Delocalization in the 1D Anderson Model with Long-Range Correlated Disorder

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We study the nature of electronic states in a tight-binding one-dimensional model with the on-site energies exhibiting long-range correlated disorder and nonrandom hopping amplitudes. The site energies 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 long-range correlated 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. [S0031-9007(98)07502-4]

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The simplest theoretical model containing the basic ingredients for studying the nature of one-electron states in disordered systems was introduced by Anderson [1] which considered one-electron moving in a lattice endowed by a random potential and allowed to hop only to nearest-neighbor sites. Anderson pointed out that if the disorder is very strong the wave function may become exponentially localized with a characteristic localization length l_c. Further, scaling arguments applied to noninteracting electron systems in the presence of uncorrelated disorder have indicated that all one-electron states are exponentially localized in one and two dimensions for any amount of disorder, with a true metal-insulator transition taking place only in 3D on which one-electron states may remain extended for weak disorder [2,3].

The scaling prediction of the absence of extended states in one dimension agrees with a series of analytical results which show that all wave functions must have an exponentially decaying envelope whenever the potential assumes random values uncorrelated from site to site [4]. In recent years, there has been a growing interest in the study of the role played by correlations in the nature of the one-electron states of low-dimensional disordered systems. The reason for that is based on the fact that 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 [5–13]. 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 [5,9,11] have been reported to display delocalized states. More recently, thermally annealed disordered chains with the on-site energies correlated as $\langle \epsilon_i \epsilon_j \rangle \propto e^{-|i-j|/\xi}$ have also been investigated [14]. It has been shown that the localization length monotonically increases with the correlation length ξ, but all states remain localized due to the absence of typical resonances. A common point on all these models is the fact that localization properties are modified when some kind of short-range correlation is introduced in the disorder distribution.

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 [15]. These sequences usually have an approximate power-law spectral density of the form $S(k) \propto 1/k^{\alpha}$, where $S(k)$ is the Fourier transform of the two-point correlation function $\langle \epsilon_i \epsilon_j \rangle$ and k is related to the wavelength λ of the undulations on the random parameter landscape by $k = 1/\lambda$. The widespread occurrence in nature of sequences with $1/k^{\alpha}$ noise, as, for example, the nucleotide sequency in DNA molecules [16], seems to be related to the general tendency of large driven dynamical systems to evolve for a self-organized critical state [17].

In this work, we investigate the nature of one-electron states of the 1D Anderson model on which the on-site energies exhibit a long-range correlated disorder distribution characterized by a power-law spectral density. The on-site energy landscape is generated by considering the potential as 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.

In what follows, we will 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

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

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 will be considered to be in such a sequency to describe the trace of a fractional Brownian motion with a specified spectral density $S(k) \propto 1/k^\alpha$. For $\alpha = 0$ one recovers the traditional Anderson model with δ-correlated disorder $\langle \epsilon_n \epsilon_{n'} \rangle = \langle \epsilon_n^2 \rangle \delta_{n,n'}$. 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 with a chosen spectral density, we followed an approach based on the use of discrete Fourier transforms to construct long-range correlated sequences [18–20]. A power-law spectral density is imposed by construction when one chooses the on-site energies to be given by the relation

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

where N is the number of sites and ϕ_k are $N/2$ independent random phases uniformly distributed in the interval $[0, 2\pi]$. In what follows we will normalize the energy sequency to have $\langle \epsilon_n \rangle = 0$ and $\Delta\epsilon = \sqrt{\langle \epsilon_n^2 \rangle - \langle \epsilon_n \rangle^2} = 1$. In Fig. 1, we plot typical traces generated by the preceding relation. Notice the smoothening of the energy landscape for persistentlike sequences ($\alpha > 2; H > 1/2$). These have the feature of displaying well defined power-law spectral densities in contrast to real correlated sequences which exhibit a noisy power-law spectrum. We expect that the present filtering of the noise in the amplitudes of the Fourier components of the potential does not include or remove any relevant feature associated with the underlying correlations.

