New Class of Level Statistics in Correlated Disordered Chains

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We study the properties of the level statistics of 1D disordered systems with long-range spatial correlations. We find a threshold value in the degree of correlations below which in the limit of large system size the level statistics follows a Poisson distribution (as expected for 1D uncorrelated-disordered systems), and above which the level statistics is described by a new class of distribution functions. At the threshold, we find that with increasing system size, the standard deviation of the function describing the level statistics converges to the standard deviation of the Poissonian distribution as a power law. Above the threshold we find that the level statistics is characterized by different functional forms for different degrees of correlations.

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Investigating statistical properties of the energy spectrum and the behavior of the level statistics proved to be a useful approach to study electronic properties of disordered systems [1–3]. In 3D disordered systems, the Anderson transition between metallic and insulating phase is associated with a transition in the level statistics distribution from a Wigner-Dyson form to Poisson distribution [4,5]. In 1D disordered systems, for any degree of disorder, the level statistics is described by the Poisson distribution in the limit of large system size corresponding to electronic localization and insulating behavior [6].

Recently, it has been demonstrated numerically that introducing long-range correlations in the spatial order of atoms with different energies in a chain can lead to electronic delocalization [7], creating an interesting debate [8]. Further, it has been shown that there is a localization-delocalization transition at a critical value of the degree of correlations imposed on the disorder in the system, and later works extended these results to other models [9–12]. Also, this type of transition can be found in quasiperiodic systems, as the Aubrey-Andre model and other models[13], indicating the importance of some type of ordering. These theoretical findings are supported also by experimental results showing delocalization and electronic transport driven by extended states in correlated-disordered $GaAs/Ga_{0.7}Al_{0.3}$ superlattices [14]. Recently, a metal-insulator transition has been reported in 2D correlated-disordered systems [15].

Here we hypothesize that, as the localization properties of the electronic states in a disordered system are affected by the degree of spatial correlations [7,12], the properties of the level statistics of the energy spectrum of such correlated-disordered systems could also change. Specifically, we investigate how the functional form of the distribution describing the level statics is affected by the degree of correlations introduced in the system. We demonstrate that the Poissonian form describing the level statistics in disordered 1D systems in the thermodynamic limit is preserved even when a certain degree of spatial correlations is introduced. Further, we find a critical threshold for the degree of correlations above which in the thermodynamic limit there is a transition to a different class of distribution functions for the level statistics. We consider systems without electronic interactions, which may also influence the properties of the level statistics [16] in addition to the correlations in the disorder.

We consider the standard 1D tight-binding Hamiltonian with nearest-neighbor interaction

$$H = \sum_i \xi_i |i\rangle\langle i| + \sum_{\langle i,j\rangle} V|i\rangle\langle j|, \tag{1}$$

where V is the coupling energy and i ranges from 1 to N, where N is the system size. To fix the energy scale, we choose $V = 1$. In the case of uncorrelated disorder, the site energies $\{\xi_i\}$ are randomly drawn from a certain probability distribution, commonly a box (uniform) distribution or a Gaussian. This is equivalent to consider the series of site energies as white noise. In contrast, for systems with correlated disorder, we introduce spatial long-range correlations in the series of site energies $\{\xi_i\}$, so that their sequence describes the trace of a fractional Brownian motion. To this end, we obtain the site energies using the inverse Fourier transform

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

where ϕ_k are $N/2$ random phases uniformly distributed in the interval $[0, 2\pi]$ [7,17,18]. Thus, by construction, the power spectrum of the series $\{\xi_i\}$ is of the type $1/k^\beta$. By choosing different values for the exponent β, we generate series of site energies with different degrees of spatial correlations: for $\beta = 0$, we have pure disorder (white noise), $\beta < 0$ corresponds to anticorrelations, and $\beta > 0$ represents positive correlations in the series of site ener-

gies $\{\xi_i\}$. In our study, we consider only systems with positive correlations ($\beta \geq 0$).

