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Correlation-induced metal-insulator transition in the one-dimensional Anderson model

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Abstract

We study the nature of the electronic states in tight-binding one-dimensional models with long-range correlated disorder. In particular, we study both diagonal and off-diagonal chains. The energies are considered to be in such a sequency to describe the trace of a fractional Brownian motion with a specified spectral density $S(k) \propto 1/k^{\alpha}$. Using a renormalization group technique, we show that for random on-site energy sequences with anti-persistent increments ($\alpha < 2$) all energy eigenstates are exponentially localized. On the other hand, for on-site energy sequences with persistent increments ($\alpha > 2$), the Lyapunov coefficient (inverse localization length) vanishes within a finite range of energy values revealing the presence of an Anderson-like metal–insulator transition. In the case of off-diagonal disorder a phase of delocalized states becomes stable for any $\alpha > 1$.

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In the recent years, a series of one-dimensional versions of the Anderson model has been shown to exhibit a breakdown of Anderson's localization induced by internal correlations on the disorder distribution [1–5]. Most of these models consider on-site energies ε_n distributed in such a way that the impurity always appears in finite segments of fixed size. Extended states arise from resonant modes which present no backscattering through these finite structures. Such states form a discrete set of energy values. Therefore, these models do not present a true disorder induced metal–insulator transition in the thermodynamic limit which is characterized by the presence of mobility edges separating extended and localized energy eigenstates. Also, chains with correlated off-diagonal interactions [1,3,4] have been reported to display delocalized states.

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Within this context, a natural question to be made is about the possible effects due to long-range correlations in the disorder distribution. Several stochastic processes in nature are known to generate long-range correlated random sequences which have no characteristic scale [6,7]. These sequences usually have an approximate power-law spectral density of the form $S(k) \propto 1/k^{\alpha}$, where k is related to the wavelength λ of the undulations on the random parameter landscape by $k = 1/\lambda$. In a recent work, Russ et al. [8] have shown that the states near the center of the bond are strongly sensitive to long-range correlations in the disordered potential.

In this work, we further investigate the nature of one-electron states of the 1D Anderson model with long-range correlated disorder characterized by a power-law spectral density. The energy landscape is derived from the trace of a fractional Brownian motion. By using a renormalization group method, we show that all one-electron states remain localized for $\alpha < 2$, but there is a finite range of energy values with extended eigenstates for $\alpha > 2$ even in the thermodynamic limit.

At first, we consider a Hamiltonian model describing one electron moving in a chain with a single orbital per site and nearest-neighbor interactions. In the atomic orbital wave function basis $\{|n\rangle\}$ the Hamiltonian is expressed as

$$H = \sum_n \varepsilon_n |n\rangle\langle n| + t \sum_n [|n\rangle\langle n+1| + |n\rangle\langle n-1|] , \tag{1}$$

where ε_n is the energy at site n and t is the first-neighbor hopping amplitude. Hereafter we will use energy units of $t = 1$. In the standard Anderson model the site energies are considered to assume random values uncorrelated from site to site exhibiting, therefore, a white noise spectrum $S(k) \propto k^0$.

In order to introduce long-range correlations in the disorder distribution, the site-energies ε_n are derived from the trace of a fractional Brownian motion with a specified spectral density $S(k) \propto 1/k^{\alpha}$. For $\alpha = 0$ one recovers the traditional Anderson model with δ-correlated disorder $\langle \varepsilon_n \varepsilon_{n'} \rangle = \langle \varepsilon_n^2 \rangle \delta_{n,n'}$. In the case of $\alpha = 2$ the sequency of site energies resembles the trace of the usual Brownian motion. The exponent α is directly related to the Hurst exponent H of the rescaled range analysis ($\alpha = 2H + 1$) which describes the self-similar character of the series and the persistent character of its increments. To generate the trace of a fractional Brownian motion, we followed an approach based on the use of discrete Fourier transforms [9–12]. A power-law spectral density is imposed by construction when one chooses the on-site energies to be given by the relation

$$\varepsilon_i = \sum_{k=1}^{N/2} \left[k^{-\alpha} \left(\frac{2\pi}{N} \right)^{(1-\alpha)} \right]^{1/2} \cos\left(\frac{2\pi i k}{N} + \phi_k \right) , \tag{2}$$

where N is the number of sites and ϕ_k are $N/2$ random phases uniformly distributed in the interval $[0, 2\pi]$. In what follows we will normalize the energy sequence to have $\langle \varepsilon_n \rangle = 0$ and $\langle \varepsilon_n^2 \rangle = 1$.

