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Delocalization in disordered chains with random symmetrical impurities

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Abstract. We study in this paper, with the context of a tight-binding on-side model, the electronic properties of one-dimensional random lattices with correlated impurities. We show that, when symmetrical impurities $\varepsilon_{\rm b}\varepsilon_{\rm c}\varepsilon_{\rm b}$ are inserted in a host chain of site energy $\varepsilon_{\rm a}$ and a constant hopping interaction V, diffusion will occur even when $\varepsilon_{\rm c}$ is random. We provide analytic expressions for the transmittance and confirm the theoretical results by a great deal of numerical calculations. When $\varepsilon_{\rm b} = V$, we find that the mean-square displacement (MSD) follows the law $\langle m^2 \rangle \propto t^{\beta}$ with $\beta = 2.0$ for $\varepsilon_{\rm c}$ = constant and $\beta = 1.0$ for $\varepsilon_{\rm c} = \varepsilon_{\rm r}$ = random, respectively.

PACS. 71.55.Jv Disordered structure; amorphous and glassy solids – 72.15.Rn Localization effects (Anderson or weak localization) – 71.23.-k Electronic structure of disordered solids

1 Introduction

In the past few decades, there has been much interest in the problem of electronic localization in random systems. It is well-known that all the electronic states are localized even for infinitesimal disorder in one-dimensional lattice [1,2]. However, during the last decade analytical and numerical studies revealed that delocalized electronic states can exist in one-dimensional lattices with short-range correlations [3–6]. In the theory of Anderson localization [1], the random on-site energy value is chosen as a set of uncorrected random values. In 1990, Dunlap *et al.* (DWP) [3] introduced the random dimer model (RDM) in which the on-site energy takes two possible values $\epsilon_{\rm A}$, $\epsilon_{\rm B}$ and a constant nearest-neighbor matrix element V. When the same value of site energy is assigned at random to two succeeding lattice sites, they found the absence of localization when $|\epsilon_{\rm A} - \epsilon_{\rm B}| \leq 2V$. Furthermore, they found dynamically that the mean-square displacement (MSD) of an initially localized particle will grow with time as $t^{3/2}$, provided that $|\epsilon_{\rm A} - \epsilon_{\rm B}| < 2V$. When $\epsilon_{\rm A} - \epsilon_{\rm B} = \pm 2V$, the MSD grows as t, and when $|\epsilon_{\rm A} - \epsilon_{\rm B}| > 2V$, the MSD will be bounded, consequently, the particle will be localized. Furthermore, they claimed that there are $\sqrt{N}$ extended states in RDM, where N is the number of lattice sites of the sample. In the later papers [4–6], it was suggested that a metal insulator transition is possible in polyaniline and the highly doped transpolyacetylene. Ever since, physicists have paid more and more attention to these systems, and have made extensive investigations. Bovier [7] confirmed the conclusion of DWP from perturbative calculations. Evangelou and Economou [8] generalized this random dimer model to "random N-mer" case and calculated the localization length of these systems. Flores and Hilke [9] reported the divergence of localization length around perfect transmission energy is $1/\sqrt{E}$ at outer edges. Lavarda *et al.* [10] constructed the so-called "asymmetrical dimer" and showed that in RDM model internal symmetry is not a necessary condition for dimers to produce near resonant scattering of Bloch states in one-dimensional system. Huang *et al.* [11] studied the number of extended states at the band center and the band edge of RDM, respectively, and found that it is of order $\sqrt{N}$ for both cases. Stimulated by the RDM-like correlations, other kinds of correlations have been considered by many authors [12–22]. More recently, the experimental evidence of delocalization in correlated disorder superlattices was reported by Bellani *et al.* [23,24]. From the above review, we find that the correlations among the defects played a important role in the localization problem. Some kind of correlations of defects can alter the localization length of the disordered system at some special energies.

In this paper, we will consider a new kind of correlated defects in a certain segment of one-dimensional disordered lattice. The defect consists of two types of atoms

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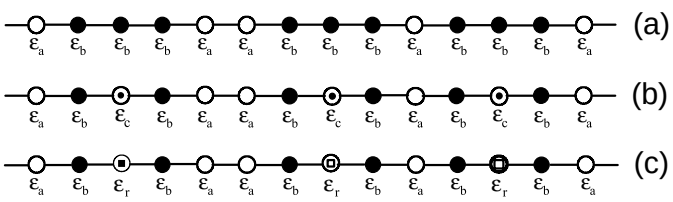

Fig. 1. The scheme of random lattices with different defects: (a) trimer defects, (b) symmetric defects, here ε_c is a constant and (c) random symmetric defects, here ε_r is randomly distributed in a given region.

and has symmetric internal structure. In the following section, we introduce our models. In Section 3, when a single defect is inserted in a perfect lattice, we derive exactly the reflection coefficient for the model through a transfer-matrix technique. Then, we perform numerical simulations of transmission coefficient for the case when a finite concentration of impurities is added. In Section 4, we numerically study the spatial distribution of electronic states near the resonant energies. Finally, the propagation of the particle in the studied systems is discussed by the corresponding mean-square displacement (MSD).