Once the series $\{\xi_i\}$ is obtained, we normalize it to zero mean and unit standard deviation, thus fixing the width of the site energy distribution to unity. This is equivalent to keeping the "traditional disorder" of the system fixed, since the standard deviation of the distribution of $\{\xi_i\}$ quantifies the variety in the site energies of the atoms forming the chain, while their spatial order is quantified by the exponent β. Note that for uncorrelated-disordered systems ($\beta = 0$), the disorder is quantified by the standard deviation in the case of site energies randomly drawn from a Gaussian distribution, or by the width of the box in the case of a box distribution.

After the normalization of the site energies, we diagonalize the Hamiltonian (1) to obtain the energy spectrum $\{E_i\}$, where $E_1 < E_2 < \ldots < E_N$. For any system size N and any value of the correlation exponent β in our numerical calculations, we diagonalize $2^{24}/N$ realizations of the Hamiltonian (1). Thus we have a sufficiently large ensemble of realizations to avoid statistical fluctuations in our results, while we consider the same number of 2^{24} energy levels for any N.

Once the energy spectrum is obtained, we study the distribution of the spacings between consecutive energy levels. Since the density of energy levels is not constant throughout the energy band, and thus the local average energy spacing is not constant either, one cannot compare fluctuations in the spacings obtained from different regions of the band. To avoid this problem, we normalize to unity the local average energy spacing from different regions of the energy band, thus effectively normalizing all energy spacings to the same scale. This "unfolding" of the energy spectrum is a procedure commonly used in the study of level statistics of disordered systems [19]. In brief, the unfolding procedure consists of the following steps: we first introduce the integrated density of energy levels $g(E)$ defined as

$$g(E_i) = i. \tag{3}$$

Thus, $g(E_i)$ is the number of energy levels below the energy E_i. Second, we fit $g(E)$ using a polynomial function. This fit represents the averaged integrated density of energy levels $\overline{g}(E)$. Next, the unfolded energy spectrum $\{\varepsilon_i\}$ is obtained from the map

$$\varepsilon_i = \overline{g}(E_i). \tag{4}$$

To avoid unfolding problems related to irregular behavior of $g(E)$ at the borders of the energy band, we consider only energy levels from the central region of the band. Specifically for a system of size N, we obtain N energy levels [eigenvalues of the Hamiltonian (1)], and we consider the central part of the spectrum $\{E_i\}$, where $i \in [N/3 + 1, 2N/3]$. We obtain the averaged integrated density of levels $\overline{g}(E)$ by fitting $g(E)$ with a cubic polynomial in the interval $[E_{N/3+1}, E_{2N/3}]$.

Using the unfolded spectrum $\{\varepsilon_i\}$, we study the normalized distribution function of energy spacings $P(s)$, where $s_i \equiv \varepsilon_{i+1} - \varepsilon_i$. From Eqs. (3) and (4), we have that the average level spacing is $\langle s \rangle = 1$.

For the classical cases of 1D and 2D uncorrelated-disordered systems in the limit of large system size, $P(s)$ follows the Poisson distribution

$$P_{\mathrm{P}}(s) = e^{-s}. \tag{5}$$

A Poisson distribution for $P(s)$ indicates strong clustering between energy levels because it reaches maximum when $s \to 0$ (Fig. 4).

In our analysis, we characterize $P(s)$ using its standard deviation σ. For the classical case of Poissonian form for $P(s)$ (5), we have $\sigma \equiv \sigma_{\mathrm{P}} = 1$. For convenience, we study the behavior of $\hat{\sigma} \equiv 1 - \sigma$. In Fig. 1 we show $\hat{\sigma}$ as a function of the system size N for different values of the correlation exponent β. For uncorrelated disorder ($\beta = 0$) and for large N, $\hat{\sigma} \to 0$ (or equivalently $\sigma \to 1$), indicating Poissonian behavior for $P(s)$ as expected for 1D disordered systems [6].

