Statistics of the Lyapunov Exponent in 1D Random Periodic-on-Average Systems

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(Received 2 April 1998)

By means of Monte Carlo simulations we show that there are two qualitatively different modes of localization of classical waves in 1D random periodic-on-average systems. States from pass bands and band edges of the underlying band structure demonstrate single parameter scaling with universal behavior. States from the interior of the band gaps do not have universal behavior and require two parameters to describe their scaling properties. The transition between these two types of behavior occurs in an extremely narrow region of frequencies. When the degree of disorder exceeds a certain critical value the single parameter scaling is restored for an entire band gap. [S0031-9007(98)07924-1]

PACS numbers: 72.15.Rn, 03.65.Sq, 05.45.+b, 42.25.Bs

In this paper we numerically study localization properties of band gap states in a one-dimensional periodic-on-average random system (PARS). These kinds of systems were extensively studied in the past in the context of electron localization, where they were known as Kronig-Penny-like models (see, for example, Refs. [1–3], and references therein). Classical wave versions of 1D PARS also recently attracted considerable attention [4–7]. Most of these studies focused upon localization properties of states from pass (conduction) bands of the respective initial periodic systems, or states at band edges of the original spectrum. They were found to behave similarly to the one-dimensional Anderson model, demonstrating single-parameter scaling (SPS) and universality [8].

Disorder, however, not only localizes states in the conduction bands of 1D systems, it also gives rise to localized states inside band gaps of the original spectrum. This is well known in the physics of disordered semiconductors, where a vast literature on properties of localized states arising within forbidden gaps of semiconductors exists (see, for example, book [9]). In the case of one-dimensional models, however, these states have been studied surprisingly little. Particularly, statistical properties of the Lyapunov exponent (the inverse localization length), λ, for these states have not been studied at all. At the same time, it turns out that the variance, var(λ), of the Lyapunov exponent contains important information about spectral properties of these systems. From the frequency dependence of the variance, we find that the band gap states can be divided into two groups with qualitatively different localization properties separated by a sharp boundary. This means that though all states in 1D systems are localized, there might be two qualitatively different regimes of localization. The first regime corresponds to the band and band edge states, and has regular Anderson behavior (if disorder is locally weak). The second regime, associated with the gap states, does not obey SPS and is not universal. The regular tight-binding Anderson model also demonstrates violation of SPS, when disorder becomes *locally* strong [10,11]. It should be emphasized, therefore, that in our case the absence of SPS is caused not by the strength of disorder, but by the different nature of the gap states. Studying how var(λ) and the Lyapunov exponent (LE) itself depend upon the degree of disorder (rms fluctuations of a random parameter, σ) we find that there exists a critical value, σ_{cr}, at which the boundary between the groups of states with different localization properties disappears. At $\sigma > \sigma_{\mathrm{cr}}$ all the states have the regular Anderson-like behavior. It is interesting to note that in this situation SPS is *restored* when disorder becomes stronger, contrary to what one would expect in the Anderson model.

In the paper we deal with the classical wave version of PARS and consider localization properties of scalar waves in a 1D superlattice composed of two alternating layers A and B with dielectric constants ε_A and ε_B, respectively. The results, however, can also be applied to Kronig-Penny-like models of electron localization. We introduce disorder in the system forcing the thickness d_B of the B layers to change randomly assuming that d_B is drawn independently from a uniform distribution.

The structure of the described model is periodic on average with the spatial period equal to $d = d_A + \langle d_B \rangle$ and with random positions of the boundaries between different layers. The states of the model are characterized by a dimensionless wave number $k = (\omega/c)d$, where ω is the frequency and c is the vacuum speed of light.