2 Model

We start with a tight-binding monatomic chain, for which the site energy is ε_a and atoms are connected by a same hopping interaction V. In this paper, we consider three types of impurities which are randomly inserted in the host chain. The specific models (shown in Fig. 1) are the models with (a) trimer defects (TD), (b) symmetrical defects (RD), where ε_c is same, and (c) random symmetrical defects (RSD), where ε_r is random.

In the tight-binding and nearest-neighbor interaction approximation, the equation of motion is given by

$$\mathrm{i}\frac{\mathrm{d}C_n(t)}{\mathrm{d}t} = \varepsilon_n C_n(t) + VC_{n+1}(t) + VC_{n-1}(t), \qquad (1)$$

where $C_n(t)$ is the probability amplitude for an electron at the nth lattice site, ε_n is the site energy.

By making the transformation $C_n(t) = \exp(-\mathrm{i}Et)c_n$, we have the eigenvalue equation

$$(E - \varepsilon_n)c_n - Vc_{n+1} - Vc_{n-1} = 0, \qquad (2)$$

here c_n is the site amplitude for site n, equation (2) can be rewritten in the matrix form

$$\begin{bmatrix} c_{n+1} \\ c_n \end{bmatrix} = \underline{P}^{(n)} \begin{bmatrix} c_n \\ c_{n-1} \end{bmatrix}, \qquad (3)$$

and

$$\underline{P}^{(n)} = \begin{bmatrix} \dfrac{E-\varepsilon_n}{V} & -1 \\ 1 & 0 \end{bmatrix}, \qquad (4)$$

where $\underline{P}^{(n)}$ is the transfer matrix which connects the adjacent site amplitudes c_n and $c_{n\pm1}$. In what next section, we study the transmission properties of the models which are shown in Figure 1. Since the physical properties depend on the difference of site energies but not the actual values of ε_a, ε_b and ε_c separately. For the sake of simplicity, in the following discussions, we can set the host site energy $\varepsilon_a = 0$.

3 Electronic transmission

3.1 Theoretical analyses for single impurity

To study the problem of the localization properties of the models shown in Figure 1. Let us consider a single defect that occupies m sites and suppose the defect is placed at site $n+1$ to $m+n+1$ in an otherwise perfect lattice. Then, we have the site amplitudes to both sides of the defect as

$$c_j = \begin{cases} \mathrm{e}^{\mathrm{i}kj} + r\mathrm{e}^{-\mathrm{i}kj} & \text{for } j \le n+1, \\ t\mathrm{e}^{\mathrm{i}kj} & \text{for } j \ge n+m+1. \end{cases} \qquad (5)$$

From equation (5), the relation of the site amplitudes which connects both ends of the defect is

$$\begin{bmatrix} c_{n+m+1} \\ c_{n+m} \end{bmatrix} = \underline{P}_m \begin{bmatrix} c_{n+1} \\ c_n \end{bmatrix}, \qquad (6)$$

where $\underline{P}_m$ is the total transfer matrix, it is given by

$$\underline{P}_m = \left[\prod_{j=n+1}^{n+m+1} \underline{P}^{(j)} \right]. \qquad (7)$$

Using the definition of equations (5) and (6), Wu *et al.* [6] have found the reflection amplitude r

$$r = -Z^{2n} \frac{\alpha^T \Gamma \underline{P}_m \alpha}{\alpha^T \Gamma \underline{P}_m \alpha^*}, \qquad (8)$$

where $Z = \mathrm{e}^{\mathrm{i}k}$, $\Gamma = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$, $\alpha = \begin{bmatrix} Z \\ 1 \end{bmatrix}$, and α^T, the transpose of α.

