

$$\langle g_m^{(j)}(t, t') \rangle = \langle g_m^{(o)}(t, t') \rangle + \int dt_1 \int dt_2 \langle g_m^{(o)}(t, t_1) \rangle \langle \sum_m^{(j)}(t_1, t_2) \rangle \langle g_m^{(o)}(t_2, t') \rangle + \dots + \int dt_1 \dots \int dt_{2n} \langle g_m^{(o)}(t, t_1) \rangle \langle \sum_m^{(j)}(t_1, t_2) \rangle \langle g_m^{(o)}(t_2, t_3) \rangle \dots \langle \sum_m^{(j)}(t_{2n-1}, t_{2n}) \rangle \langle g_m^{(o)}(t_{2n}, t') \rangle + \dots \tag{10}$$

Using Equations (4) and (5) the averaged value of renormalized hoppings can be calculated once the averaged on-site Green's function is determined.

3. Applications and Results

In this section the formalism of time-dependent renormalization group will be used to study the effects of noisy leads on the densities of states of a single and chains of quantum dots. For simplicity, we consider a quantum wire in TB approximation where all the sites, except a finite number of them, are driven by time-dependent random potential, $V_m(t)$. For simplicity, we assume that the hoppings between the leads and the quantum dots are equal to the hoppings within the leads and they are independent of time. The Hamiltonian of the dots and the leads takes the simple form

$$H(t) = \sum_{m=-\infty}^{\infty} [V_m(t) + v_m] a_m^\dagger a_m + \sum_m T [a_m^\dagger a_{m-1} + a_m^\dagger a_{m+1}] \tag{11}$$

where v_m 's are the on-site static potentials and $V_m(t)$'s are zero on the dots. We, also, choose $V_m(t)$ to be Gaussian noise with

$$\langle V_m(t) V_n(t') \rangle = F_m \delta(t - t') \delta_{nm} \tag{12}$$

where F_m 's are parameters defining the distribution and the brackets $\langle \dots \rangle$ indicate statistical averages and n, m corresponding to the sites in the leads.

The Gaussian noise is completely defined by its generating function

$$\left\langle \exp \left(i \sum_n \int_{-\infty}^{\infty} dt \Phi_n(t) V_n(t) \right) \right\rangle = \exp \left(-\frac{1}{2} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \Phi_n(t) \Phi_m(t') \langle V_n(t) V_m(t') \rangle \right) \tag{13}$$

where $\Phi_n(t)$'s are test functions. Functionally differentiating the generating function with respect to $\Phi_m(t)$'s r -times and setting $\Phi_m(t)$'s to zero after differentiation, we obtain the statistical average of $\langle V_{m_1}(t_1) \dots V_{m_r}(t_r) \rangle$. For the above Hamiltonian, the on-site retarded Green's function has the form

$$g_m^{(o)}(t, t') = -\frac{i}{\hbar} \theta(t - t') \exp \left(\frac{-i}{\hbar} v_m(t - t') \right) \exp \left(\frac{-i}{\hbar} \int_{t'}^t dt_1 V_m(t_1) \right), m = 0, \pm 1, \pm 2, \dots \tag{14}$$

and its statistical average is given by

$$g_m^{(o)}(t, t') = -\frac{i}{\hbar} \theta(t - t') \exp \left(\frac{-i}{\hbar} v_m(t - t') \right) \left\langle \exp \left(\frac{-i}{\hbar} \int_{t'}^t dt_1 V_m(t_1) \right) \right\rangle, m = 0, \pm 1, \pm 2, \dots \tag{15}$$

Using the generating functional for Gaussian noise, Equation (13), the right hand side of the Equation (15) can be determined exactly and the averaged on-site

Green's function is given by

$$\begin{aligned} \langle g_m^{(o)}(t, t') \rangle = & \\ & -\frac{i}{\hbar} \theta(t-t') \exp\left(\frac{-i}{\hbar} V_m(t-t')\right) \\ & \exp\left(\frac{-1}{2} F_m |t-t'|\right) \end{aligned} \quad (16)$$