To study the properties of the one-electron states of the above model, we applied the general renormalization technique to the one-dimensional nearest-neighbor tight-binding model. The method is based on the particular form assumed by the equation of motion

satisfied by the Green's operator matrix elements $[G(z)]_{mn} = \langle m|1/(z-\mathscr{H})|n\rangle$ [13,14]:

$$(z-\varepsilon^0_{n+\mu})[G(z)]_{n+\mu,\,n} = \delta_{\mu,\,0} + t_{n+\mu,\,n+\mu-1}[G(z)]_{n+\mu-1,\,m,} + t_{n+\mu,\,n+\mu+1}[G(z)]_{n+\mu+1,\,n,} \tag{3}$$

where $\varepsilon^0_i = \varepsilon_i, t^0_{i,\,i+1} = t$ and $\mu = 0, \pm 1, \pm 2, \ldots$.

After eliminating the elements associated with a given site, the remaining set of equations of motion can be expressed in the same form as the original one but with site energies and hopping amplitude renormalized. The operation of renormalization consists in removing iteratively the sites $1, 2, 3, \ldots, N$ of the lattice, obtaining the effective energies of the extremal sites and the effective hopping interaction between them through the following three iterative equations:

$$\varepsilon^{(N+1)}_0(E) = \varepsilon^{(N)}_0(E) + t^{(eff)}_{0N}\frac{1}{E-\varepsilon^{(N-1)}_N(E)}t^{(eff)}_{0N}\,, \tag{4}$$

$$\varepsilon^{(N)}_{N+1}(E) = \varepsilon_{N+1} + t\frac{1}{E-\varepsilon^{(N-1)}_N(E)}t\,, \tag{5}$$

$$t^{(eff)}_{0,\,N+1}(E) = t^{(eff)}_{0N}(E)\frac{1}{E-\varepsilon^{(N-1)}_N(E)}t\,, \tag{6}$$

where $\varepsilon^{(N)}_0(\varepsilon^{(N)}_{N+1})$ is the effective energy at site 0 $(N+1)$ after the dizimation of the N internal sites and $t^{(eff)}_{0,\,N+1}$ is the effective hopping between sites 0 and $N+1$.

We investigate the nature of the electronic states by computing the Lyapunov coefficient γ (inverse localization length). Farchioni et al. [14] have shown that, after a large number of iterations, γ is asymptotically related to the effective hopping amplitude as

$$\gamma(E) = \lim_{N\to\infty}\left[\frac{1}{N}\ln\left|\frac{G_{N,\,N}(E)}{G_{0,\,N}(E)}\right|\right] = -\lim_{N\to\infty}\frac{1}{N}\ln\,|t^{(eff)}_{0,\,N}(E)|\,. \tag{7}$$

Therefore, a linear regression of $\ln|t^{(eff)}_{0,\,N}(E)|$ versus N allows for a direct extrapolation of the Lyapunov coefficient in the thermodynamic limit after a finite, although large, number of iterations. The effective interaction $t^{(eff)}_{0N}(E)$ presents an oscillating behavior in the case of extended states (which implies in a vanishing γ) and an exponentially decreasing behavior for exponentially localized states (finite γ).

We computed $\gamma(E)$ within the band of allowed energies for distinct values of the exponent α. In Fig. 1 we show plots of γ versus E for two typical values of α corresponding to an anti-persistent ($\alpha = 1.0$) and a persistent ($\alpha = 2.5$) sequency as obtained from chains with $N = 10^4$ sites. Data from larger chains produce curves indistinguishable to the eyes and, therefore, the observed trends shall remain even in the thermodynamical limit. For random sequences with anti-persistent increments, we obtained that the Lyapunov coefficient is finite within the entire band of allowed energies indicating that all electronic eigenstates remain exponentially localized, with the localization being more pronounced near the band edges, as usual. However, this picture is qualitatively different for potentials with persistent increments ($\alpha > 2$). The Lyapunov

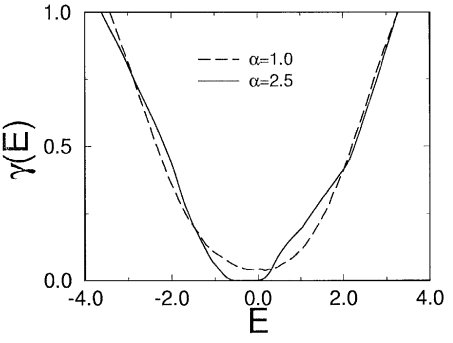

Fig. 1. Lyapunov coefficient γ versus E as obtained from the renormalization procedure on chains with random on-site energies, $N = 10^4$ sites and $\alpha = 1.0$ (on-site energy landscape with anti-persistent increments) and $\alpha = 2.5$ (on-site energy landscape with persistent increments). The vanishing of the Lyapunov coefficient within a finite range of energy values for $\alpha = 2.5$ indicates the presence of a phase of extended states near the center of the band. Data from larger chains produce curves indistinguishable to the eyes.

