Statistics of the Lyapunov exponent in 1-D random periodic-on-average systems

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By means of Monte Carlo simulations we show that there are two qualitatively different modes of localization of classical waves in 1-D 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.

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 system were extensively studied in the past in the context of electron model, demonstrating single-parameter scaling (SPS) and universality [9]. Classical wave versions of 1-D PARS also recently attracted a considerable attention [4–8]. 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 [9].

Disorder, however, not only localizes states in the conduction bands of 1-D 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 [10]). 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 1-D 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 [11,12]. 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, σcr, at which the boundary between the groups of states with different localization properties disappears. At σ > σcr 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 1-D superlattice composed of two alternating layers A and B with dielectric constants εA and εB, 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 dB of the B layers to change randomly assuming that dB is drawn independently from a uniform distribution.

The structure of the described model is periodic on average with the spatial period equal to d = dA + ⟨dB⟩ and with random positions of the boundaries between different layers. The states of the model are characterized by a dimensionless wave number k = (ω/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 un with components representing the wave field, En, and its spatial derivative, En′. The evolution of the vector un is
controlled by the matrix $X_n$: $u_{n+1} = X_n u_n$, where $X_n$ is determined as follows:

$$X_n = \begin{pmatrix} \cos(k_n d_n) & \frac{1}{k_n} \sin(k_n d_n) \\ -k_n \sin(k_n d_n) & \cos(k_n d_n) \end{pmatrix},$$  
(1)

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

$$\lambda = \lim_{L \to \infty} \frac{1}{L} \mathbb{E} \left[ \ln \left( \frac{\| X^{(N)} u_0 \|}{\| u_0 \|} \right) \right],$$  
(2)

where $L$ is the length of the system, the matrix $X^{(N)}$ is a product of all $X$-matrices corresponding to each layer, $X^{(N)} = \prod_1^N X_n$, and $u_0$ is a generic vector. 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 $X$-matrices in accord with the model described above. The parameters of the model were chosen as follows: $\epsilon_A = 1$, $\epsilon_B = 1.2$; $d_A = 1$ and the mean width of the $B$ layers $\langle d_B \rangle = 1$. The standard deviation $\sigma$ of $d_B$ is a measure of the disorder in the model. The results of the calculations are presented in figures below. Fig. 1 shows the frequency dependence of LE and its variance, $\var(\lambda) = \langle \lambda^2 \rangle - \langle \lambda \rangle^2$, for frequencies covering one of the band-gaps. The behavior of $\lambda$ coincides with the results reported previously in Refs. [4,5,8]. The variance of $\lambda$ at the same time demonstrates anomalous non-monotonic behavior with two maxima inside the band. In the region between the maxima, $\var(\lambda)$ changes oppositely to $\lambda$, approaching its minimum value at the center of the gap. Such a behavior is clearly inconsistent with SPS, which dictates that $\var(\lambda) = (2/L) \lambda$ [1,3]. When the dispersion of our random variable increases, the maxima of $\var(\lambda)$ moves toward the center of the gap, and the central minimum raises. At some critical value, $\sigma_{cr}$, double-peaked structure of $\var(\lambda)$ dissapear, and at $\sigma > \sigma_{cr}$ the variance exhibits only one maximum and goes along with 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 LE upon $\sigma$ 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 LE corresponding to the states from the pass band and the gap was previously discussed in Refs. [1,3,4]. 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 $\var(\lambda)$. For $\sigma > \sigma_{cr}$, where $\sigma_{cr}$ corresponds to the transformation between different types of behavior of $\var(\lambda)$, all functions $\lambda(\sigma)$ for different $k$ merge together demonstrating behavior independent of frequency of the states.

Fig. 3 presents $\var(\lambda)$ directly plotted versus $\lambda$. In order to obtain this figure, we combine frequency dependences of 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 non-linear dependence of $\var(\lambda)$ versus $\lambda$ is caused by the states from the inner region of the band gap between the two maxima of $\var(\lambda)$. 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 inset 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 of the dependence of $\var(\lambda)$ versus $\lambda$ with an increase of the value of the standard deviation, $\sigma$, of the layers’ thickness. One can observe that with an increase of $\sigma$, the variance of $\lambda$ approaches a regular linear dependence upon $\lambda$. 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 $\sigma$ at which the maxima on the frequency dependence of $\var(\lambda)$ 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. Therefore, different branches of the graph in Fig. 4 return to the universal behavior at different values of the disorder parameter, $\sigma$.

The presented results suggest that the probability distribution function of 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 $\var(\lambda) \propto 1/L$. 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.
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 $\text{var}(\lambda)$. It is more convenient to start with the states arising in the center of the forbidden band, which exhibit the smallest fluctuations of $\lambda$. 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, [5]) 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 $\lambda$ 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 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 LE becomes more effective, leading, therefore, to the decrease of $\text{var}(\lambda)$. The interplay between these two tendencies generates nonmonotonic behavior of $\text{var}(\lambda)$ presented in Fig. 1.

Arguments similar to that presented above can explain the difference in the the $\sigma$-dependence of LE for states from the inner part of the band-gaps and boundary states. The behavior of 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 $\sigma \to 0$, LE for states from the band-gap tends to a non zero value, which is just an inverse penetration length through the forbidden band. This penetration length obviously decreases when frequency moves from 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 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 $\text{var}(\lambda)$. It is interesting, however, to examine this behavior from the standpoint of general arguments leading to SPS [9]. According to these arguments, SPS is realized when the localization length $l_{\text{loc}} = \lambda^{-1}$ is much greater than the phase randomization length $l_{\text{ph}}$. In the random phase model [9] it is assumed that phase randomization occurs at a microscopic scale, and, violation of the inequality $l_{\text{loc}} \gg l_{\text{ph}}$ 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 $l_{\text{ph}}$ 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 $l_{\text{ph}} > l_{\text{loc}}$ 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 $\chi^2$ statistical tests to check the uniformity of the distribution. We used the plane wave representation for the transfer-matrix, and following Ref. [12], define the phase, as a relative phase responsible for the scaling behavior of 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 $\text{var}(\lambda)$. We also found that the transition from the inequality $l_{\text{ph}} < l_{\text{loc}}$ to $l_{\text{ph}} > l_{\text{loc}}$ 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 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 $\text{var}(\lambda)$ upon 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 $l_{ph} < l_{loc}$, and $l_{ph} > l_{loc}$ 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.

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Fig. 1. Frequency dependence of the Lyapunov exponent, $\lambda$, and its variance, $\text{var}(\lambda)$, 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, $\lambda$, upon the standard deviation, $\sigma$, of the random layers’ thicknesses for different $k$ in the vicinity of $k = 2.835$, which approximately corresponds to the left maximum of $\text{var}(\lambda)$ shown in Fig. 1.

Fig. 3. Variance of $\lambda$ versus $\lambda$. The graph was obtained by means of combining frequency dependencies of $\text{var}(\lambda)$ and $\lambda$ for the frequency region covering four band-gaps of the parent periodic structure. The insert corresponds to frequencies from the left half of the second band-gap.

Fig. 4. Evolution of the graph from Fig. 3 with increase of $\sigma$. 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 $\sigma$ that marks the start of the universal behavior of the graphs in Fig. 2.
