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Delocalization and wave-packet dynamics in one-dimensional diluted Anderson models

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Abstract. We study the nature of one-electron eigen-states in a one-dimensional diluted Anderson model where every Anderson impurity is diluted by a periodic function $f(l)$. Using renormalization group and transfer matrix techniques, we provide accurate estimates of the extended states which appear in this model, whose number depends on the symmetry of the diluting function $f(l)$. The density of states (DOS) for this model is also numerically obtained and its main features are related to the symmetries of the diluting function $f(l)$. Further, we show that the emergence of extended states promotes a sub-diffusive spread of an initially localized wave-packet.

PACS. 63.50.+x Vibrational states in disordered systems – 63.22.+m Phonons or vibrational states in low-dimensional structures and nanoscale materials – 62.30.+d Mechanical and elastic waves; vibrations

1 Introduction

The nature of electronic states in disordered tight-binding models with site-diagonal uncorrelated disorder was firstly studied by Anderson [1] when the localization of quantum states was discussed in connection with the transport properties of a random lattice. One of the most remarkable effects of disorder, which has been demonstrated by several authors, is the exponential localization of all one-electron eigen-states in the one-dimensional Anderson model, irrespective to the strength of disorder [2]. The electron localization in random lattices is a result of destructive quantum interference due to incoherent backscattering. Therefore, the localization phenomenon occurs in general model systems involving wave propagation in random media.

Recently, the existence of delocalized states in several variants of the low-dimensional Anderson models has been reported [3–19]. In these works, the presence of short or long-range correlations appears as the fundamental mechanism responsible for the emergence of extended states. This theoretical prediction about suppression of localization was recently confirmed experimentally in doped polyaniline [20], semiconductor superlattices with intentional correlated disorder [21] as well as microwave transmission spectra of single-mode waveguides with inserted correlated scatterers [22]. Among these models, the diluted Anderson chain has attracted a renewed interest [23–27]. Hilke [23] introduced an Anderson model with diagonal disorder diluted by an underlying periodicity. The model consisted of two interpenetrating sub-lattices, one composed of random potentials (Anderson lattice) and the other composed of non-random segments of constant potentials. Due to the periodicity, special resonance energies appear which are related to the lattice constant of the non-random lattice. The number of resonance energies is independent of the system size and, therefore, it was conjectured that these states shouldn't have any influence on the transport properties in the infinite size limit. In reference [25] the authors presented a simple model for alloys of compound semiconductors by introducing a one-dimensional binary random system where impurities are placed in one sublattice while host atoms lie on the other sublattice. The existence of an extended state at the band center was demonstrated, both analytic and numerically. The diluted Anderson model was recently extended to include a general diluting function which defines the on-site energies within each non-random segment [24]. Using a block decimation approach, it was demonstrated that this model displays a set of extended states, the number of which strongly depends on the length of the diluting segments and the symmetries of the diluting function.

In this work we will use the matrix decimation method and the transfer matrix technique to provide accurate estimates of the set of extended states in general 1D diluted Anderson models. The density of states (DOS) will be shown to display a set of gaps whose number and width

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depend on the set of impurities used to dilute the disordered lattice. Further, we will investigate the influence of such resonant extended states on the wave-packet dynamics. Our results suggest that, in spite of the number of resonance energies being independent of the system size [23], these extended states induce a sub-diffusive spread of an initially localized wave-packet.

2 Model and formalism

The standard one-dimensional Anderson model is described by a tridiagonal Hamiltonian

$$H = \sum_j \epsilon_j |j\rangle\langle j| + t\sum_j [|j\rangle\langle j+1| + |j\rangle\langle j-1|] \quad (1)$$

where disorder is introduced on the site energies ϵ_j which are uncorrelated random numbers chosen from a previously defined distribution. In our calculations, we will use energy units such that the hopping term $t = 1$ and the random site energies will be taken uniformly from the interval $[-0.5, 0.5]$. The diluted Anderson model is constructed by introducing a sequence of k new sites between each original pair of neighboring sites. These sequences are all identical and the on-site energies within such sequences are given by $f(l)$, $l = 1, 2, ..., k$.