For a single symmetrical defect $\varepsilon_b\varepsilon_c\varepsilon_b$, the following reflection coefficient is easily obtained by equation (8)

$$R = |r|^2 = \frac{(Y + 2X\cos k)^2}{(2X + Y\cos k)^2 + (Y + 2C)^2 \sin^2 k}, \qquad (9)$$

where $X = BC - 1$, $Y = 2B - C - B^2C$, $B = (E - \varepsilon_b)/V$ and $C = (E - \varepsilon_c)/V$.

Equation (9) is a general equation for the reflection coefficient due to scattering by the defect $\varepsilon_b\varepsilon_c\varepsilon_b$. In this case, the vanishing of the reflection coefficient occurs when $\cos k$ satisfies

$$\cos k = \frac{\varepsilon_b^2 + \varepsilon_b\varepsilon_c \pm \sqrt{\varepsilon_b^2\varepsilon_c(\varepsilon_b - \varepsilon_c)^2 + 4\varepsilon_b V^2(2\varepsilon_b - \varepsilon_c)}}{4\varepsilon_b V}. \qquad (10)$$

Obviously, when $\varepsilon_{\rm b} = \varepsilon_{\rm c}$, the symmetric defect $\varepsilon_{\rm b}\varepsilon_{\rm c}\varepsilon_{\rm b}$ is exactly the trimer case and the corresponding resonances of equation (10) satisfy $|\cos k| = |\varepsilon_{\rm b}/2V \pm 1/2| \leq 1$, which are obtained by Wu *et al.* in their paper [6]. In this paper, we concentrate our attention on a particular case ($\varepsilon_{\rm b} = V$) of equation (10). When $\varepsilon_{\rm b} = V$, it follows from equation (10) that

$$|\cos k| = \left|\frac{\varepsilon_{\rm c} - V}{2V}\right| \leq 1, \tag{11}$$

and

$$|\cos k| = 1. \tag{12}$$

Since $E = 2V\cos k$, one resonant energy $E = \varepsilon_{\rm c} - V$ can be readily obtained by equation (11), provided that $-V \leq \varepsilon_{\rm c} \leq 3V$. And the dependence of equation (12) has a remarkable property that there is always one resonance at the energy $E = 2V$, regardless of the value of the site energy $\varepsilon_{\rm c}$.

It is of special interest to explain these resonant behaviors with the view of the property of the corresponding transfer matrix. From the equation (8), Wu *et al.* [6] have pointed out that the reflection coefficient will vanish only when the matrix $\underline{P}_m$ is proportional to (a) the unit matrix or (b) the transfer matrix for the ordered system (or some linear combination of both).

For the single defect $\varepsilon_{\rm b}\varepsilon_{\rm c}\varepsilon_{\rm b}$, when $\varepsilon_{\rm b} = V$, we find the corresponding transfer matrix across the defect is

$$\underline{P}_{\rm bcb} = \begin{bmatrix} F & -D \\ D & 0 \end{bmatrix} + \left(\frac{\varepsilon_{\rm c} - E}{V}\right)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{13}$$

where

$$F = \frac{E^3 + 2E\varepsilon_{\rm c}V + 2V^2(V - \varepsilon_{\rm c}) - E^2(\varepsilon_{\rm c} + 2V)}{V^3}, \tag{14}$$

and

$$D = \frac{(E - \varepsilon_{\rm c})(E - V) - V^2}{V^2}\cdot \tag{15}$$

When $E = \varepsilon_{\rm c} - V$, where $-V \leq \varepsilon_{\rm c} \leq 3V$, equation (13) reduces to

$$\underline{P}_{\rm bcb} = \left(\frac{V - \varepsilon_{\rm c}}{V}\right)\begin{bmatrix} \frac{E}{V} & -1 \\ 1 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{16}$$

when $E = 2V$, we obtain

$$\underline{P}_{\rm bcb} = \left(\frac{V - \varepsilon_{\rm c}}{V}\right)\begin{bmatrix} \frac{E}{V} & -1 \\ 1 & 0 \end{bmatrix} + \left(\frac{\varepsilon_{\rm c}}{V} - 2\right)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{17}$$

where we use the condition $\varepsilon_{\rm a} = 0.0$. Evidently, for both cases, the defect transfer matrix in this model reduces to the linear combination of unit matrix and the ordered system transfer matrix. Especially, for the case of $E = 2V$, the reflection coefficient will vanish for any given $\varepsilon_{\rm c}$.