The analytical arguments used to demonstrate the complete localization in one-dimensional disordered chains cannot be extended to the present model. Complete localization is a consequence of a limiting theorem (Furstenberg theorem) about the product of *uncorrelated* random variables [4]. Contrary to short-range correlations, long-range ones cannot be removed by any coarse-graining procedure. 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 whose Schroedinger equation reads

$$\epsilon_n u_n + t(u_{n-1} + u_{n+1}) = E u_n , \quad (3)$$

where $|\Psi\rangle = \sum_n u_n |n\rangle$ is an eigenstate with energy E. The method is based on the particular form assumed by the equation of motion satisfied by the Green's

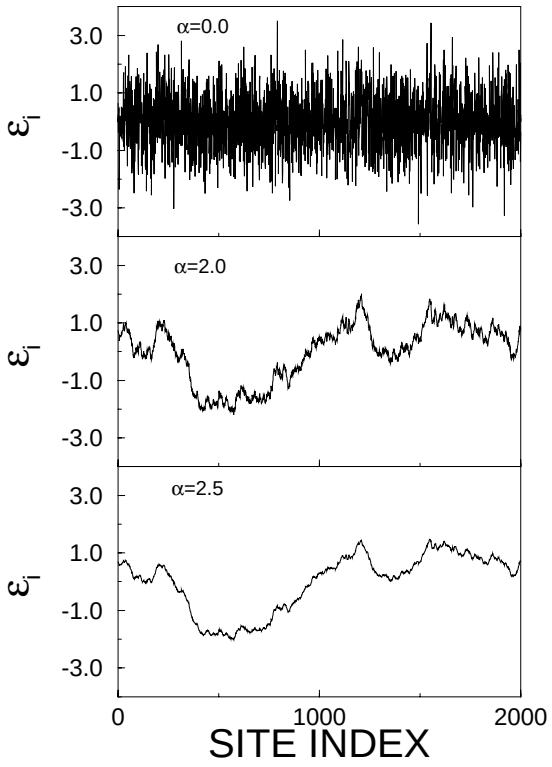

FIG. 1. Typical on-site energy landscapes generated from relation (2) with $N = 4096$: $\alpha = 0.0$: uncorrelated random sequency; $\alpha = 2.0$: trace of a usual Brownian motion; $\alpha = 2.5$: trace of a fractional Brownian motion with persistent increments. Notice the smoothening of the energy landscape for increasing values of α.

operator matrix elements $[G(z)]_{mn} = \langle m | \frac{1}{z - \mathcal{H}} | n \rangle$ [21,22]:

$$\begin{aligned}(z - \epsilon^0_{n+\mu})[G(z)]_{n+\mu,n} = \delta_{\mu,0} \\ + t^0_{n+\mu,n+\mu-1}[G(z)]_{n+\mu-1,n} \\ + t^0_{n+\mu,n+\mu+1}[G(z)]_{n+\mu+1,n} ,\end{aligned} \quad (4)$$

where $\epsilon^0_i = \epsilon_i$, $t^0_{i,i+1} = t^0_{i,i-1} = t$, 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. Therefore, 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:

$$\epsilon_0^{(N+1)}(E) = \epsilon_0^{(N)}(E) + t_{0N}^{(\mathrm{eff})} \frac{1}{E - \epsilon_N^{(N-1)}(E)} t , \quad (5)$$

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

$$t^{(\mathrm{eff})}_{0,N+1}(E) = t^{(\mathrm{eff})}_{0N}(E)\,\frac{1}{E - \epsilon^{(N-1)}_{N}(E)}\,t\,, \qquad (7)$$

where $\epsilon^{(N)}_0$ ($\epsilon^{(N)}_{N+1}$) is the effective energy at site 0 ($N+1$) after the decimation of the N internal sites and $t^{(\mathrm{eff})}_{0,N+1}$ 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.* [22] have shown that, after a large number of iterations, γ is asymptotically related to the effective hopping amplitude as

$$\gamma(E) = \lim_{N\to\infty}\left[\frac{1}{N}\ln\left|\frac{G_{N,N}(E)}{G_{0,N}(E)}\right|\right] = -\lim_{N\to\infty}\frac{1}{N}\ln|t^{(\mathrm{eff})}_{0,N}(E)|\,. \qquad (8)$$