To study the properties of the one-electron eigenstates, we employ a transfer matrix calculation (TM) in order to obtain the Lyapunov exponent defined as the inverse of the localization length L_c. The Schrödinger equation for the present tight-binding model is:

$$\epsilon_n c_n + c_{n-1} + c_{n+1} = E c_n, \quad (2)$$

where $\Phi = \sum_n c_n |n\rangle$ is an eigenstate with energy E. The above equation can be rewritten as a transfer matrix equation

$$\begin{pmatrix} c_{n+1} \\ c_n \end{pmatrix} = \begin{pmatrix} E-\epsilon_n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_n \\ c_{n-1} \end{pmatrix}, \; n = 0, 1, 2, ..., N. \quad (3)$$

Based on the asymptotic behavior of the matrix product $\prod_{n=1}^{N} Q_n$, where Q_n are 2×2 transfer matrices, the Lyapunov exponent γ can be defined as:

$$\gamma = \lim_{N\to\infty} \frac{1}{N} \log \frac{|\prod_{n=1}^{N} Q_n z(0)|}{|z(0)|}, \quad (4)$$

where $z(0) = \binom{u_1}{u_0}$ is a generic initial condition. In addition, the Lyapunov exponent can be obtained using a decimation renormalization-group (DRG) technique which is based on the particular form of the equation of motion satisfied by the Green's operator matrix elements $[G(E)]_{i,j} = \langle i|1/(E-H)|j\rangle$ [12]:

$$\begin{aligned}(E-\epsilon^0_{n+\mu})[G(E)]_{n+\mu,n} &= \delta_{n+\mu,n} \\ &+ t^0_{n+\mu,n+\mu-1}[G(E)]_{n+\mu-1,n} \\ &+ t^0_{n+\mu,n+\mu+1}[G(E)]_{n+\mu+1,n}, \quad (5)\end{aligned}$$

where $\epsilon^0_n = \epsilon_n$ and $t^0_{n,n+1} = t^0_{n-1,n} = t$. After eliminating the matrix elements associated with a given site, the remaining set of equations can be expressed in the same form as the original one, but with energies and hopping amplitudes renormalized. Therefore, the decimation-renormalization technique consists in removing iteratively the sites $1, 2, ..., N-1$ of the system obtaining in that way the effective energies of the external sites and the effective hopping between them by using the iterative equations

$$\epsilon_N^{(N-1)}(E) = \epsilon_N + t_{N-1,N} \frac{1}{E - \epsilon_{N-1}^{(N-2)}(E)} t_{N-1,N}, \quad (6)$$

$$t_{0,N}^{(eff)}(E) = t_{0,N-1}^{(eff)} \frac{1}{E - \epsilon_{N-1}^{(N-2)}(E)} t_{N-1,N}, \quad (7)$$

where, after $N-1$ decimations, ϵ_N^{N-1} denotes the renormalized diagonal element at site N and $t_{0,N}^{(eff)}$ indicates the effective renormalized hopping connecting the sites 0 and N. The behavior of the effective interaction $t_{0,N}^{(eff)}$ during the decimation procedure can be used as another evidence of the localized/delocalized nature of the one-electron states. An oscillatory behavior of $t_{0,N}^{(eff)}$, as a function of N, signals an extended state. On the contrary, an exponentially localized state results in an exponential decrease of $t_{0,N}^{(eff)}$ as the decimation process proceeds. After a large number of decimation steps, the Lyapunov exponent is asymptotically related to the effective hopping $t_{0,N}^{(eff)}$ in the following way:

$$\gamma(E) = -\lim_{N\to\infty} \left[\frac{1}{N} \ln \left| t_{0,N}^{(\mathrm{eff})}(E) \right| \right].$$