3.2 Numerical results for random symmetrical impurities

Thus far, we have shown theoretically that for a given symmetric defect ($\varepsilon_{\rm b}\varepsilon_{\rm c}\varepsilon_{\rm b}$), when $\varepsilon_{\rm b}$ is equal to the hopping interaction V, the randomness of $\varepsilon_{\rm c}$ doesn't influence the vanishing of the reflection coefficient in the system. When a large number of such defects are randomly placed in the host chain, the transmission properties can be investigated by direct numerical computation of the reflection or transmission coefficients through transfer matrix method. Generally, we can first consider electronic transmission through a one-dimensional chain of length N. We embed this chain in an infinite perfectly ordered atom chain. Then, in the conducting region to the left and the right of the chain, the normalized wave functions can be written as

$$c_n = \begin{cases} {\rm e}^{{\rm i}kn} + f_{\rm r}{\rm e}^{-{\rm i}kn} & \text{for } -\infty < n \leq 1, \\ f_{\rm t}{\rm e}^{{\rm i}kn} & \text{for } N+1 \leq n < \infty. \end{cases} \tag{18}$$

We define the transfer matrix $Q(N)$ by

$$\begin{bmatrix} f_{\rm t} \\ {\rm i}f_{\rm t} \end{bmatrix} = T(N)\begin{bmatrix} 1 + f_{\rm r} \\ {\rm i}(1 - f_{\rm r}) \end{bmatrix}, \tag{19}$$

here

$$Q(N) = S^{-1}M(N)S, \tag{20}$$

where $M(N)$ is the total transfer matrix and S is given by

$$S = \begin{bmatrix} \cos k & \sin k \\ 1 & 0 \end{bmatrix}. \tag{21}$$

Because $Q(N)$ is unimodular, thus, one can calculate the transmission coefficient in the relationship

$$T = \frac{4}{2 + \sum_{i,\,j=1}^{2} |Q(N)_{ij}|^2}\cdot \tag{22}$$

By applying the equation (22), we calculate the transmission coefficient as a function of energy for four cases. In each case, we take the size of systems $N = 10\,000$, the hopping interaction $V = 1$, the site energy $\varepsilon_{\rm b} = V = 1$ and a defect concentration $p = 0.5$. The numerical results are shown in Figure 2. In Figure 2a, transmittance *versus* energy for the trimer model (Fig. 1a) is shown. It is well known that there are two peaks ($E = 0.0$ and $E = 2.0$) in the transmission spectrum. In Figures 2b and 2c, we present the results for the model of Figure 1b for $\varepsilon_{\rm c} = 0.0$ and $\varepsilon_{\rm c} = 20.0$, respectively, where two peaks ($E = -1.0$ and $E = 2.0$) appear in the former figure, but only one maximum $E = 2.0$ has survived in the latter figure. These results can be well explained by equation (10). As we can see when $\varepsilon_{\rm c} = 0.0$, the resonant energies are

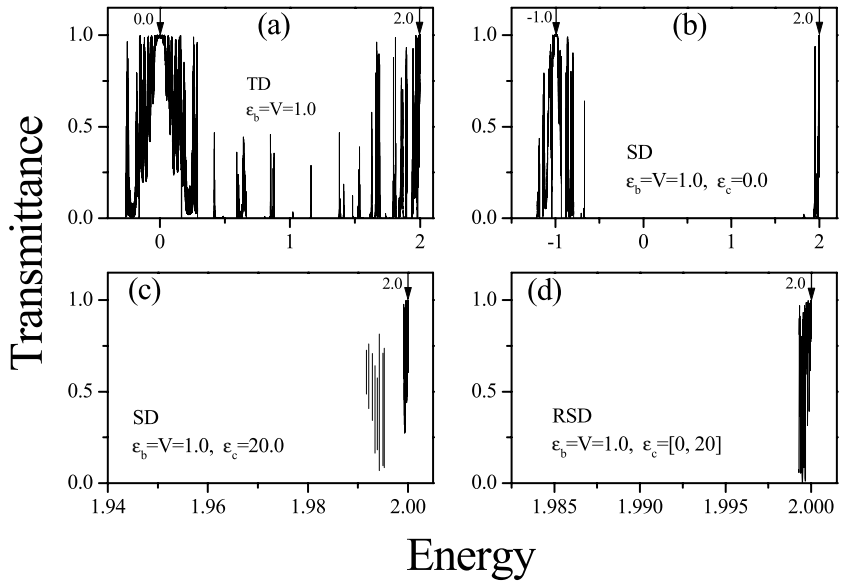

Fig. 2. Transmittance as a function of the energy for the systems of Figure 1 with 10 000 lattice sites, hopping interaction $V = 1.0$ and defect concentration $p = 0.5$. (a) the model of Figure 1a with $\varepsilon_\mathrm{b} = 1.0$; (b) and (c) the same model of Figure 1b, $\varepsilon_\mathrm{c} = 0.0$ for former figure, $\varepsilon_\mathrm{c} = 20.0$ for latter figure; and (d) the model Figure 1c with $\varepsilon_\mathrm{r} = [0, 20]$.