Therefore, a linear regression of $\ln|t^{(\mathrm{eff})}_{0,N}(E)|$ 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 $t^{(\mathrm{eff})}_{0N}(E)$ presents an oscillating behavior in the case of extended states (which implies 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. The density of states (DOS) was numerically obtained using Dean's method, which is based on the negative eigenvalue theorem [23]. In Fig. 2 we show typical plots of the DOS as obtained from particular energy sequences on chains with 10^4 sites. Notice that the DOS becomes less rough as the characteristic exponent α is increased, but the imposed normalization makes its width α independent. The density of states has no sharply defined band edges but stretches for energies outside the Lifshitz boundaries ($E/t = \pm 4$) because ranges of additional states become available through the disordered potential distribution [24].

In Fig. 3 we show plots of γ versus E for typical values of α. For $\alpha = 0$, 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. We also included the Lyapunov coefficient obtained for a chain with random uncorrelated on-site energies whose spectrum has also $\alpha = 0$ but exhibits a white noise in the Fourier component amplitudes. Both curves show similar trends which indicates that the filtering of the amplitude noise does not influence the localization properties, as expected. We found that $\gamma(E)$ is finite within the entire band of allowed energies for all potentials which have antipersistent increments ($\alpha < 2$). However, this picture is qualitatively different for potentials with persistent increments ($\alpha > 2$). The Lyapunov coefficient vanishes within a finite range of energy values revealing the presence of a phase of extended states near the center of the band. In this phase, the error inherent to the numerical regression, although very small, is such that $\gamma = 0$ is within the error bar. Further, the effective hopping does not show any tendency of vanishing within this range as the renormalization procedure goes on. It oscillates around a constant value which is a typical signature of extended states, as shown in Fig. 4. We have studied chains with size ranging from 10^4 up to 10^5 sites. All $\gamma(E)$ curves appear to be the same (within the error bars) with no identifiable shrinking of the extended phase as larger chains are considered. This finite size analysis gives a strong support to the hypothesis that the extended phase is stable in the thermodynamic limit.

In Fig. 5, we show the phase diagram in the (E, α) plane as obtained from chains with $\Delta\epsilon/t = 1$ and the same random phase sequence which generates landscapes similar to the ones displayed in Fig. 1. For $\alpha = 2.0$ the

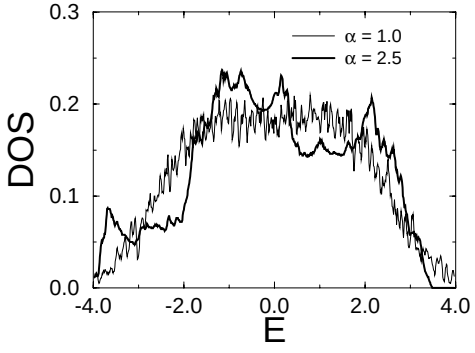

FIG. 2. DOS versus E for chains with $N = 10^4$ sites: $\alpha = 1.0$: energy landscape with antipersistent increments; $\alpha = 2.5$: energy landscape with persistent increments. Notice that the DOS becomes less rough as α is increased.