3 Results and discussion

In the present study, we use chains with 10^7 sites in order to calculate the Lyapunov exponent within the entire energy band. We start our analysis investigating the main features of a diluted 1D Anderson model with segments consisting of two sites with identical on-site energies ϵ_0. The emergence of extended states for this particular dilution was analytically demonstrated in [23,24]. The density of states (DOS) for general 1D tight-binding models can be obtained by using the negative eigenvalue theorem [35]. In Figure 1a we show typical plots of the DOS of chains with $N = 10^5$ sites and several ϵ_0 values. In this diluted chain, the density of states displays two pseudo-gaps for $\epsilon_0 > 0$. The widths of these pseudo-gaps increase as a function of ϵ_0. These pseudo-gaps are reminiscent of the gaps present in the absence of disorder and their width is proportional to ϵ_0 for any length of the diluting segment (see Fig. 1b), thus following a similar trend of the gap found in the two band model [37]. The presence of disorder rounds one of the band edges which displays an exponentially decaying tail. On the other hand, the opposite band edge remains as a singularity of the DOS. The surviving of this singularity in the presence of disorder

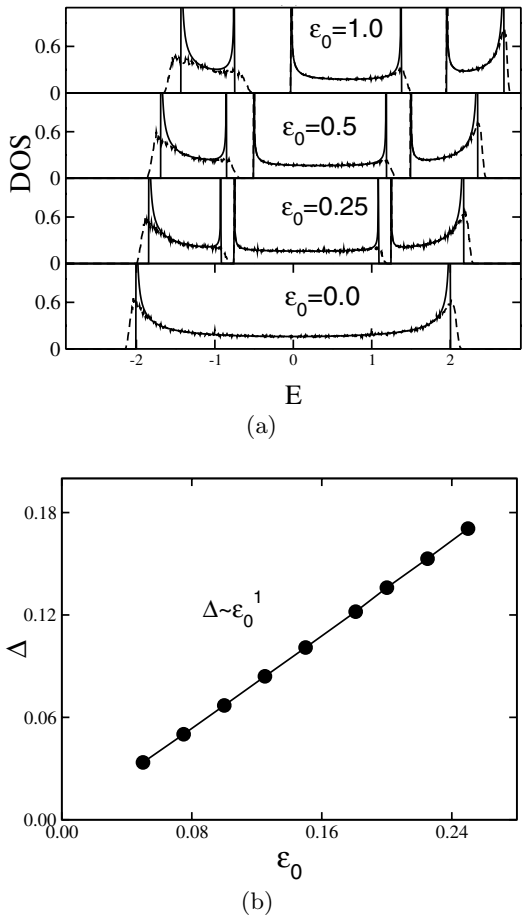

Fig. 1. (a) Dashed lines represent the normalized density of states (DOS) as a function of energy E obtained using the Dean's method for a chain with $N = 10^5$ sites of the diluted 1D Anderson model with dimer segments of identical on-site energies ϵ_0. The DOS displays two pseudo-gaps for $\epsilon_0 > 0$, which are reminiscent of the gaps present in the DOS of the corresponding pure models (shown as solid lines). (b) The width of the gap (Δ) for a diluted chain without disorder versus ϵ_0. The width Δ displays a linear behavior $\Delta \propto \epsilon_0^1$ for any length of the diluting segment.