$E = \varepsilon_\mathrm{c} - V = -1.0$ and $E = 2V = 2.0$. When $\varepsilon_\mathrm{c} = 20.0$, the resonant energy $E = \varepsilon_\mathrm{c} - V = 19.0 > 2V$ is forbidden, consequently, only the peak $E = 2V = 2.0$ is remained. Finally, for the model of disordered $\varepsilon_\mathrm{c} = [0, 20]$ of Figure 1c, only one resonant peak ($E = 2.0$) can be found in Figure 2d.

4 Wave functions and MSD

4.1 Periodic-like wave functions

In the previous study of the transmission coefficient of states we have shown that there exist resonant energies where the electronic states remain unscattered by the symmetric defect of $\varepsilon_\mathrm{b}\varepsilon_\mathrm{c}\varepsilon_\mathrm{b}$. It should be noted that, the result does not necessarily mean that those states are true extended. This fact requires us to seek a different approach to study the localization of the eigenstates. The spatial distribution of wave functions have been considered as the most solid evidence of the localization in low dimensional random and pseudorandom systems.

As is well known, in a one-dimensional perfect lattice, the eigenstates are simply Bloch states of the form $\mathrm{e}^{\mathrm{i}kn}$. When the defects $\varepsilon_\mathrm{b}\varepsilon_\mathrm{c}\varepsilon_\mathrm{b}$ are embed in the perfect lattice because the eigenstates near the resonant energies have unit transmission (see Sect. 3), we can ensure that the electron wave functions for the resonant energies are still of the Bloch form. For simplicity, we consider the single symmetric defect to occupy sites 0, 1 and 2. Then the electron wave function before and after it has interacted with the impurity has the form $\mathrm{e}^{\mathrm{i}kn}$ for $n \leq 0$ and $\mathrm{e}^{\mathrm{i}kn+\mathrm{i}\Omega}$ for $n \geq 2$, where Ω is the phase shift. To proceed we study the phase shift for the resonant electronic states in an otherwise ordered lattice containing one single symmetric defect. In the case of $E = 2V$, from the eigenvalue equations for site 0 and 2, we obtain that the phase shift through a symmetric defect is $\Omega = -3k + \pi$. As a result, the wave function amplitudes around the defect satisfy $c_{-1} = \mathrm{e}^{-\mathrm{i}k}$, $c_0 = 1$, $c_1 = 1 - \mathrm{e}^{-\mathrm{i}k}$, $c_2 = -\mathrm{e}^{-\mathrm{i}k}$, $c_3 = -1$. For another resonant energy $E = \varepsilon_\mathrm{c} - V$, we find that the state satisfies $\mathrm{e}^{\mathrm{i}kn}$ for $n \leq 0$ and $-\mathrm{e}^{\mathrm{i}k(n-1)}$ provided that $-V \leq \varepsilon_\mathrm{c} \leq 3V$. The corresponding phase shift is $\Omega = -k + \pi$.

Below we study numerically the electron wave functions for the three models of correlated site energies defined in Section 2, and some wave functions are obtained at the special energies $E = -1.0$, 1.0 and 2.0.

In Figure 3, we show some extended electronic states with eigenvalues nearest to $E = 2.0$ for the three models of Figure 1 with the same site number $N = 1000$ and hopping interaction $V = 1$, respectively. Among which Figures 3a–c are for the trimer defects of Figure 1a with site energies $\varepsilon_\mathrm{b} = 1.0$, Figures 3d–f are for the model of Figure 1b with site energies $\varepsilon_\mathrm{b} = 1.0$ and $\varepsilon_\mathrm{c} = 50$, the rest three figures (Figs. 3g–i) are for the model of Figure 1c with same site energies $\varepsilon_\mathrm{b} = 1.0$, but random distribution of $\varepsilon_\mathrm{c} = [0, 50]$.