We study the model by means of the transfer-matrix method. The state of the system is described by the vector $\mathbf{u}_n$ with components representing the wave field, E_n, and its spatial derivative, E_n'. The evolution of the vector $\mathbf{u}_n$ is controlled by the matrix $\mathbf{X}_n$: $\mathbf{u}_{n+1} = \mathbf{X}_n \mathbf{u}_n$, where $\mathbf{X}_n$ is determined as follows:

$$\mathbf{X}_n = \begin{pmatrix} \cos(k_n d_n) & \frac{1}{k_n}\sin(k_n d_n) \\ -k_n \sin(k_n d_n) & \cos(k_n d_n) \end{pmatrix}, \qquad (1)$$

where $k_n = k\sqrt{\epsilon_n}$. The LE can be computed in accordance with the following definition:

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$$\lambda = \lim_{L\to\infty} \frac{1}{L} \left\langle \ln\left(\frac{\| \mathbf{X}^{(N)}\mathbf{u}_0 \|}{\| \mathbf{u}_0 \|} \right) \right\rangle, \qquad (2)$$

where L is the length of the system, the matrix $\mathbf{X}^{(N)}$ is a product of all $\mathbf{X}$ matrices corresponding to each layer, $\mathbf{X}^{(N)} = \prod_1^N \mathbf{X}_n$, and $\mathbf{u}_0$ is a generic vector. The LE determined according to Eq. (2) is a self-averaging quantity. For finite systems, however, it exhibits fluctuations that are the main object of study of this paper.

In computer simulations we generated a sequence of random $\mathbf{X}$ matrices in accord with the model described above. The parameters of the model were chosen as follows: $\varepsilon_A = 1$, $\varepsilon_B = 1.2$; $d_A = 1$ and the mean width of the B layers $\langle d_B \rangle = 1$. The standard deviation σ of d_B is a measure of the disorder in the model. The results of the calculations are presented in figures below. Figure 1 shows the frequency dependence of the LE and its variance, $\mathrm{var}(\lambda) = \langle \lambda^2 \rangle - \langle \lambda \rangle^2$, for frequencies covering one of the band gaps. The behavior of λ coincides with the results reported previously in Ref. [4,5]. The variance of λ at the same time demonstrates anomalous nonmonotonic behavior with two maxima inside the band. In the region between the maxima, $\mathrm{var}(\lambda)$ changes *oppositely* to λ, approaching its minimum value at the center of the gap. Such a behavior is clearly inconsistent with SPS, which dictates that $\mathrm{var}(\lambda) = (2/L)\lambda$ [8,10,12]. When the dispersion of our random variable increases, the maxima of $\mathrm{var}(\lambda)$ moves toward the center of the gap, and the central minimum raises. At some critical value, σ_{cr}, double-peaked structure of $\mathrm{var}(\lambda)$ disappear, and at $\sigma > \sigma_{\mathrm{cr}}$ the variance exhibits only one maximum and goes along with the LE itself. The results presented in this figure show that localization properties of band and band-edge states are different from those of the gap states. This difference sharply manifests itself in the dependence of the LE upon σ shown in Fig. 2 for different k. This dependence undergoes a strong qualitative change when the wave number moves toward the center of the gap. The difference in behavior of the LE corresponding to the states from the pass band and the gap was previously discussed in Refs. [6,7,13]. Our results show that the change between different shapes of the function $\lambda(\sigma)$ occurs within a narrow frequency interval of the order of magnitude of 0.01% suggesting existence of a well-defined boundary between different groups of state. It is remarkable that this boundary coincides with the position of the respective maximum of $\mathrm{var}(\lambda)$. For $\sigma > \sigma_{\mathrm{cr}}$, where σ_{cr} corresponds to the transformation between different types of behavior of $\mathrm{var}(\lambda)$, all functions $\lambda(\sigma)$ for different k merge together demonstrating behavior independent of frequency of the states.

Figure 3 presents $\mathrm{var}(\lambda)$ directly plotted versus λ. In order to obtain this figure, we combine frequency dependences of the LE and its variance in the region covering several bands of the parent periodic system. This figure illustrates the violation of the SPS in our system. It is clear from comparison between this plot and the plot in Fig. 1 that anomalous nonlinear dependence of $\mathrm{var}(\lambda)$ versus λ is caused by the states from the inner region of the band gap between the two maxima of $\mathrm{var}(\lambda)$. The multibranch structure of the plot shows the lack of universality in this dependence: it is different for different band gaps. Indeed, we checked that different branches originate from frequencies corresponding to different band gaps. Double lines, which form each of the branches, correspond to different halves of the same band gap. The insert in Fig. 3 presents one of the branches that was obtained by filtering out all the frequencies except those that belong to one half of a band gap.