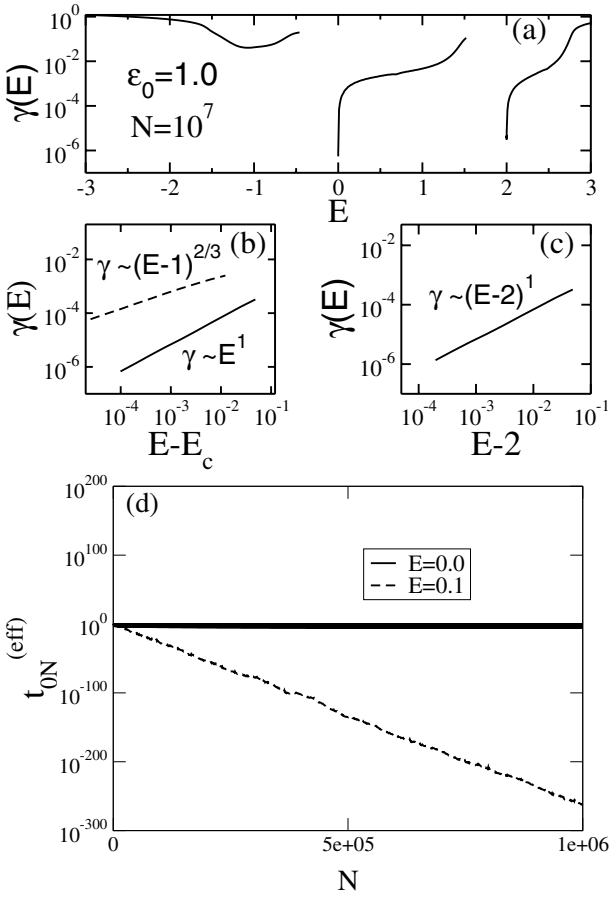

Fig. 2. a) Lyapunov exponent γ versus E for a chain with $N = 10^7$ sites diluted by dimers with $\epsilon_0 = 1.0$. We found that γ is finite for all energies except at the two resonance energies where γ vanishes linearly (see b) and c)). For $\epsilon_0 = 0.0$, one has a slower non-linear vanishing of $\gamma \propto (E - E_c)^{(2/3)}$ (see long-dashed line in Fig. b). (d) The effective hopping $t_{0,N}^{(\mathrm{eff})}$ displays an oscillating behavior as a function of N for $E = 0.0$ (extended state) and an exponentially decaying behavior for $E = 0.1$ (localized state).

will be shown to influence the wave-packet dynamics of the diluted Anderson model.

In Figure 2a we depict the Lyapunov exponent γ versus E for chains with $N = 10^7$ sites and $\epsilon_0 = 1.0$. We calculate γ using both transfer matrix and decimation renormalization group approaches. The results were identical within our numerical accuracy. We found that $\gamma(E)$ is finite for all energies except at the two resonance energies ($E = 0.0$ and $E = 2.0$) where the Lyapunov exponent is of the order $\frac{1}{N}$. Therefore, all states are exponentially localized except at these two resonance energies where γ vanishes in the thermodynamic limit. This result coincides with the analytical prediction of extended states at $E = \epsilon_0 \pm 1$ [24]. In Figures 2b and c, we point out the linear vanishing of γ around $E = 0$ and $E = 2.0$ (see full lines in Figs. 2b and 2c). For $\epsilon_0 = 0.0$, we found a slower non-linear vanishing of $\gamma \propto (E - E_c)^{(2/3)}$ (see dashed line in Fig. 2b), in perfect agreement with reference [23]. The larger exponent found for $\epsilon_0 \neq 0$ can be attributed to fact that the resonance energies for $\epsilon_0 \neq 0$ are precisely at the DOS band edge singularities, which are absent for $\epsilon_0 = 0$. To further characterize the extended nature of these resonant states, we plot in Figure 2d the effective interaction $t_{0,N}^{(eff)}$ versus N. For the resonant state at $E = 0.0$ the Lyapunov exponent γ vanishes due to the oscillating behavior of $t_{0,N}^{(\mathrm{eff})}$. The extended character of this state is, therefore, reflected by a finite effective hopping amplitude between the sites located at the chain ends. For $E = 0.1$ the effective hopping decreases exponentially, indicating the localized character of non-resonant states. We have also considered longer diluting sequences with constant on-site energy. The number of extended states always corresponds to the number of sites in the sequence, as expected [23,24].

From the theoretical point of view, the basic condition to find delocalized states in diluted disordered systems is the existence of some symmetries in the periodic function $f(l)$ which defines the site energies $\epsilon_l = f(l)$ within the