Considering that

$$T_n^o(t, t') = T \delta(t-t') \quad (17)$$

for the Hamiltonian given by Equation (11), we can use the recursion relations (4), and (5), and Equations (7), and (8), after averaging the decimated sites, to obtain the renormalized hoppings and on-site Green's function. For Gaussian noise the averaged retarded on-site Green's function is a function of time-difference. Thus, we can solve Equation (10) using Fourier Transform (FT) with respect to time variable. This reduces the integral Equation (10) to algebraic equation

$$\begin{aligned} \langle g_m^{(j)}(E) \rangle = & \langle g_m^{(o)}(E) \rangle + \\ & \langle g_m^{(o)}(E) \rangle \langle \sum_m^{(j)}(E) \rangle \langle g_m^{(o)}(E) \rangle + \\ & \dots + \langle g_m^{(o)}(E) \rangle \langle \sum_m^{(j)}(E) \rangle \langle g_m^{(o)}(E) \rangle \dots \\ & \langle \sum_m^{(j)}(E) \rangle \langle g_m^{(o)}(E) \rangle + \dots \end{aligned} \quad (18)$$

or

$$\begin{aligned} \langle g_m^{(j)}(E) \rangle = & \langle g_m^{(o)}(E) \rangle + \\ & \langle g_m^{(o)}(E) \rangle \langle \sum_m^{(j)}(E) \rangle \langle g_m^{(j)}(E) \rangle \end{aligned} \quad (19)$$

which has the form of Dyson equation. Equation (19) can be solved for $\langle g_m^{(j)}(E) \rangle$, which gives us

$$\langle g_m^{(j)}(E) \rangle = \frac{\langle g_m^{(o)}(E) \rangle}{1 - \langle g_m^{(o)}(E) \rangle \langle \sum_m^{(j)}(E) \rangle} \quad (20)$$

We can, also, FT the recursion relations, Equations (4) and (5), for renormalized hoppings and Equation (7) for $\sum_m^{(j)}(t, t')$. This reduces Equations (4), (5) and (7), respectively, to

$$\begin{aligned} T_{m, m+2^{(j)}}^{(j)}(E) = & \\ & -T_{m, m+2^{(j-1)}}^{(j-1)}(E) g_{m+2^{(j-1)}}^{(j-1)}(E) T_{m+2^{(j-1)}, m+2^{(j)}}^{(j-1)}(E) \end{aligned} \quad (21)$$

$$\begin{aligned} T_{m, m-2^{(j)}}^{(j)}(E) = & \\ & -T_{m, m-2^{(j-1)}}^{(j-1)}(E) g_{m+2^{(j-1)}}^{(j-1)}(E) T_{m-2^{(j-1)}, m-2^{(j)}}^{(j-1)}(E) \end{aligned} \quad (22)$$

and

$$\begin{aligned} \sum_m^{(j)}(E) = & \\ & -T_{m, m+2^{(j-1)}}^{(j-1)}(E) g_{m+2^{(j-1)}}^{(j-1)}(E) T_{m+2^{(j-1)}, m+2^{(j)}}^{(j-1)}(E) - \\ & T_{m, m-2^{(j-1)}}^{(j-1)}(E) g_{m-2^{(j-1)}}^{(j-1)}(E) T_{m-2^{(j-1)}, m-2^{(j)}}^{(j-1)}(E) \end{aligned} \quad (23)$$

Equations (20)-(23) including Equation (16) constitute the renormalized recursion relation for a system driven by a Gaussian noise.