The nonuniversal behavior of states from different band gaps and a violation of SPS are closely related phenomena. The intimate relationship between nonuniversality and SPS is demonstrated in Fig. 4. These plots show the evolution

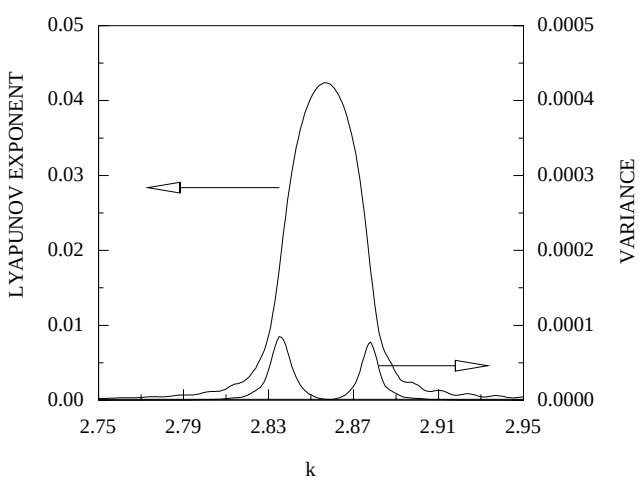

FIG. 1. Frequency dependence of the Lyapunov exponent λ and its variance $\mathrm{var}(\lambda)$ for the frequencies covering a band gap ($2.83 < k < 2.88$) and band edges of the underlying structure. The graph was obtained for a system with 200 layers, so that states with $2.82 < k < 2.89$ have localization lengths shorter than the system's size.

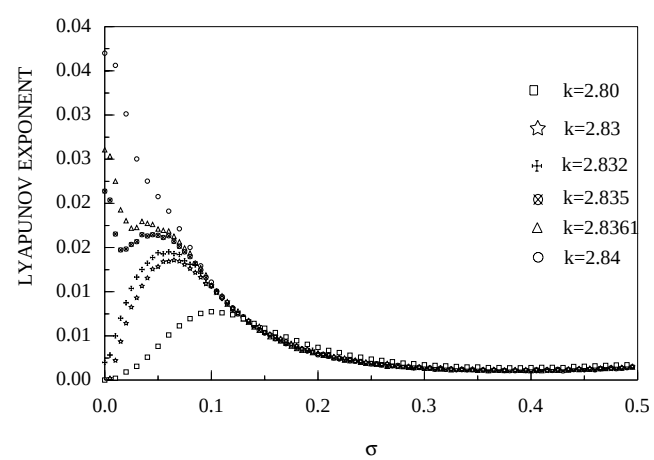

FIG. 2. The dependence of the Lyapunov exponent λ upon the standard deviation σ of the random layers' thicknesses for different k in the vicinity of $k = 2.835$, which approximately corresponds to the left maximum of $\mathrm{var}(\lambda)$ shown in Fig. 1.

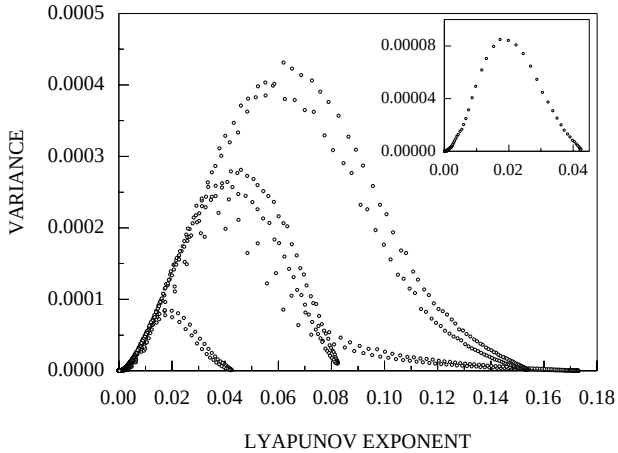

FIG. 3. Variance of λ versus λ. The graph was obtained by means of combining frequency dependencies of var(λ) and λ for the frequency region covering four band gaps of the parent periodic structure. The inset corresponds to frequencies from the left half of the second band gap.

of the dependence of var(λ) versus λ with an increase of the value of the standard deviation, σ, of the layers' thickness. One can observe that with an increase of σ, the variance of λ approaches a regular linear dependence upon λ. And along with this, all the branches from the different band gaps merge into one universal curve. It happens at approximately the same values of σ at which the maxima on the frequency dependence of var(λ) disappear, signaling about complete eroding of the initial band structure by the disorder. However, a destruction of the initial spectrum is not a uniform (in terms of frequencies) process—some bands disappear at smaller disorder than others.