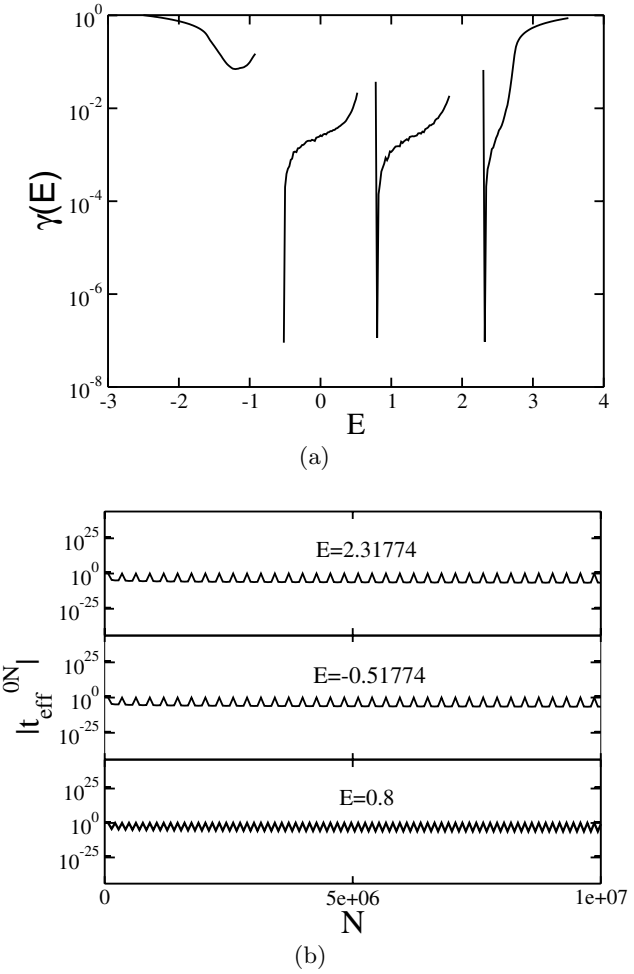

Fig. 3. a) The Lyapunov exponent γ versus E for an Anderson chain diluted by segments with $k = 3$ sites exhibiting specular symmetry $f(l) = \{\epsilon_2, \epsilon_3, \epsilon_2\}$ where $\epsilon_2 = 0.8$ and $\epsilon_3 = 1.0$. All calculations were performed for a chain with $N = 10^7$ sites. (b) The effective hopping $t^{(eff)}_{0,N}$ as a function of N for the resonance energies $E_c = \{0.8, 2.31774, -0.51774\}$ corresponding to extended states.

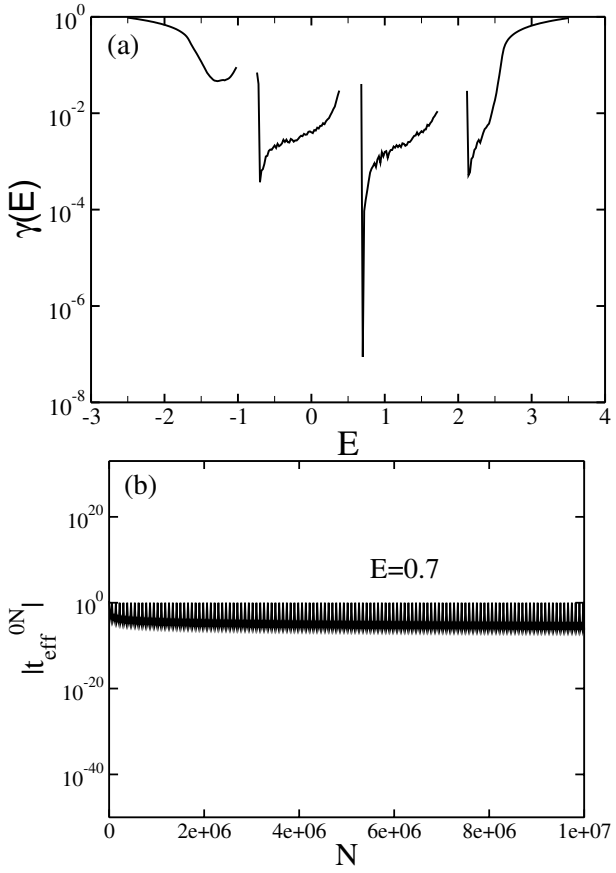

Fig. 4. (a) The Lyapunov exponent γ versus E for an Anderson chain with $N = 10^7$ sites diluted by segments with $k = 3$ sites exhibiting the distance to center symmetry $f(l) = \epsilon_l = \{0.8, 0.7, 0.6\}$. In this case, there is a single extended state located at the resonance energy $E = 0.7$. (b) The effective hopping $t^{(eff)}_{0,N}$ as a function of N for $E = 0.7$ shows the oscillating behavior characteristic of extended states.

diluting segment. The relevant symmetries are [24]:
a) Specular reflection symmetry with respect to center of the diluting segment, namely, $f(l) = f(k + 1 - l)$, with $l = 1, 2, ...k$.
b) Distance to the center symmetry, namely, $|f(l_0) - f(l_0 - j)| = |f(l_0) - f(l_0 + j)|$, with j ranging from $j = 1$ to $j = (k-1)/2$ and l_0 being the position of the central segment site. This kind of symmetry can be present only in segments with an odd number of sites.