In Figure 4, we show some periodiclike electron wave functions in the model of Figure 1b. For the model with $\varepsilon_\mathrm{b} = 1$ and $\varepsilon_\mathrm{c} = 2$, we show the three states (Figs. 4a–c) with eigenvalues nearest to the resonant energy $E = \varepsilon_\mathrm{c} - V = 1.0$. The Figures 3d–f are obtained for the electronic states around the resonant energy $E = \varepsilon_\mathrm{c} - V = -1.0$ for the model with $\varepsilon_\mathrm{b} = 1.0$ and $\varepsilon_\mathrm{c} = 0$. Of course, the resonant energy $E = 2.0$ exists in both cases and the corresponding electron wave functions are similar to Figure 3. Although the studied systems are different, it is easy to conclude that these figures have a similar characteristic of periodic-like extended states as the results of RDM [11]. These results are in agreement with that obtained in Section 3, where we have indicated that the perfect transmission can be found in the corresponding systems near the resonant energies.

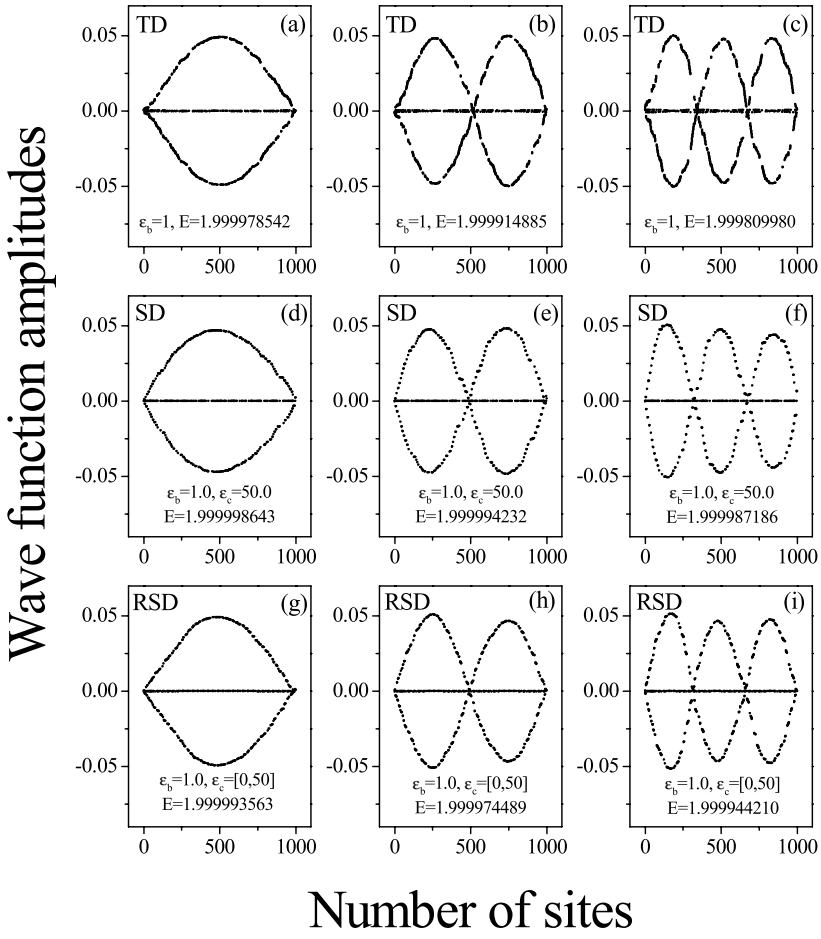

Fig. 3. The periodiclike wave functions for the systems of Figure 1 with size of sample $N = 1000$, $V = 1.0$. (a−c) for the case of Figure 1a, (d−f) for the case of Figure 1b, and (g−i) for the case of Figure 1c.

