# Localization and delocalization of a one-dimensional system coupled with the environment*

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We investigate several models of a one-dimensional chain coupling with surrounding atoms to elucidate disorder-induced delocalization in quantum wires, a peculiar behaviour against common wisdom. We show that the localization length is enhanced by disorder of side sites in the case of strong disorder, but in the case of weak disorder there is a plateau in this dependence. The above behaviour is the conjunct influence of the coupling to the surrounding atoms and the antiresonant effect. We also discuss different effects and their physical origin of different types of disorder in such systems. The numerical results show that coupling with the surrounding atoms can induce either the localization or delocalization effect depending on the values of parameters.

**Keywords:** delocalization, localization, one-dimensional chain, surrounding atoms
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With the advent of miniaturization and fabrication of various quantum structures,[1] it is possible to use quantum wires such as carbon nanotubes[2,3] as wiring to connect nanodevices. For this purpose, good conduction for these quantum wires is necessary. However, impurities and dislocations which cause disorders therein always occur during fabrication. Thus, it is ineluctable to import disorder into a quantum wire. The situation is similar to molecular chains although they are supposed to be defect-free. Especially, the latter can be subject to random interactions with their surroundings, e.g., the ligands of DNA molecules.[4] As common wisdom, in such low-dimensional systems the localization of electron states is induced by disorder even though it is produced by the environment, and the conductance should be poorer when the environmental disorder increases.[5] However, several experimental studies[6,7] have shown that in some parameter regions the conductivity of ideal nanowires can be enhanced by increasing environmental disorder. Theoretically, Zhong and Malcolm[8] investigated a shell-doped nanowire with a model of one ideal chain coupled with several disordered chains serving as environmental disorder, and Xiong[4] studied a one-dimensional (1D) tight-binding ideal chain subject to random interactions with disordered side sites. The behaviours they obtained are similar to those observed in experiments and some possible explanations are provided for the observed phenomena.

In this paper we generalize the 1D tight-binding model in Ref. [4] to investigate the effects of different types of disorder in the environment and the couplings with it. The model is shown in Fig. 1, in which every side site couples with two host sites as a bridge, different from the situation in Ref. [4] where every side site couples with one site in the host chain. The disorder can occur in the site energies of the side sites or in the coupling strengths between the host and side sites. Our numerical results show that the Lyapunov exponent (the inverse of the localization length of electronic states) is reduced by disorder of side sites in the region of strong disorder, similar to what Zhong and Malcolm[8] and Xiong[4] have found, but in the region of weak disorder, a plateau appears in the curve of the Lyapunov exponent versus the disorder strength. Using the real-space decimation renormalization technique[9] and considering the so-called antiresonant effect,[10] we show that the above behaviour observed in our results is the conjunct influence of the effective coupling between the conduction states of the ideal chain and the localized states in disordered side sites and the antiresonant effect which generally oc-

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curs in 1D systems. Based on this we discuss different effects and their physical origin of different types of disorder in such systems.

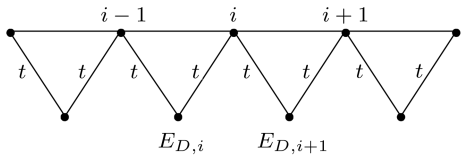



**Fig. 1.** Schematic illustration of the model. $E_{D,i}$ is the energy of the $i$th side site and $t$ is the hopping integral between the ideal chain and the side sites.

The Hamiltonian of the system in Fig. 1 is

$$\hat{H} = \hat{H}_P + \hat{H}_D + \hat{H}_{DP}, \tag{1}$$

where the sub-Hamiltonian of the host chain is

$$\hat{H}_P = \sum_{i=1}^{N} \hat{C}^{\dagger}_{P,i}\hat{C}_{P,i+1} + \text{H.c.}\ . \tag{2}$$

Here the on-site energy is taken as the energy reference point and the intersite hopping integral is taken as the energy units, for the sake of convenience in our numerical calculations. Obviously, we have the eigenenergy band of $\hat{H}_P$ as $E(k) = 2\cos k$.