Introducing a certain degree of spatial correlations ($\beta > 0$) in the system, we find that in the limit of large N, the level statistics exhibits again Poissonian behavior [$\hat{\sigma} \to 0$, Fig. 1(a)], indicating energy level clustering and electronic localization. This finding indicates that Poissonian behavior in the level statistics exists even in the presence of long-range correlations. However, we find that the convergence of $P(s)$ to the Poisson distribution

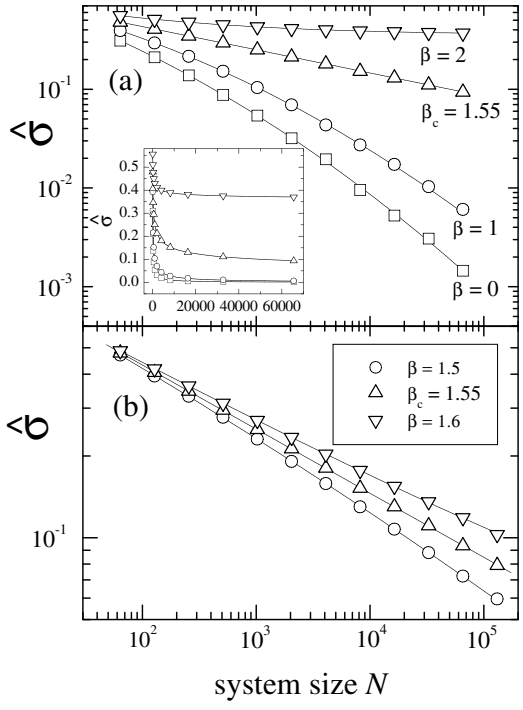

FIG. 1. (a) Log-log plot of $\hat{\sigma}$ as a function of the system size N for different values of the correlation exponent β. Inset: same dependence in linear scales. Solid lines represent fits with Eqs. (6)–(8). (b) Same as in (a) for β close to β_c.

with increasing N is much slower in the case of correlated disorder ($\beta > 0$) compared to the case of uncorrelated disorder ($\beta = 0$) (Figs. 1 and 2).

Increasing the strength of the long-range correlations, we find a threshold value, a critical exponent β_c, above which the functional form of $P(s)$ does not converge to Poisson distribution—i.e., $\hat{\sigma}$ does not converge to zero in the limit of large N [Figs. 1(a) and 2]. At the critical value β_c, we find that for increasing N, the level statistics converges very slowly to Poisson distribution and $\hat{\sigma} \to 0$ as a power law [Fig. 1(b)].

We next investigate the functional dependence of $\hat{\sigma}$ on the system size N for the three regimes: (i) $\beta < \beta_c$; (ii) $\beta = \beta_c$; and (iii) $\beta > \beta_c$. Based on simulations of various systems sizes up to $N = 2^{17}$, we model the behavior of $\hat{\sigma}$ using the following expressions:

$$\hat{\sigma} = a_1 N^{-b_1 - c_1 \log N} (\beta < \beta_c), \tag{6}$$

$$\hat{\sigma} = a_2 N^{-b_2} (\beta = \beta_c), \tag{7}$$

$$\hat{\sigma} = \hat{\sigma}_\infty + a_3 N^{-b_3} (\beta > \beta_c), \tag{8}$$

where all the parameters are positive and in general depend on the correlation exponent β. To test the validity of these expressions, we use the Levenberg-Mardquardt (L-M) algorithm [20] to fit the data in Fig. 1(a) and 1(b) and to estimate the optimal values of the parameters. Although we have tried more expressions to fit the data, those in Eqs. (6)–(8) are the best based on two criteria: good description of data and less number of parameters.

We note that for $\beta < \beta_c$, the behavior of $\hat{\sigma}$ vs N on a log-log plot presents negative curvature [Fig. 1(a)], while for $\beta = \beta_c$, $\hat{\sigma}$ depends on N as a power law with a negative slope, so that in both cases for $N \to \infty$, $\hat{\sigma} \to 0$ [Fig. 1(b)], indicating that in the thermodynamic limit the level statistics is Poissonian. In contrast, for $\beta > \beta_c$, the dependence of $\hat{\sigma}$ on N has positive curvature [Fig. 1(b)], indicating a decay slower than a power law. We find that data are best modeled (with best fit based on the L-M algorithm) as a power law with an additive positive constant $\hat{\sigma}_\infty$ such that $\hat{\sigma} = \hat{\sigma}_\infty$ for $N \to \infty$ (8). Thus our results suggest that for $\beta > \beta_c$, in the thermodynamic limit $\hat{\sigma}$ does not converge to zero, and that the level statistics is not of Poissonian type.