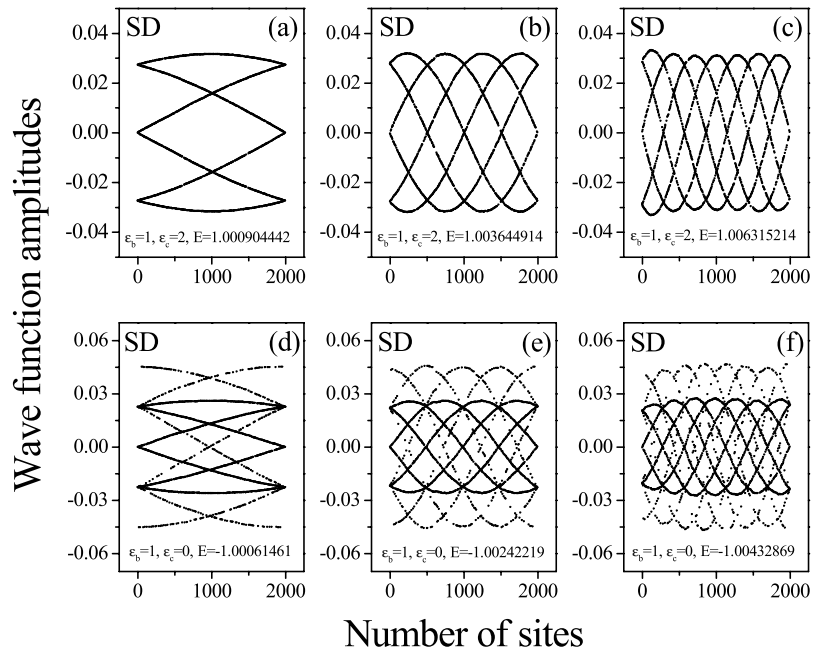

Fig. 4. The periodic-like wave functions for the system of Figure 1b with size of sample $N = 2000$, $\varepsilon_b = V = 1.0$. (a–c) for the case $\varepsilon_c = 2.0$ (d–f) for the case $\varepsilon_c = 0.0$.

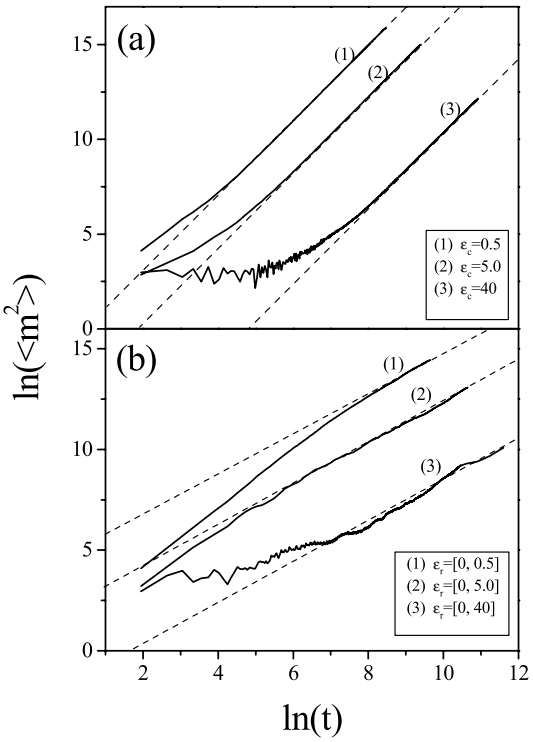

Fig. 5. Mean-square displacement for the systems of Figures 1b and 1c, respectively. (a) Constant ε_c of three values: 0.5, 5 and 40, (b) random ε_r of three distributions: $[0, 0.5]$, $[0, 5]$ and $[0, 40]$. The dotted parallel lines are those with a slope of 2 for (a), and 1 for (b). Consequently, the MSD behaves as t^2 for constant ε_c, and t for random ε_r, respectively.

4.2 Mean-square displacement

Since the pioneering work of Anderson [1], the problem of the absence of diffusion in certain random and aperiodic systems is studied by evaluating the time evolution of mean-square displacement (MSD). As mentioned in the introduction, Dunlap *et al.* [3] have shown the diffusion and superdiffusive behaviors in RDM. In a recent work, Brito *et al.* [25] have studied the propagation of carriers in 1D Fibonacci and Thue-Morse lattices, in the field-free case, they have found the MSD grow as t^α with $\alpha = 1.55$ for the Fibonacci and $\alpha = 1.65$ for the Thue-Morse lattice, respectively.

For the dynamical localization problem, one usually starts from investigating the time evolution of a particle using the time-dependent Schrödinger equation (1). The propagation of initially localized particle in a lattice can be characterized by the mean square displacement (MSD) which is defined as

$$\left\langle m^2 \right\rangle = \sum_m m^2 \left| C_m \right|^2 . \tag{23}$$

The MSD usually follows a power law

$$\left\langle m^2 \right\rangle \sim t^\beta . \tag{24}$$

When $\beta = 0$ the particle is localized, when $0 < \beta < 1$ it is subdiffusive, $\beta = 1$ corresponds to a diffusive behavior, $1 < \beta < 2$ is for superdiffusive, $\beta = 2$ means that the motion is ballistic.

