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Sensitivity to initial conditions of the wave-packet dynamics in diluted Anderson chains

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Abstract

We study the one-electron wave-packet dynamics in the one-dimensional diluted Anderson model which is composed of two interpenetrating chains with pure and random on-site potentials, respectively. This model presents extended states at a particular resonance energy. Starting with one electron fully localized at the site closer to the chain center, we solve the set of coupled motion equations and calculate the time evolution of the wave-packet width. We report on a long-time memory effect which is reflected by distinct asymptotic dynamics governing the wave-function spread for electrons initially localized at random or pure sites. This anomalous behavior is discussed under the light of the Bloch character of the extended resonant state.

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Keywords: Anderson localization; Electronic transport; Diluted disorder

1. Introduction

The problem involving the spread of one-electron wave-functions in low-dimensional disordered systems is a well-known issue with several connections with transport properties [1–3]. In general lines, the wave-function of an electron moving in a perfectly periodic potential spreads linearly in time. In the presence of uncorrelated disorder, the scaling theory predicts the absence of extended eigenstates [4] in one-dimensional (1D) systems. Therefore, the width of the time-dependent wave-function saturates in the long time limit, i.e., the electron wave-function remains localized in a finite region around the initial position. The scaling theory prediction of exponential localization of all one-electron eigenfunctions in 1D systems can be violated when special short-range [5] or long-range [6,7] correlations are present in the disorder distribution. The influence of scale-free disorder in the 3D Anderson transition has also been recently addressed [8]. In particular, the presence of dimer-like correlations on a N-site binary chain produces $\sqrt{N}$ extended states. These states have random phase changes when crossing the dimer impurities which results in a finite coherence length. If the energy of the resonant extended state is within the band of allowed states of the underlying pure chain, the electron wave-packet experiences a superdiffusive spread [5].

It has been reported that the fractal dimensions D_2^{μ} and D_2^{ϕ} associated with the energy spectra and eigenfunctions, respectively, determine the spread of the wave-function [9] for systems where the shape of wave-packet is preserved. The kth moments of the wave-function increase as $t^{k\gamma}$ with $\gamma = D_2^{\mu}/D_2^{\phi}$ and the return probability decrease as $t^{-D_2^{\mu}}$. In fact, it was numerically verified that the dynamical behavior of the Anderson model at the quantum Hall regime is connected with the energy spectra and eigenfunctions using exactly the above relations between dynamical exponents and the fractal dimensions [10,11]. More recently, the metal–insulator transition in the two-dimensional Anderson model with long-range correlations was characterized by measuring the participation number exponent

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D_2^{μ} from the long-time behavior of the wave-function spacial distribution [12].

Within the field of electrons in solids with correlated disorder, the diluted Anderson chain has attracted a renewed interest [13–17]. Hilke [13] introduced an Anderson model with diagonal disorder diluted by an underlying periodicity. The model consists of two interpenetrating sublattices, 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 with vanishing wave-function amplitudes on the random lattice. The extended states in the diluted Anderson model are in fact Bloch waves with infinite coherence length. In Ref. [15], 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 [14]. 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. Recently, accurate estimates of the set of extended states in general 1D diluted Anderson models was presented [18]. The authors also showed that such resonant extended states influence the wave-packet dynamics. Recently, the diluted Anderson model was extended for a 2D lattice [19]. Using analytical and numerical methods, it was shown that the 2D diluted Anderson model displays a metal–insulator transition which was compared with recent experimental results in 2D disordered samples [20].

The diluted Anderson model has a quite particular feature related to the infinite coherence length of their resonant states. As the extended states do not probe the underlying randomness, they provide a distinct framework for electronic transport in systems with correlated disorder, as compared to models with dimer-like correlated disorder whose extended state depicts random phase changes [5]. In this work we address to this important question and provide a detailed study of wave-packet spread by numerically solving the time-dependent Schrödinger equation for the complete Hamiltonian in a 1D diluted Anderson chain. We restrict our analysis to the simplest case where every Anderson impurity is diluted by a single pure site with on-site energy equal to ϵ_0. Starting with one electron fully localized at the site closer to the chain center, we will solve the set of coupled motion equations and calculate the time-evolution of the wave-packet spacial distribution. In particular, we will show that the dynamics of the wave-packet spread is strongly dependent on the initial condition, thus revealing a long-time memory effect.