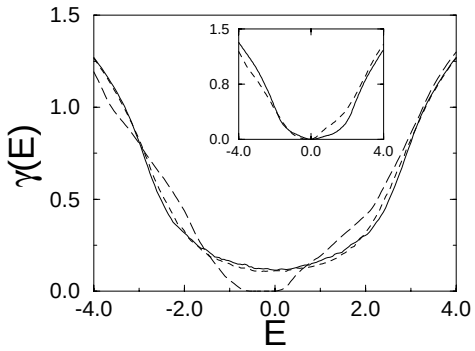

FIG. 3. Lyapunov coefficient γ versus E as obtained from chains with $N = 10^4$ sites. For $\alpha = 0$ (continuous line) all states are localized as expected. The results for a random sequency with white noise in the Fourier component amplitudes (dashed line) show that the filtering of the amplitude noise does not influence the localization properties. For $\alpha = 2.5$ (long-dashed line), which corresponds to an on-site energy landscape with persistent increments, γ vanishes within a finite range of energy values indicating the presence of extended states near the center of the band. In the inset, we show data for $\alpha = 2.0$ with (dashed line) and without (continuous line) amplitude noise filtering, above which the delocalized phase emerges. Data from longer chains produce curves indistinguishable to the eyes.

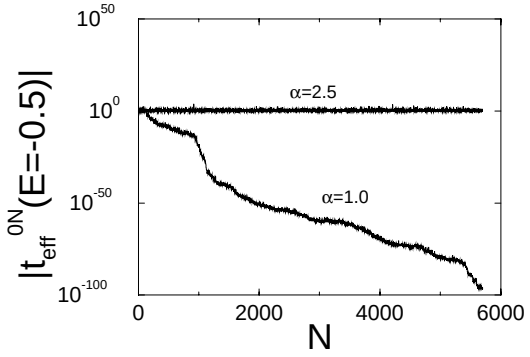

FIG. 4. The effective interaction $|t^{(\mathrm{eff})}_{0,N}(E)|$ versus N for a sequency with originally 10^4 sites and $E = -0.5$. $\alpha = 1.0$, for which the one-electron states are localized (exponentially decaying effective interaction); $\alpha = 2.5$, showing the oscillatory behavior typical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

Lyapunov coefficient vanishes in a single energy (see inset of Fig. 4) 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 and with the width of the extended phase saturating as $\alpha \to \infty$. The boundary asymmetry is inherent to the particular long-range correlated sequency used. It can be removed after a configurational average, although a series of recent works have questioned the physical meaning of self-averaging techniques in long-range correlated disordered systems due to the presence of large sample-to-sample fluctuations [25].

In summary, we found that the one-dimensional Anderson model with long-range correlated diagonal disorder displays a phase of extended electronic states once the on-site energy disorder distribution exhibits a power-law spectral density $S(k) \propto 1/k^{\alpha}$ with $\alpha > 2$, i.e., whenever the energy sequency increments have a long-range persistent character ($H > 1/2$). Contrary to dimerlike models where delocalization is observed only at particular resonance energies, this model exhibits a true Anderson transition with mobility edges separating localized and thermodynamically extended states and, in this sense, has a behavior similar to the one obtained for chains with incommensurate deterministic potentials [22]. This result has significant technological interest since it predicts that polymeric chains with long-range correlated disorder may present unusual transport properties. It would certainly be valuable to understand the observed delocalization transition from analytical grounds as well as to perform a large scale numerical effort to obtain the full phase diagram in the (E, α) space for distinct $\Delta\epsilon/t$ and to establish the corresponding universal scaling exponents.

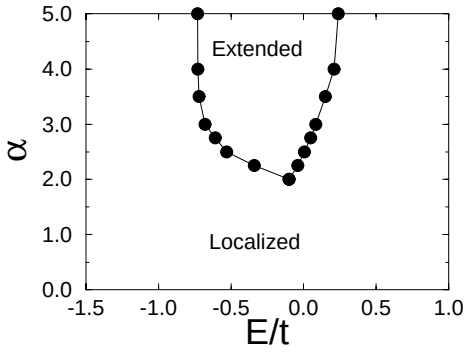

FIG. 5. Phase diagram in the $(E/t, \alpha)$ plane. Data were obtained from chains with 10^4 sites, $\Delta\epsilon/t = 1.0$, and the same random phases sequency. The phase of extended states emerges for $\alpha > 2$, and its width saturates as $\alpha \to \infty$. The band of allowed states ranges approximately from $-4.0 < E < 4.0$ and is independent of α by construction (see text).

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