The sub-Hamiltonian of the side sites is

$$\hat{H}_D = \sum_{i=1}^{N} E_{D,i}\hat{C}^{\dagger}_{D,i}\hat{C}_{D,i} + \text{H.c.}\ , \tag{3}$$

here $E_{D,i}$ is the random on-site energies distributed in the region $[E_c - W, E_c + W]$, $E_c$ is the average value of the random energies and $W$ is the disorder strength. The coupling between the host chain and the side sites is

$$\hat{H}_{DP} = t\sum_{i=1}^{N}(\hat{C}^{\dagger}_{P,i}C_{D,i} + \hat{C}^{\dagger}_{P,i}C_{D,i+1}) + \text{H.c.}\ , \tag{4}$$

where $t$ is the coupling strength. At first we set $t$ as a constant for all side sites.

The eigenstate of the Hamiltonian with energy $E$ can be written as a linear combination of orbitals on the sites

$$|\Psi(E)\rangle = \sum_i (\Gamma_{P,i}C^{\dagger}_{P,i}|0\rangle + \Gamma_{D,i}C^{\dagger}_{D,i}|0\rangle)\ , \tag{5}$$

where $|0\rangle$ is the vacuum state, $\Gamma_{P,i}$ and $\Gamma_{D,i}$ are amplitudes of the wave function on the $i$th host site and on the $i$th side site, respectively. From the Schrödinger equation

$$H|\Psi(E)\rangle = E|\Psi(E)\rangle, \tag{6}$$

we obtain a set of equations for the amplitudes,

$$E\Gamma_{P,i} = \Gamma_{P,i-1} + \Gamma_{P,i+1} + t(\Gamma_{D,i} + \Gamma_{D,i+1})\ , \tag{7}$$

$$(E - E_{D,i})\Gamma_{D,i} = t(\Gamma_{P,i} + \Gamma_{P,i-1}). \tag{8}$$

Then, by decimating $\Gamma_{D,i}$ and $\Gamma_{D,i+1}$ in equations (7) and (8) as shown in Fig. 2, we have

$$\begin{aligned}&(E - \Delta E_{D,i} - \Delta E_{D,i+1})\Gamma_{P,i}\\ &= (1 + \Delta E_{D,i+1})\Gamma_{P,i+1} + (1 + \Delta E_{D,i})\Gamma_{P,i-1},\end{aligned} \tag{9}$$

in which

$$\Delta E_{D,i} = \frac{t^2}{E - E_{D,i}}. \tag{10}$$

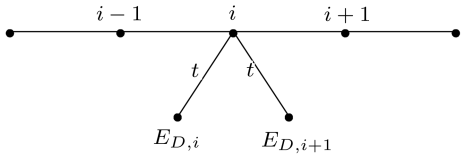



**Fig. 2.** A site of the host chain coupled with two side sites with on-site energies $E_{D,i}$ and $E_{D,i+1}$ respectively.

From equation (9) we can construct the transfer matrix $\boldsymbol{T}_i$,

$$\boldsymbol{T}_i = \begin{pmatrix} \dfrac{E - \Delta E_{D,i} - \Delta E_{D,i+1}}{1 + \Delta E_{D,i+1}} & -\dfrac{1 + \Delta E_{D,i}}{1 + \Delta E_{D,i+1}} \\ 1 & 0 \end{pmatrix}, \tag{11}$$

by which amplitudes $\Gamma_{P,i+1}$ can be calculated from $\Gamma_{P,i}$ and $\Gamma_{P,i-1}$

$$\begin{pmatrix} \Gamma_{P,i+1} \\ \Gamma_{P,i} \end{pmatrix} = \boldsymbol{T}_i \begin{pmatrix} \Gamma_{P,i} \\ \Gamma_{P,i-1} \end{pmatrix}. \tag{12}$$

Then the total transfer matrix which provides the relation between amplitudes at two ends of a system with $N$ sites in the host chain becomes $\boldsymbol{T} = \boldsymbol{T}_N\boldsymbol{T}_{N-1}\ldots\boldsymbol{T}_i\ldots\boldsymbol{T}_1$. By using the transfer matrix and the standard method of Gram–Schmidt reorthonormalization, we can calculate the Lyapunov exponent (LE) of wave functions. The numerical results of LE versus $W$ are shown in Fig. 3 for various electron energies and different average energies of the side sites. It can be seen that the curves of the LE versus $W$ are not monotonic. The turning point $W_c$, where the LE is changed from increasing with $W$ to decreasing with $W$, is increased with increasing electron energy $E$ when the average side site energy $E_c$ is within the host band [the curve in Fig. 3(a)], but it is decreased with increasing $E$ when $E_c$ is out of the host band [the curve in Figs. 3(b) and 3(c)].