We now consider the effects of noisy leads with Gaussian distributions on the local densities of states of a single and finite chain of quantum dots. For a single quantum dots, we assume that the dot is located at the site $m=0$ and the Gaussian noise acts on all the sites of left and right leads with a same strength. Figure 1 represents the local densities of states for three different values of $F'_m s$. Figures 2 and 3 depict, respectively, the local densities of states of a quantum dot located at site $m=0$ within the chains with 11 and 19 quantum dots for two different values of $F'_m s$. We observe from Figure 1 that in the case of a single quantum dot the noise in the leads causes the states of the dot to become more localized around zero energy state. The effect of localization also appears in the chains. For weak noise it manifests itself as an oscillation in the local densities of states. As the strength of noise increases, the states of quantum dot become more localized around definite

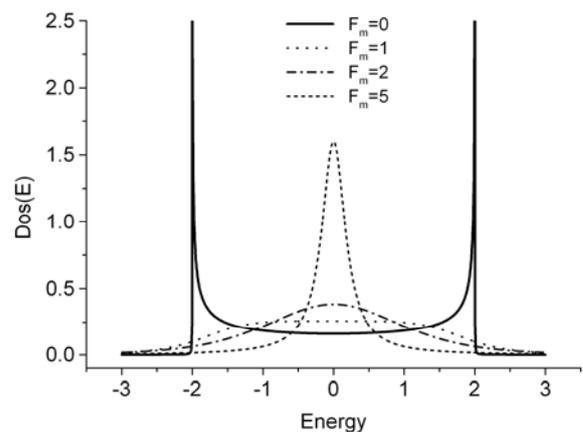


Figure 1. The local densities of states of a single quantum dot connected to noisily leads, for four different values of $F'_m s$ in unit of hopping integral.

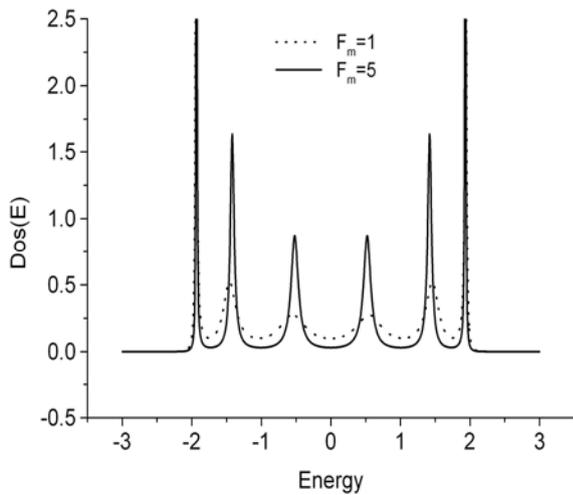


Figure 2. The local densities of states of a quantum dot located at $m=0$ within the chain of eleven quantum dots, connected to noisy leads for two different values of $F'_m s$ in unit of hopping integral.

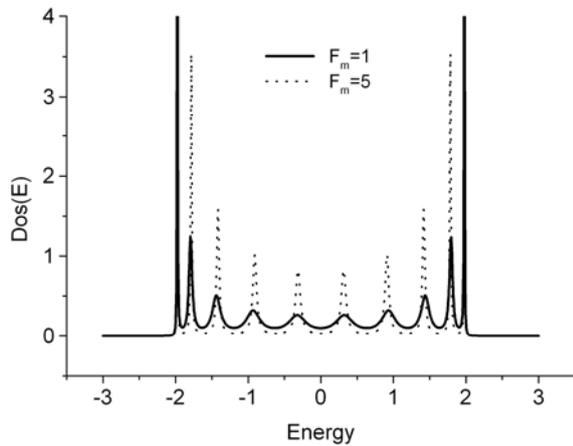


Figure 3. The local densities of states of a quantum dot located at $m=0$ within the chain of nineteen quantum dots, connected to noisy leads for two different values of $F'_m s$ in unit of hopping integral.

energy values. These behaviors of local densities of states are reminiscent of a leaky double barriers; *i.e.* each noisy lead acts as a leaky barrier for electrons in the quantum dot or in the chains.

In conclusion, in this paper we have presented the time-dependent real space renormalization group method which is a versatile numerical technique for studying the effects of various time-dependent random potentials with any kinds of distributions [13,14]. We have then used the proposed method for studying the effects of noisy leads with Gaussian distribution on the densities of states of single and chains of quantum dots. The method can, also, be extended to include, concurrently, static as well as time-dependent random potentials and hopping integrals.

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