To determine β_c, we use the following procedure: (i) starting from small values of β for which the dependence of $\hat{\sigma}$ on N follows Eq. (6), we increase β and observe that the fitting parameter c_1 decreases, and for a given value of β becomes zero, so that Eq. (6) is not valid anymore; (ii) starting from large values of β for which $\hat{\sigma}$ follows Eq. (8), we decrease β and observe that the fitting parameter $\hat{\sigma}_\infty$ decreases, and for a given value of β becomes zero, so that Eq. (8) is not valid anymore. We find that for both (i) and (ii), the transitions occur at a critical value of $\beta \equiv \beta_c = 1.55 \pm 0.05$ (Figs. 1 and 2), where the behavior of $\hat{\sigma}$ is described by Eq. (7).

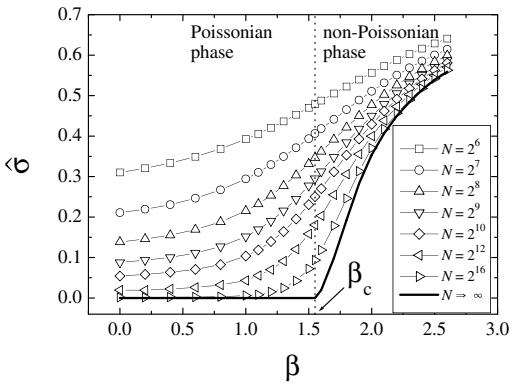

FIG. 2. Dependence of $\hat{\sigma}$ on the correlation exponent β for varied system size N. The solid line represents the behavior of $\hat{\sigma}$ in the limit of $N \to \infty$ (i.e., $\hat{\sigma}_\infty$)—a phase transition from Poissonian ($\hat{\sigma} = 0$) to non-Poissonian ($\hat{\sigma} \neq 0$) level statistics at the critical value β_c.

We next obtain a phase diagram of the properties of the level statistics as a function of the degree of spatial correlations in the system. We systematically investigate the asymptotic behavior of $\hat{\sigma}$ in the limit of large system size N as a function of the correlation exponent β (Fig. 2). For a fixed system size N, we calculate how $\hat{\sigma}$ depends on the spatial correlations choosing a dense set of β values. We then repeat the calculations for increasing N. We find that $\hat{\sigma}$ is an increasing function of β, and that for each value of N, a relatively flat region at small β is followed by a sharp increasing in $\hat{\sigma}$ for large β (Fig. 2). This behavior becomes more pronounced with increasing N. Further, we find that the flat region in $\hat{\sigma}$ extends to intermediate values of β and rapidly approaches zero with increasing N. This is in agreement with our finding of level statistics of Poissonian type even in the presence of a moderate degree of spatial correlations in the system and with the predictions of Eqs. (6) and (7). In contrast, for large values of β, the values of $\hat{\sigma}$ remain large and do not decrease substantially with increasing the system size N. Thus, we observe a transition in $\hat{\sigma}$ centered at intermediate values of β, which becomes more abrupt with

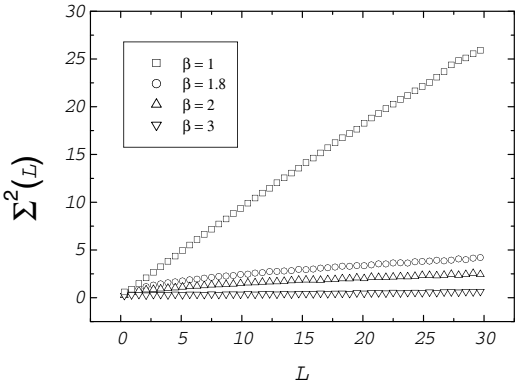

FIG. 3. Behavior of Σ^2 as a function of L for spectra obtained for different values of β and for a system size $N = 2^{17}$.