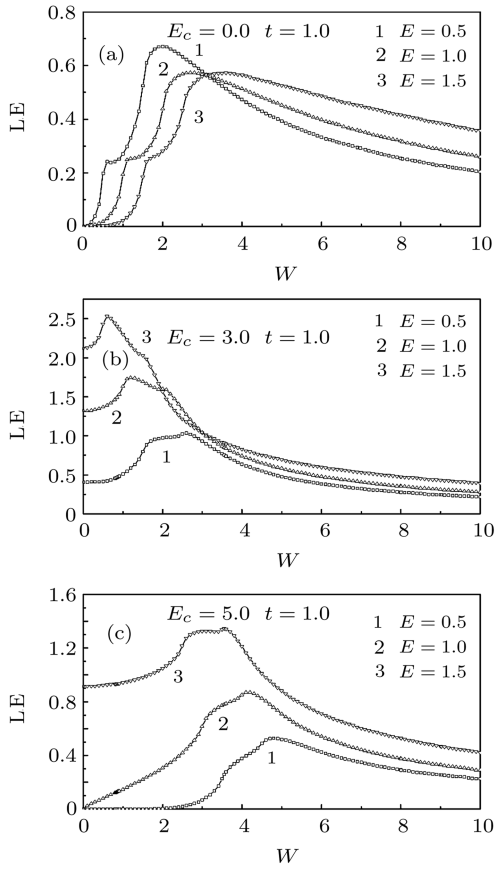



**Fig. 3.** Lyapunov exponent versus $W$ with $E = 0.5$, 1.0, 1.5 and $t = 1.0$ for (a) $E_c = 0.0$, (b) $E_c = 3.0$, and (c) $E_c = 5.0$.

In Fig. 3(a), it is interesting to see that a plateau appears below the turning point $W_c$. This implies that there exists a range of $W$ where the opposite effects (localization and delocalization) of the increase of the disorder strength are in balance. This plateau does not appear in the case of $E_c$ out of the host band.

From the renormalized on-site energy $\Delta E_{D,i} + \Delta E_{D,i+1}$ and renormalized hoppings $(1+\Delta E_{D,i+1})$ or $(1+\Delta E_{D,i})$ in Eq. (9), we can see that the increase of the side site energies not only enhances the disorder of the renormalized on-site energies, but also changes the renormalized band width of the host chain. The former is the cause of localization of electron states in the system, the latter may serve as the origin of delocalization for the states if the effective hoppings increase with $W$. When $W$ is comparable with or larger than the band width of the host chain, the width of the renormalized band begins to increase with $W$. This results in the enhancement of the delocalization effect, reflected by the decrease with $W$ in the range $W > W_c$. When $W$ is small, the band width cannot be efficiently increased by increasing $W$, resulting in the general trend of increase of LE with $W$. There may be some complicated behaviour of the curves in this region due to the singularities of $\Delta E_{D,i}$. By decimating both the site in the ideal chain and the side sites coupled with it as shown in Fig. 4(a),[8] we obtain the renormalized intersite hopping integral as

$$t_i' = \frac{(E - E_{D,i+1} + t^2)(E - E_{D,i} + t^2)}{E(E - E_{D,i})(E - E_{D,i+1}) - t^2(2E - E_{D,i} - E_{D,i+1})}. \tag{13}$$

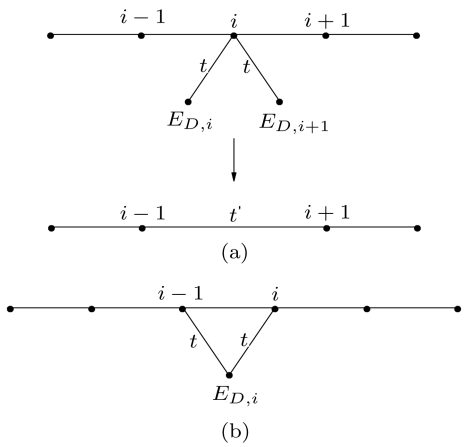



**Fig. 4.** (a) Renormalization of both the on-site energy and the intersite hoppings by decimating both the sites on the host chain and the side sites coupled with it. (b) A unit-cell of our model.