Delocalized states emerge whenever the diluting function exhibits one of the above symmetries. In the following, we consider two examples using diluting segments with either one of the above symmetries present.

To observe the emergence of extended states in the diluted Anderson model with specular reflection symmetry, we considered a diluting segment with $k = 3$ sites: $f(l) = \{\epsilon_2, \epsilon_3, \epsilon_2\}$, where the site energies are $\epsilon_2 = 0.8$ and $\epsilon_3 = 1.0$, respectively. In Figure 3a we show the Lyapunov exponent γ versus E. All calculations were performed for $N = 10^7$ sites. After executing the renormalization process, we found that the Lyapunov exponent vanishes for $E_c \approx \{0.8, 2.31774, -0.51774\}$, in agreement with the block decimation result [24]. In addition, we show in Figure 3b the oscillating pattern exhibited by the effective hopping $t^{(eff)}_{0,N}$ as a function of N for the same critical energies, thus confirming the extended nature of these states.

A similar analysis can be made to investigate a diluted Anderson chain with the distance to the center symmetry. We considered, for this case, the following diluting function: $f(l) = \epsilon_l = \{0.8, 0.7, 0.6\}$. From the theoretical calculation of [24], one can anticipate that this chain will have only one extended state with energy $E_c = 0.7$. Figures 4a and b clearly show that the Lyapunov exponent vanishes only for $E_c = 0.7$ and the effective hopping $t^{(eff)}_{0,N}$ displays an oscillating behavior at this critical energy.

In order to investigate the influence of the above resonant extended states on the transport properties of the diluted Anderson model, we calculate the time dependence of the mean-square displacement of an initially localized wave-packet. Starting with one electron fully localized at

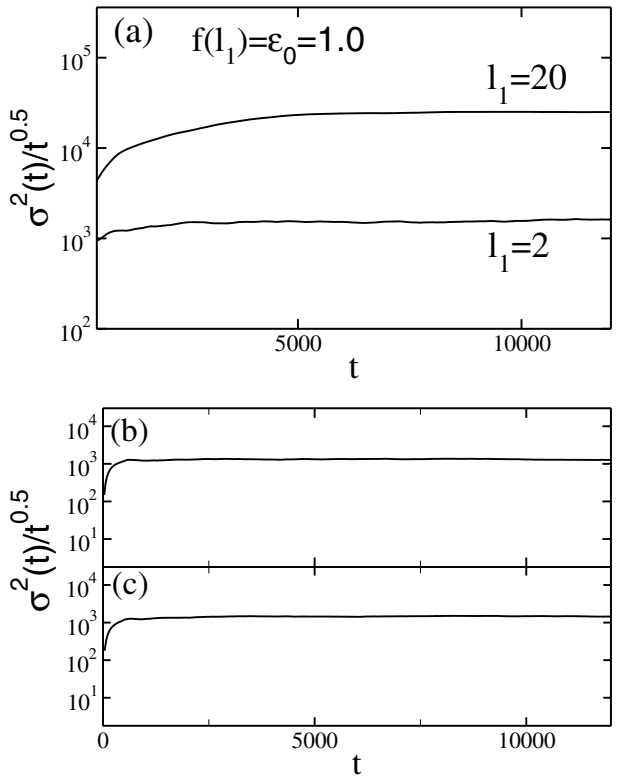

Fig. 5. The scaled mean-square displacement $\sigma^2(t)/t^{0.5}$ versus times t for the 1D diluted Anderson model with 7×10^4 sites for: a) Constant diluting function $\epsilon_0 = f(l_1) = \epsilon_0 = 1$ with $l_1 = 2, 20$. (b) Diluting function with specular reflection symmetry $f(l) = \{\epsilon_2, \epsilon_3, \epsilon_2\}$ with $\epsilon_2 = 0.8$ and $\epsilon_3 = 1.0$ (c) Diluting function with the distance to center symmetry $f(l) = \{0.8, 0.7, 0.6\}$. A sub-diffusive behavior $\sigma^2 \propto t^{0.5}$ takes place for any symmetry supporting extended states.