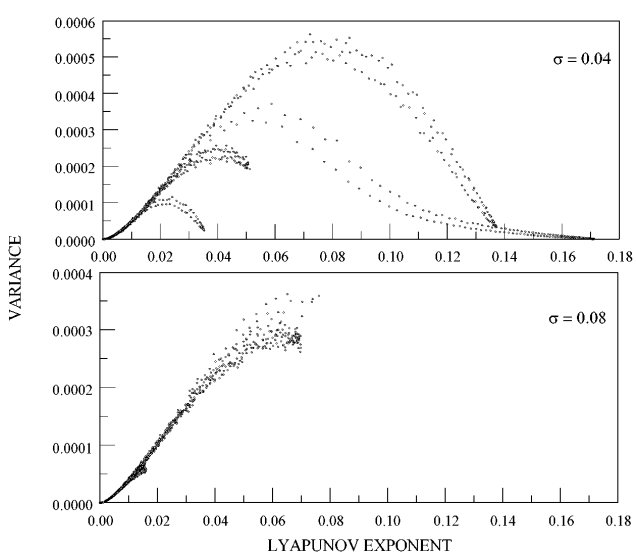

FIG. 4. Evolution of the graph from Fig. 3 with increase of σ. It is seen how different branches raise gradually and form the universal curve corresponding to the prediction of SPS. Note that $\sigma = 0.08$ on the second graph is close to, but still smaller than, the critical value of σ that marks the start of the universal behavior of the graphs in Fig. 2.

Therefore, different branches of the graph in Fig. 4 return to the universal behavior at different values of the disorder parameter, σ.

The presented results suggest that the probability distribution function of the LE, $P(\lambda)$, in the case of the inner gap states, cannot be described by a single parameter. We find, however, that in the asymptotic limit $L \to \infty$, $P(\lambda)$ retains its Gaussian form with var(λ) $\propto 1/L$. That means that statistical properties of the gap states are characterized by two independent parameters. The similar situation occurs in the Anderson model in the case of locally strong scattering [10,11]. In our situation the local scattering, characterized by the mismatch between the dielectric parameters of the layers, is weak. The considered system, therefore, presents an example when two-parameter scaling occurs due to properties of the initial spectrum of the system rather then due to the strength of the disorder.

To suggest a qualitative explanation of the results let us first consider the nonmonotonic behavior of var(λ). It is more convenient to start with the states arising in the center of the forbidden band, which exhibit the smallest fluctuations of λ. The reason for this behavior lies in the fact that states deep in the forbidden band can only arise due to a strong deviation from the initial periodic structure. The probability of such events is small, and such defect configurations, occurring at different parts of the structure, are separated from each other by distances much greater than localization lengths of states emerging due to these deviations. The wave functions corresponding to different states do not overlap and such configurations can be considered as isolated defects. It is well known (see, for example, [2]) that the localization length in this case is determined solely by the initial spectrum of the system and the frequency of the corresponding local state. Therefore, fluctuations of λ would be equal to zero in the idealized situation of isolated defects. In the real case, we have small fluctuations due to overlap of exponential tails of different states, and rare occasions when two defects appears close to each other.

When k moves from the center of the band gap toward the boundary, the density of the configurations responsible for the states at corresponding frequencies and their localization lengths increase. First this leads to an increase in the fluctuation of the LE because the localization length is determined now by complexes of several interacting defect configurations, and becomes sensitive to the fluctuating structure of such complexes. However, as the band boundary is approached, the effect of self-averaging comes into play. With an increase of spatial overlap between states localized at different centers, self-averaging of the LE becomes more effective, leading, therefore, to the decrease of var(λ). The interplay between these two tendencies generates nonmonotonic behavior of var(λ) presented in Fig. 1.