From Eq. (13) we can see that the renormalized intersite coupling $t_i'$ approaches zero when $(E - E_{D,i+1} + t^2)$ or $(E - E_{D,i} + t^2)$ becomes zero. Moreover, the transmission coefficient through a unit cell of our model, as shown in Fig. 4(b), is given by

$$|\boldsymbol{T}(E)|^2 = \frac{1}{1 + \dfrac{t^4(2+E)}{(E - E_{D,i} + t^2)(2-E)}}. \tag{14}$$

We can see that when $(E - E_{D,i} + t^2) \to 0$, the transmission coefficient $|\boldsymbol{T}(E)|^2$ also becomes zero, this is just the antiresonant effect.[9] This leads to another value of $W$ around $|E + t^2 - E_c|$ in the curves of LE versus $W$, which corresponds to the boundary of the antiresonant effect and is reflected in the LE-$W$ curves as a plateau. In summary, the behaviour of Lyapunov

exponent versus $W$ is the conjunct influence of two different effects: the antiresonant effect[9] and the effective coupling between the conduction states of the host chain and the localized states of disordered side sites.

We also carry out calculations on systems where the disorder appears in the host chain only. In this case the side site energy is taken as the energy reference point, and the intersite hopping integral is also taken as the energy unit for the sake of convenience. The on-site energies of the sites in the host chain $E_{P,i}$ are distributed in the region $[E_c - W, E_c + W]$, with $E_c$ being the centre of the random energies and the strength of disorder $W$. Similar to the analytical treatment above, in this case we have

$$\left(E - E_{P,i} - \frac{2t^2}{E}\right) \Gamma_{P,i} = \left(1 + \frac{t^2}{E}\right) \Gamma_{P,i+1} + \left(1 + \frac{t^2}{E}\right) \Gamma_{P,i-1}. \quad (15)$$

We can see that the influence of the side sites on conduction states in the chain appears only in the renormalized hoppings as a correction $2t^2/E$ which is a constant when $t$ and $E$ are given. Meanwhile the randomness in the host chain takes place in the renormalized on-site energies. Then we can conclude that the influence of the side sites coupled with the disordered host chain should not change the common wisdom about the behaviour of the localization length. We also calculated the renormalized intersite hopping integral as shown in Fig. 4(a), it is given by

$$t_i' = \frac{\left(1 + \frac{t^2}{E}\right)^2}{E - E_{P,i} - \frac{2t^2}{E}}. \quad (16)$$

We can see that here the antiresonant effect[10] is absent, which is in agreement with Wang *et al.* in Ref. [9]. From this we may expect that the LE (the inverse of the localization length) should increase with the increase of the disorder strength $W$, consistent with common wisdom. The numerical results, as shown in Fig. 5, are consistent with this conclusion when the electron energy is within the host band. The initial parts of the curve in Fig. 5(b) with $E = 0.5$ and the curves in Fig. 5(c) seem to have opposite features as they decrease with increasing $W$. This is just because these curves correspond to the electron energies which are out of the host band for small $W$. The localization length can be increased when the electron energy is moved towards the band centre.