2. Model

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

$$H = \sum_j \epsilon_j |j\rangle\langle j| + t \sum_j \big[|j\rangle\langle j+1| + |j\rangle\langle j-1|\big], \tag{1}$$

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 $[-5, 5]$. Weaker disorder leads typically to longer localization lengths and consequently longer transient times prior to the asymptotic dynamical regime. The diluted Anderson model we are going to consider is constructed by introducing a pure site with on-site energy ϵ_0 between each original pair of neighboring Anderson sites [13]. Another version of the diluted Anderson model considers the diluting site with on-site energy $\epsilon_0 = 0$ and the random potential with a tunable average value [15]. The above two versions are actually equivalent differing only up to a constant shift in the potential.

To study the wave-packet dynamics, we follow the time evolution of an initially localized electron. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation as

$$i\dot{\phi}_n(t) = \epsilon_n \phi_n(t) + \big(\phi_{n-1}(t) + \phi_{n+1}(t)\big), \quad n = 1, 2, \ldots, N. \tag{2}$$

We consider a wave packet initially localized at site i_0, i.e., $\phi_i(t=0) = \delta_{i,i_0}$. A fourth-order Runge–Kutta method is used to solve the above set of coupled differential equations. We will be particularly interested in calculate the wave-packet spacial distribution $|\phi_i(t)|^2$ as well as the square root of the electron mean-square displacement defined by

$$\sigma(t) = \sqrt{\sum_{i=1}^{N} \big(i - \langle i(t)\rangle\big)^2 \big|\phi_i(t)\big|^2}, \tag{3}$$

where $\langle i(t)\rangle = \sum_{i=1}^{N} i|\phi_i(t)|^2$ is the average electron position at time t. We choose the initial site i_0 close to the chain center. To minimize end effects, our numerical calculations were performed in long chains with $N \approx 6 \times 10^4$ sites. As a consequence, the wave-function amplitudes at the ends of the chain ($\phi_1(t)$ and $\phi_N(t)$) were always negligible within the finite time intervals we considered. However, these were much larger than the initial transient time and, therefore, we could infer about the asymptotic scaling regime which sets up in the long-time domain. We choose two distinct kinds of initial conditions: i_0 being an Anderson site (a random site) and i_0 being a pure site of the diluting sublattice.

3. Results and discussion

The numerical integration of Eq. (2) was performed using the Runge–Kutta algorithm with time step $\Delta t = 10^{-2}$. An average of the time history over 100 distinct disorder configurations was performed. We start our analysis investigating the main features of a diluted 1D Anderson model with $\epsilon_0 = 1$. The emergence of extended states for this particular dilution was analytically and numerically demonstrated in Refs. [13–15,18].

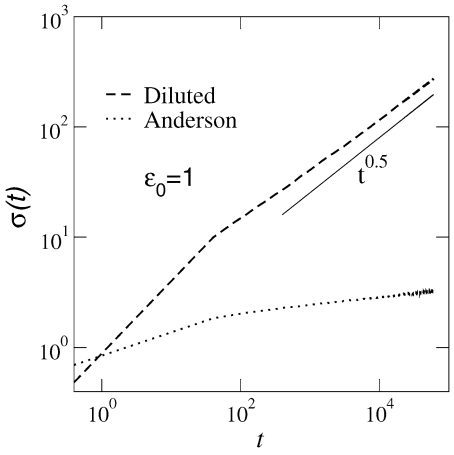

Fig. 1. The scaled root mean-square displacement of the electron $\sigma(t)$ versus times t for the 1D diluted Anderson model with 6×10^4 sites, $\epsilon_0 = 1$. i_0 was chosen to be an Anderson site (dotted line) in and a diluting site (dashed line). The distinct scaling exponents characterize the strong sensitivity to the initial condition exhibited by the wave-function spread.

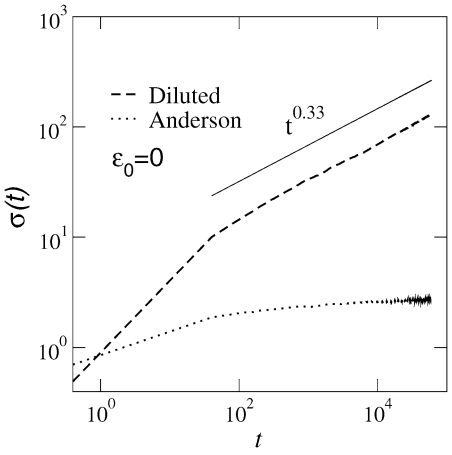

Fig. 2. The scaled root mean-square displacement of the electron $\sigma(t)$ versus times t for the 1D diluted Anderson model with 6×10^4 sites, $\epsilon_0 = 0$. i_0 was chosen as an Anderson site (dotted line) and a diluted site (dashed line). Notice again the sensitivity to the initial condition presented by the wave-function spread which is reflected by distinct asymptotic scaling behaviors.