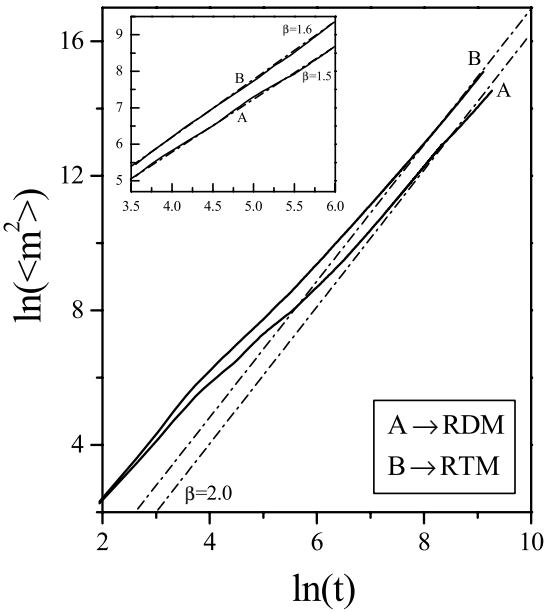

Fig. 6. Mean-square displacement for the systems of the RDM and RTM with the parameters $\varepsilon_a = 0.0$, $\varepsilon_b = \varepsilon_c = 1.0$, and $V = 1.0$.

In this section, we focus on the study of the influence of ε_c on the propagation of particle in the systems of Figure 1b and Figure 1c. The numerical calculations performed here are based on the same treatment of DWP in their paper [3]. In order to avoid the influence of boundaries, we can treat the lattice in a self-expanding manner. In the calculations, we examine the amplitudes of wave function on the last atoms, and if the amplitudes approach the preset small value, then we can add some atoms to the lattice.

The results from the random model of Figure 1b for three different values of ε_c are shown in Figure 5a. From this figure, we have $\beta = 2.00 \pm 0.09$ and the MSD follow the law t^2 for all three cases considered. In other word, the particle will propagate ballistically in the system despite of the value of ε_c. For large ε_c, it takes longer times to reach the ballistic regime. In Figure 5b, the results for three cases of Figure 1c are shown. We consider that the ε_c are randomly distributed within the interval: (a) $\varepsilon_c = [0, 0.5]$, (b) $\varepsilon_c = [0, 5]$ and (c) $\varepsilon_c = [0, 40]$, respectively. From the figure, we can see clearly that, unlike the cases of constant ε_c, here $\beta = 1.00 \pm 0.15$ and the MSD grow as t in all three cases. Consequently, we have diffusive behaviors under the condition of random ε_c.

When $\varepsilon_c = 1.0$, the corresponding system of Figure 1b is exactly the random trimer model (RTM). One would have thought that both lattices (RDM and RTM) would behave identically. In reference [3], the authors found superdiffusive transport for the RDM. Surprisingly, we observe the ballistic motion in the RTM for sufficiently long times. To settle this disagreement, we calculate the MSD for the RDM and RTM with the same parameters. The numerical results are shown in Figure 6, though, the exponents have quite some uncertainly, we find that, for long times, the exponent for the RDM is much greater than 1.5.

We note that, in reference [3], the numerical results were obtained when $Vt < 10^4$. In fact, our numerical result (see the Fig. 6 inset) illustrates that, when $Vt < 10^6$, the MSD of the RDM is well represented by $t^{1.5}$ line. This result is in agreement with that obtained in reference [3]. In addition, in our previous publication [11], we numerically proved that, for the RDM systems with different exponents ($\beta = 1.5$ and $\beta = 1.0$), the number of extended states are proportional to $C\sqrt{N}$, where C is a constant and N is the atom number. Though, our numerical results here indicate that, for the given parameter $\varepsilon_{\rm b} = 1.0$ of RDM, the exponent $\beta > 1.5$, yet we consider the argument that the number of extended states $\tilde{}\sqrt{N}$ is correct.

5 Summary

We have investigated three one dimensional tight-binding on-site models with special correlated random site energies. In the work we have studied, mainly by numerical calculations, the transmission coefficient, the wave function and the mean-square displacement. For the symmetric defect ($\varepsilon_{\rm b}\varepsilon_{\rm c}\varepsilon_{\rm b}$) of one-dimensional chain (host site energies $\varepsilon_{\rm a} = 0$ and hopping interaction V), we have found that, when $\varepsilon_{\rm b} = V$, there exists always one resonant energy $E = 2V$ which is independent of the choice of site energy $\varepsilon_{\rm c}$. We have given an analytical explanation of the phenomenon by making use of the transfer matrix method. For three different distributions of $\varepsilon_{\rm c}$, we have presented some periodic-like wave functions near the resonant energies. For any constant $\varepsilon_{\rm c}$, we have found ballistic transport for sufficiently long times. When $\varepsilon_{\rm c}$ is randomly distributed in a given region, diffusive behavior is observed.

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