Arguments similar to that presented above can explain the difference in the σ dependence of the LE for states from the inner part of the band gaps and boundary states.

The behavior of the LE for states from the pass bands and states at the band edges is well understood: $\lambda \propto \sigma^2$ for states from the pass bands, and $\lambda \propto \sigma^{2/3}$ at the band edges [4]. It is also clear that when $\sigma \rightarrow 0$, the LE for states from the band gap tends to a nonzero value, which is just an inverse penetration length through the forbidden band. This penetration length obviously decreases when frequency approaches the center of the band gap. Disorder results in emergence of a small number of states with frequencies in the inner part of the gap. These states enhance propagation of waves due to a process similar to resonant tunneling, reducing by this means the LE. These arguments cannot be applied to states at the band edge because their penetration length at $\sigma = 0$ is so large that even small disorder makes them indistinguishable from the states at the pass-band side of the edge.

It is clear from the presented results that the violation of SPS and the absence of universality in the considered system are due to nonmonotonic behavior of var(λ). It is interesting, however, to examine this behavior from the standpoint of general arguments leading to SPS [8]. According to these arguments, SPS is realized when the localization length $l_{\mathrm{loc}} = \lambda^{-1}$ is much greater than the phase randomization length l_{ph}. In the random phase model [8] it is assumed that phase randomization occurs at a microscopic scale, and, violation of the inequality $l_{\mathrm{loc}} \gg l_{\mathrm{ph}}$ means that the localization length also becomes of microscopic size. It is natural, therefore, not to expect universality in this case. In our situation, however, localization length remains macroscopical even for states deep inside the gap. Therefore, the absence of SPS is not related to the influence of microscopic details of the system. At the same time one could expect the increase in l_{ph} in this spectral region, because the phase of a wave changes only when it crosses a localized state, which are very rare in this spectral region. One can assume, therefore, that for the state from the inner region of the band gap one can have $l_{\mathrm{ph}} > l_{\mathrm{loc}}$ even though both these lengths remain *macroscopical*. In order to check this assumption, we studied a distribution of the phase, and determined the phase randomization length using simple Neyman-Person χ^2 statistical tests to check the uniformity of the distribution. We used the plane wave representation for the transfer matrix, and following Ref. [11], define the phase, as a relative phase responsible for the scaling behavior of the LE. The results of the simulation confirm that the phase randomization length increases inside the gap, and exceeds the localization length for the states between maxima of var(λ). We also found that the transition from the inequality $l_{\mathrm{ph}} < l_{\mathrm{loc}}$ to $l_{\mathrm{ph}} > l_{\mathrm{loc}}$ occurs approximately in the same critical region, which separates the band-edge states from the inner states in Figs. 1 and 2.

To conclude, Monte-Carlo computer simulation of wave localization properties of a one-dimensional random periodic-on-average system shows that the spectrum of the system can be divided into two groups of states with qualitatively different statistical behavior of the Lyapunov exponent and a narrow critical region separating these groups. The first group combines states from pass bands of the parent periodic system and band-edge states from the band gaps. The statistical properties of this group are similar to the properties of the Anderson model and can be described by the single-parameter-scaling. The other group consists of states from the inner region of the band gaps and demonstrate a number of anomalies. The variance of the LE, for this group decreases when the frequency approaches the center of a band gap resulting in a strong deviation from single-parameter scaling-like behavior. The dependence of var(λ) upon the LE is nonuniversal for these states and is different for different band gaps. The transition between the two groups is also accompanied by the reversal of the relationship between the localization length and phase randomization length: for a pass band and band-edge states $l_{\mathrm{ph}} < l_{\mathrm{loc}}$, and $l_{\mathrm{ph}} > l_{\mathrm{loc}}$ for inner band-gap states. An increase in the degree of randomness beyond a well-defined critical value erodes the difference between the groups and returns the system to the regular single-parameter-scaling mode of behavior. This can be interpreted as a complete destruction of the original band structure by disorder.

We are pleased to acknowledge stimulating discussions with B. L. Altshuler. We wish to thank S. Schwarz for reading and commenting on the manuscript. This work was supported by the NSF under Grant No. DMR-9632789, and by a CUNY collaborative grant.

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