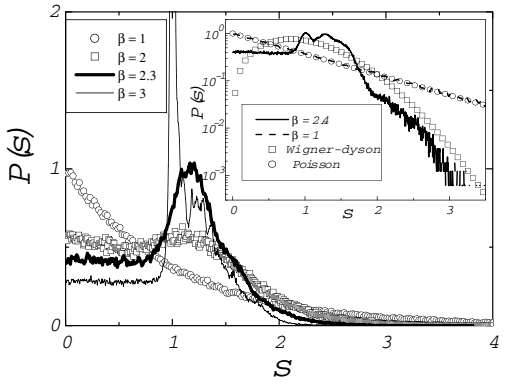

FIG. 4. Distribution functions $P(s)$ obtained for different values of β and for $N = 2^{17}$. Inset: log-linear plot of $P(s)$ for two values of β and for Poisson and Wigner-Dyson (WD) distributions. For $\beta = 1 < \beta_c$, $P(s)$ is Poissonian, while for $\beta = 2.4 > \beta_c$, the tail of $P(s)$ decays even faster than for WD.

increasing N. To extrapolate the behavior of the level statistics in the thermodynamic limit and for large β, we use Eq. (8), since for $N \to \infty$, $\hat{\sigma} \to \hat{\sigma}_\infty$. We estimate $\hat{\sigma}_\infty$ for a dense set of large and decreasing values of β—the solid thick line in Fig. 2, which sharply decreases to $\hat{\sigma}_\infty = 0$ for $\beta \equiv \beta_c = 1.55$. This suggests a phase transition from a Poissonian behavior of the level statics characterized by $\hat{\sigma}_\infty = 0$ for $\beta < \beta_c$, indicating strong clustering between energy levels, to a non-Poissonian phase defined by $\hat{\sigma}_\infty \neq 0$ for $\beta > \beta_c$. As $\hat{\sigma}_\infty$ is a function of β, this suggests that for any $\beta > \beta_c$, a different level statistics $P(s)$ is obtained. Thus we find a new class of correlated-disordered systems characterized by energy level repulsion, different values of $\hat{\sigma}_\infty$, and different distribution functions for the energy spacings $P(s)$.

Similar conclusions can be drawn with the study of $\Sigma^2(L)$, i.e., the variance of the number of levels in boxes of length L in the unfolded spectrum. It is known that for Poissonian behavior, $\Sigma^2(L)$ is linear with L with slope 1. We obtain this linear behavior for any $\beta < \beta_c$ (see the case $\beta = 1$ in Fig. 3), indicating Poissonian behavior, in agreement with our previous results. For $\beta > \beta_c$, we obtain a nonlinear and slow increasing of $\Sigma^2(L)$ as a function of L (slower for increasing β), indicating level repulsion and non-Poissonian behavior, also in agreement with our previous results, and with the behavior of the $P(s)$ functions (see below).

In Fig. 4 we show $P(s)$ for several values of β and for finite system size $N = 2^{16}$. We note that in the thermodynamic limit of large N, the form of $P(s)$ may change. However, this change is expected to be not significant, since for $N = 2^{16}$, $\hat{\sigma} - \hat{\sigma}_\infty \simeq 0.005$. In general, we obtain that for $\beta < \beta_c$, although there exists a moderate degree of correlations in the system, $P(s)$ is exponential (Poissonian) (see the case $\beta = 1$ in Fig. 4). When $\beta > \beta_c$, the Poissonian behavior is lost: as β departs from β_c, the functions $P(s)$ for low s decrease gradually, and simultaneously, an increasing peak for increasing β appears at $s = \langle s \rangle = 1$, indicating strong level repulsion. For extreme values of β, $P(s)$ for low s is very small, while the peak at $s = 1$ becomes huge (see the case of $\beta = 3$ in Fig. 4). This finding is consistent with the expectation that extreme values of β correspond to an ordered system, for which the level statistics is of the type $P(s) = \delta(s - 1)$.

In summary, we find that introducing spatial long-range correlations in 1D disordered systems leads to a transition from a Poissonian to a new class of functional forms describing the level statistics in the thermodynamic limit. Further, we find a critical value for the correlations below which the level statistics exhibit Poissonian behavior associated with energy level clustering, similar to the one observed in uncorrelated-disordered systems. Above this critical value, the system is characterized by level repulsion. These findings may relate to previous reports on localization-delocalization transition in the electronic properties of 1D systems driven by spatial correlations in the disorder [7]. In that work, the transition is detected at $\beta = 2 > \beta_c$, where we already observe non-Poissonian behavior, as expected in the extended regime.

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