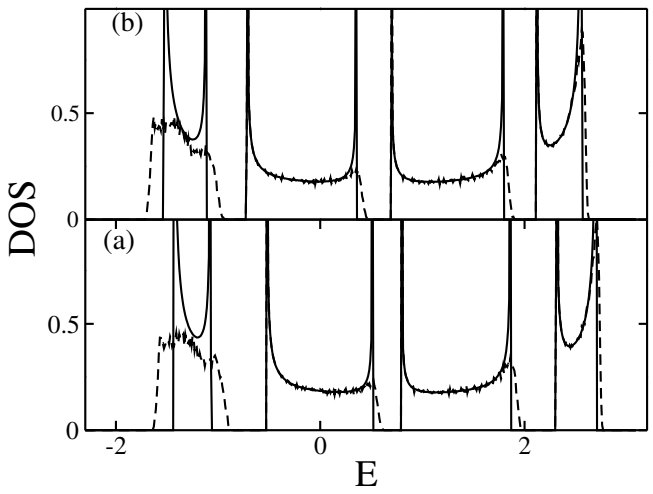

Fig. 6. Dashed lines represent the normalized density of states (DOS) for the diluted chain with a) specular reflection symmetry $f(l) = \{0.8, 1.0, 0.8\}$ and b) distance to the center symmetry $f(l) = \{0.8, 0.7, 0.6\}$. In both cases, the resonance energies associated with extended states are coincident with DOS singularities.The DOS displays pseudo-gaps for $\epsilon_0 > 0$, which are reminiscent of the gaps present in the DOS of the corresponding pure models (shown as solid lines).

the Anderson site closer to the chain center, the wave-function amplitudes $b_n(t)$ were obtained from the following equations of motion:

$$i\dot{b}_n(t) = \epsilon_n b_n(t) + (b_{n-1}(t) + b_{n+1}(t)) \qquad n = 1, 2, ..., N. \tag{8}$$

Using a Runge-Kutta algorithm, we solve the above set of coupled equations and calculate the mean-square displacement

$$\sigma^2(t) = \sum_n (n - n_0)^2 |b_n(t)|^2. \tag{9}$$

To minimize end effect, our numerical calculation was performed in a very large chain with $N = 7 \times 10^4$ sites. As a consequence, the site amplitudes at the ends of the chain ($b_1(t)$ and $b_N(t)$) are always negligible. The numerical integration of equations (8) was performed using the Runge-Kutta algorithm with precision Δt smaller than 10^{-2}. In Figures 5a–c, we exhibit our main results for the time evolution of the mean-square displacement $\sigma^2(t)$ on diluted chains considering all relevant symmetries of the diluting function. In all cases, we obtained a clear sub-diffusive behavior: $\sigma^2 \propto t^{0.5}$. This sub-diffusive spread of the wave-packet is related to the fact that the resonance energies supporting extended states occur at band edge singularities of the DOS, as depicted in Figure 6. A similar diffusive-like spread of the wave-packet has also been observed to occur with collective excitations in other disordered systems with the Lyapunov exponent vanishing at DOS singularities as, for example, in random harmonic chains [34] and disordered ferromagnetic chains [7,29].

4 Summary and conclusions

In summary, we investigated the 1D diluted Anderson model where every Anderson impurity is diluted by a set of site energies given by a diluting function $f(l)$. Using the renormalization group approach and the transfer matrix technique, we obtained the Lyapunov exponent γ in several diluting cases exploring distinct symmetries supporting extended states, such as constant diluting function, diluting function with either specular reflection or distance to the center symmetry. In all cases, we identified the resonance energies at which the model exhibit extended states, in full agreement with previous results [23,24]. We also studied the temporal spread of an initially localized electron wave-function in these diluted chains by following the time dependence of the wave-packet mean-square displacement. We found that, associated with the presence of extended states at resonance energies located at DOS band edge singularities, the electron wave-packet displays a sub-diffusive spread ($\sigma^2(t) \propto t^{0.5}$). This result is consistent with the general picture that the wave-packet dynamics depends on the relative location of resonance energies and DOS singularities [36].

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