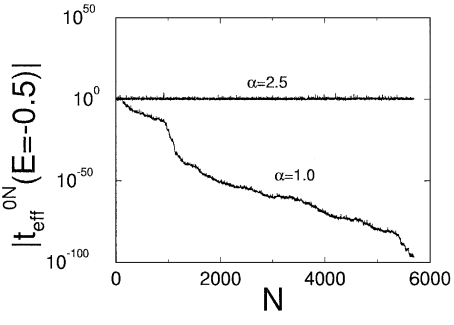

Fig. 2. The effective interaction $|t_{0,N}^{(eff)}(E)|$ versus the number of iterations N for a sequency with originally 10^4 sites and $E = -0.5$. (a) $\alpha = 1.0$ for which the one-electron states are localized (exponentially decaying effective interaction); (b) $\alpha = 2.5$ showing the oscillatory behavior typical of extended states.

coefficient vanishes within a finite range of energy values revealing the presence of a phase of extended states near the center of the band. For $\alpha = 2.0$ the Lyapunov coefficient vanishes in a single energy as $\gamma \propto |E - E_c|^{\nu}$ with $\nu = 2.0$. The range of energies corresponding to extended states increases with α, with the Lyapunov coefficient vanishing linearly near E_c for large values of α. In Fig. 2 we show the effective interaction $|t_{0,N}^{(eff)}(E)|$ versus N to exemplify the exponential decaying character of the effective interaction for localized states in contrast to its oscillating behavior in the case of extended states.

We further investigate the random hopping version of the present model whose Hamiltonian is given by

$$H = \sum_n \varepsilon |n\rangle\langle n| + \sum_n t_n [|n\rangle\langle n+1| + |n+1\rangle\langle n|] \,, \tag{8}$$

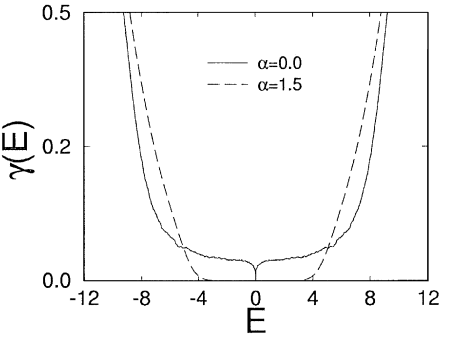

Fig. 3. Lyapunov coefficient γ versus E as obtained from the renormalization procedure on chains with random hopping amplitudes, $N = 10^4$ sites and $\alpha = 0.0$ and $\alpha = 1.5$. The results are similar to the random diagonal case with a delocalized phase emerging for $\alpha > 1$. The vanishing of γ at the center of the band for $\alpha < 1$ is associated with the presence of a quasi-delocalized state with a stretched exponential envelope [15].

where t_n are assumed to have the same Fourier decomposition as in Eq. (2). For the sake of simplicity, we will assume $\varepsilon = 0$ without any loss of generality. In order to avoid a vanishing hopping amplitude we normalize the hopping to have $\langle t_n \rangle = 4$ and $\Delta t_n = \sqrt{\langle t_n^2 \rangle - \langle t_n \rangle^2} = 1$. The Lyapunov coefficient for distinct values of α is shown in Fig. 3. It depicts a phase of delocalized states near the center of the band for $\alpha > 1$. The vanishing of γ at the center of the band for $\alpha < 1$ is associated with the presence of a quasi-delocalized state with a stretched exponential envelope [15].

In summary, we found that the one-dimensional Anderson model with long-range correlated diagonal displays a phase of extended electronic states once the disorder distribution exhibits a spectral density $S(k) \propto 1/k^{\alpha}$ with $\alpha > 2$, i.e., whenever the energy sequency increments have a long-range persistent character. In the case of off-diagonal disorder a phase of extended states becomes stable for $\alpha > 1$. Contrary to dimer-like models where delocalization is observed only at particular resonance energies, these models exhibit a true Anderson transition with mobility edges separating localized and thermodynamically extended states.

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