The density of states (DOS) exhibits a pseudo-gap, with an exponentially decaying tail as approaching $E = 1$ from below, which is reminiscent of the true band-gap appearing in a binary periodic chain. The resonant energy corresponding to the extended state is located at a DOS singularity and the localization length diverges like $\xi \propto 1/(E - E_c)$ as one approach the resonance energy [18].

In Fig. 1 we show typical plots of the scaled average electron displacement $\sigma(t)$ versus time for a chain with $N = 6 \times 10^4$ sites. i_0 was chosen to be an Anderson site (dotted line) and a diluting site (dashed line). We can see a clear dependence of the asymptotic dynamical exponent of the mean electron displacement $\sigma(t)$ on the initial electron position. For an initial condition fully localized in a pure site, the mean electron displacement $\sigma(t)$ displays a diffusive spread [$\sigma(t) \propto t^{0.50(5)}$] in contrast with the localized spread found when the electron is initially located at the random sublattice. Actually, our data cannot rule out the possibility of a very slow logarithmic spread in this case.

In Fig. 2 we report the time evolution of the root mean-square electron displacement $\sigma(t)$ in a chain with $N = 6 \times 10^4$ sites and $\epsilon_0 = 0$. In this particular case, the density of states has no pseudo-gap and the localization length exhibits a slower divergence as one approaches the resonance energy on the form $\xi \propto 1/(E - E_c)^{2/3}$ [13,18]. As in Fig. 1, i_0 was chosen to be at the Anderson sublattice (dotted line) and at the diluting sublattice (dashed line). Notice again a clear dependence of $\sigma(t)$ on the kind of initial condition. For an electron initially localized in a diluting site, the average electron displacement $\sigma(t)$ displays now a subdiffusive spread [$\sigma(t) \propto t^{0.33(5)}$] in contrast with the diffusive dynamics found for $\epsilon_0 = 1$. On the other hand, $\sigma(t)$ exhibits localized spread when one starts from an Anderson site.

The different dynamical regimes observed for the cases of $\epsilon_0 = 0$ and $\epsilon_0 = 1$ can be related to the distinct divergences exhibited by the localization length and the behavior of the density of states close to the resonance energy. $\xi \propto 1/(E - E_c)$

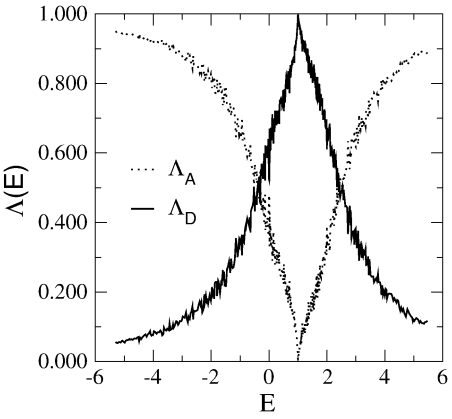

Fig. 3. The wave-function components on the random sites $\Lambda_A(E) = (\sum_{i=1,3,5,\ldots,N-1} |\phi_i(E)|^2)$ and diluting sites $\Lambda_D(E) = (\sum_{i=2,4,6,\ldots,N} |\phi_i(E)|^2)$ obtained using exact diagonalization in a chain with 500 sites, $\epsilon_0 = 1$ and periodic boundary conditions. The vanishing of $\Lambda_A(E_c)$ reflects the fact that the extended state in this model is fully localized on the diluting sublattice.

with E_c being a band gap singularity for $\epsilon_0 = 1$ while $\xi \propto 1/(E - E_c)^{(2/3)}$ with no energy gap at E_c for $\epsilon_0 = 0$. To understand the origin of the sensitivity to initial conditions of the electronic wave-function spread, one shall notice that an initially localized wave-packet has a wide spectral distribution and, therefore, has contributions coming from many energy eigenstates. However, an electron wave-packet fully localized at the random sublattice has no contribution coming from the extended state, once it has vanishing amplitudes at this sublattice. In order to better illustrate this feature, we computed the sum of the components of each wave-function belonging to the random sublattice $\Lambda_A(E) = (\sum_{i=1,3,5,\ldots,N-1} |\phi_i(E)|^2)$ and to the diluting sublattice $\Lambda_D(E) = (\sum_{i=2,4,6,\ldots,N} |\phi_i(E)|^2)$. A similar quantity has been recently used to study the localization properties of quasiperiodic chains on which the sensitivity of the wave-packet dynamics to the initial condition was reported [21]. In Fig. 3 we shown the results for $\Lambda_A(E)$ and $\Lambda_D(E)$