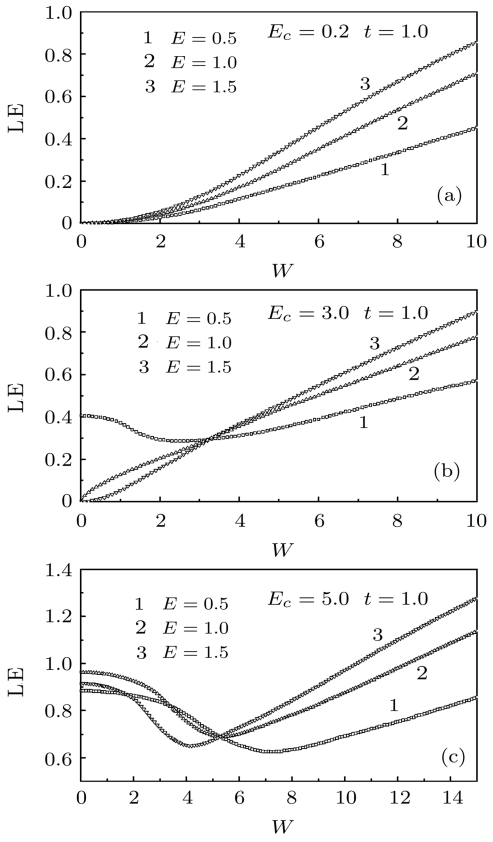



**Fig. 5.** Lyapunov exponent versus $W$ in the case of random on-site energies in the host chain, with $E = 0.5$, 1.0, 1.5 and $t = 1.0$ for (a) $E_c = 0.0$, (b) $E_c = 3.0$, and (c) $E_c = 5.0$.

Moreover, we study another case based on our initial model where the disorder appears in the hopping integrals between the host chain and the side sites only. In this case the side site energy is taken as the energy reference point, the energy of the sites in the host chain is taken as an energy constant $E_P$ and the intersite hopping in the host chain is also taken as the energy unit. The logarithms of hopping integrals between the host chain and the side sites are randomly distributed as $\ln t_i \in [-W, W]$. The sub-Hamiltonian of couplings between the host chain and the side sites is

$$\hat{H}_{DP} = \sum_{i=1}^{N} t_i (\hat{C}_{P,i}^{\dagger} C_{D,i} + \hat{C}_{P,i}^{\dagger} C_{D,i+1}) + \text{H.c.} \quad (17)$$

As the disorders appeared in the hopping integrals between the ideal chain and the side sites only, there is no antiresonant effect. Most parts of the curves of LE versus the disorder strength $W$, as shown in Fig. 6, are in agreement with common wisdom, where the LE increases with $W$.

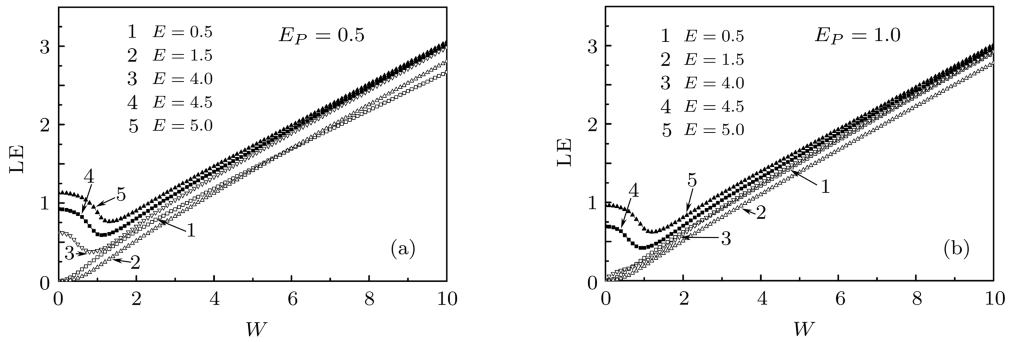



**Fig. 6.** Lyapunov exponent versus $W$ in the case of random hopping integrals between the host chain and the side sites, with $E = 0.5$, 1.5, 4.0, 4.5, 5.0 for $E_P = 0.5$ (a) and 1.0 (b).

The initial parts of some curves exhibit opposite behaviour just because the electron energy is out of the host band for small $W$ and the band is widened by increasing $W$ to include the electron energy.

In summary, we investigate the localization behaviour of electron states in a general model for different types of disorder and obtain a clear picture about the behaviour of the Lyapunov exponent versus the disorder strength $W$ in such systems. It is found that the antiresonant effect, the disorder-induced localization, and the variation of band width are physical ingredients which compete with each other and produce complicated behaviour of electron states interacting with the environment. The numerical results and theoretical analysis may shed light on the understanding of transport properties in quasi-1D systems.

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