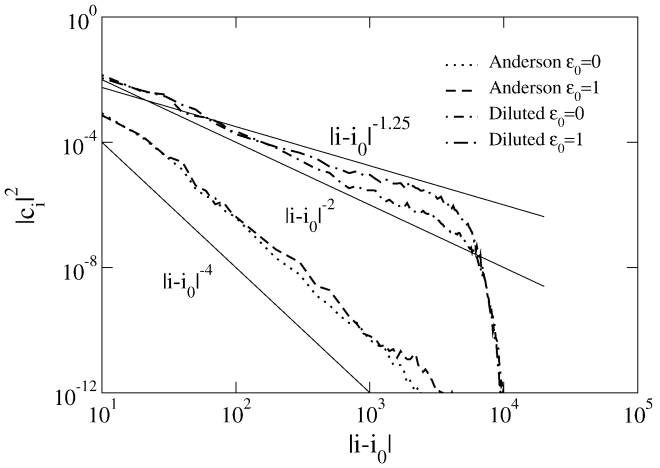

Fig. 4. Square of the average wave-function components after a long time spread ($t > 10000$) versus index site $i - i_0$ for two initial conditions and representative diluting energies. The developed power-law decay prior to the exponential cutoff is in the origin of the diffusive-like spread. The decay exponents $|\phi_j|^2 \propto 1/|i - i_0|^{D_\Phi}$ in the intermediate regime are, from the bottom to the top line, $D_\Phi = 4.0(2)$, 4.0(2), 2.0(1) and 1.25(1).

obtained from exact diagonalization of the Hamiltonian in a chain with 500 sites, periodic boundary conditions and $\epsilon_0 = 1$. These plots clearly show that the extended state in this model is fully localized on the diluting sublattice, i.e., $\Lambda_A(E_c) = 0$. Further, as one approach the resonance energy, the states have linearly vanishing amplitudes at the Anderson sublattice. Therefore, when starting with a wave-packet fully on the Anderson sublattice, there is a very small contribution coming from the effectively extended states, thus resulting in a slower wave-function spread. It is worth to mention that the energy spread on disordered harmonic chains also shows a sensitivity to initial conditions whose origin is related to the different forms the effectively extended modes contribute to the spectral decomposition of impulse and displacement excitations [22]. To complete the above picture, we plot in Fig. 4 the wave-function components $|\phi_i|^2$, after a long-time evolution ($t > 10000$) and averaged over 100 histories with distinct disorder realizations, versus site index $i - i_0$ for both initial conditions and two representative values of ϵ_0. In any case, the wave-function develops a power-law decay which is followed by an exponential tail due to the finite spreading time used. The power-law decay exponents are distinct when different initial conditions and diluting on-site energies are considered, thus supporting the sensitivity to initial condition of the asymptotic wave-packet dynamics.

4. Summary and conclusions

In summary, we investigated the 1D diluted Anderson model where every Anderson impurity is diluted by a single site with on-site energy ϵ_0. We start with one electron fully localized at the site closer to the chain center and solved the set of coupled motion equations to calculate the root mean-square displacement of the electron. Due to the presence of extended states, this model does not display the usual localization of the wave-packet in one-dimensional disordered systems. We obtain an unexpected dependence of wave-packet time-evolution with the electron initial position. Starting with one electron fully localized at a diluting site, this system presents a faster wave-function spread than that exhibited by an electron initially localized at a random site. In fact, the extended states of this model are fully localized at diluting sites. Therefore, a wave-packet fully localized on the Anderson sublattice has a small contribution coming from spectral components with large localization lengths and, as such, the wave-function spread results slower. In addition, we showed numerically that the time-dependent wave function develops a spacial distribution with a power-law tail. The characteristic scaling exponent of the wave-function distribution is different for distinct initial conditions, thus supporting the sensitivity to initial conditions of the asymptotic time evolution. Semiconductor superlattices with impurities located at alternating layers could be used as an experimental ground to observe this effect once the electronic transport properties would be sensitive to the nature of the carriers injection layer. However, incoherent scattering on the impurities and the need of single layer excitement may difficult such experimental realization. Although the carrier scattering by impurities may limit the experimental observation to thin superstructures, which would bring to the analysis finite-size effects, the single layer excitement can be optically realizable by pumping the superlattice with a focused laser.

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