Three types of spectra in one-dimensional systems with random correlated binary potential

O. V. Usatenko and S. S. Melnik, V. A. Yampol’skii
A. Ya. Usikov Institute for Radiophysics and Electronics
Ukrainian Academy of Science, 12 Proskura Street, 61085 Kharkov, Ukraine

M. Johansson, L. Kroon, and R. Riklund
Department of Physics and Measurement Technology,
IFM Linköping University SE-581 83 Linköping Sweden

The stationary one-dimensional tight-binding Schrödinger equation with a weak diagonal long-range correlated disorder in the potential is studied. An algorithm for constructing the discrete binary on-site potential exhibiting a hybrid spectrum with three different spectral components (absolutely continuous, singular continuous and point) ordered in any predefined manner in the region of energy and/or wave number is presented. A new approach to generating a binary sequence with the long-range memory based on a concept of additive Markov chains (Phys. Rev. E 68, 061107 (2003)) is used.

PACS numbers: 72.15.Rn, 03.65.Bz, 72.10.Bg

In recent years, the problem of transport of electro-magnetic waves (and various excitations in solids) in one-dimensional (1D) systems with the long-range correlated disorder has attracted much attention [1, 2, 3]. The important significance of this problem is due to exciting results that revise a commonly accepted belief that any randomness (no matter how weak the randomness is) in 1D structures results in the Anderson localization [4]. It was also believed that 1D systems could not display a complex dynamic feature such as the metal-insulator transition, which gives rise to an appearance of the mobility edges. However, in Refs. [5, 6], a highly nontrivial role of correlations was shown, the divergency of the localization length for some specific values of energy was observed. Using a perturbative approach, it was also shown in Ref. [1] that the position of the mobility edges and the windows of transparency can be controlled by the form of the binary correlator of a scattering potential, which was supposed to be continuous, of a long-range and Gaussian. If the correlations are of a long-range, i.e. they decay by the power law, a continuum of extended states may appear in the energy spectrum. In other words, the long-range correlations are necessary for the observation of the metal-insulator transition and co-existence of different type of spectra. A quite simple method was used therein to construct a random potential with a long-range correlation. From the experimental point of view, the importance of recently obtained results may be explained by a strong impact upon the creation of a new class of electron devices and electromagnetic waveguides, which can be used as window filters having new transmission properties.

In this paper we point out a new method for constructing the long range correlated sequences of a two-valued site potential \( \varepsilon(n) \) with a given correlator and prescribed probability distribution function (PDF), not only Gaussian. For this potential the method given in [1] does not work. An attempt to construct a correlated dichotomous sequence where the metal-insulator transition can be observed was made in Ref. [7]. Later, Ref. [8], this result was retracted.

We study a stationary one-dimensional tight-binding Schrödinger equation (the Anderson model [4]),

\[
\psi_{n+1} + \psi_{n-1} + (E - \varepsilon(n))\psi_n = 0, \tag{1}
\]

with a site potential \( \varepsilon(n) \) taking on two different values \( \varepsilon_0 \) and \( \varepsilon_1 \).

Equation (1) is a prototype model describing a propagation of excitations (electromagnetic waves, electrons, photons, phonons) in deterministic ordered or random disordered systems (solids or layered super-lattices). The type of ordering, i.e., the correlations in the site potential \( \varepsilon(n) \) determine the spectrum of excitation. The wave functions of excitations in such systems are usually characterized by the Lyapunov exponent \( \Lambda \). Some typical examples of sequences having different types of spectra are (spectrum is a set of allowed energies of excitations in the system):

1. A system with a regular periodic variation of the site potential \( \varepsilon(n) \) possess an absolutely continuous (AC) spectrum and describes extended, delocalized states having bounded wave functions with the Lyapunov exponent \( \Lambda = 0 \).

2. A system with a random non-correlated potential \( \varepsilon(n) \) has the allowed states with the exponentially localized wave functions and displays a point ( discrete) spectrum with the positive Lyapunov exponent (the Anderson localization).

*Electronic address: usatenko@ire.kharkov.ua
3. A potential constructed using the deterministic quasi-periodic Fibonacci chain (see the definition given below, Eq. (10)) exhibits a singular continuous (SC) Cantor-like spectrum characterized by the power-law localized wave functions with $\Lambda = 0$. The singular continuous spectrum differs essentially from the absolutely continuous one. This spectrum corresponds to a singular continuous integrated density of states (the number of states having the energies smaller then a given one). The integrated density of states is the continuous function of energy, but its derivation equals to zero almost everywhere. In terms of the forbidden and allowed energy zones, this means that the spectrum consists almost completely of forbidden gaps with the infinite number of allowed energies between them. In other words, the spectrum of quasi-periodic potential sequence possesses a fractal structure.

In each of these structures only one pure type of spectrum is presented. A nontrivial result of co-existence of continuous and point spectra in one dimensional chain with correlated disorder was presented in Ref. [4].

Correlated properties in the site potential $\varepsilon(n)$ are determined by the pair correlation function,

$$C(r) = <\varepsilon(n)\varepsilon(n + r) >_s - < \varepsilon(n) >^2, \quad < f(\varepsilon(n)) >_s = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} f(\varepsilon(n)), \quad (2)$$

where the Cezaro average $< \cdot >_s = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \cdot$ can be treated as spatial one. In the Born approximation the Lyapunov exponent is expressed, see Ref. [1], in terms of the Fourier transform $\tilde{K}$ of this two-point correlation function,

$$\Lambda(E) = \frac{(\varepsilon_1 - \varepsilon_0)^2 \tilde{K}(2k)}{32 \sin^2 k}, \quad k \in [-\pi, \pi], \quad K(r) = \frac{C(r)}{C(0)}. \quad (3)$$

The correlation function $K(r)$ and its Fourier transform are connected by the following relations,

$$\tilde{K}(k) = 1 + 2 \sum_{r=1}^{\infty} K(r) \cos(kr), \quad K(r) = \frac{1}{\pi} \int_{0}^{\pi} \tilde{K}(k) \cos(kr)dk \quad (4)$$

Here the evenness of the functions $K(r)$ and $\tilde{K}(k)$ is taking into account. The energy $E$ of the eigenstate and the wave number $k$ in Eq. (3) in zero approximation on the strength of disorder are related by the simple formula,

$$E = -2 \cos k. \quad (5)$$

Thus, there exists the relation between the correlations in the on-site potential $K(r)$ and localization properties of eigenstates expressed in terms of the Lyapunov exponent $\Lambda(E)$ (or by means of integrated density of states). This observation enables one to construct random correlates sequences with prescribed spectral properties and provides a recipe for designing filters of arbitrary complexity. Starting from a desirable spectral dependence $\Lambda(E)$ (or integrated density of states) we have to solve the inverse problem of construction a sequence of "symbols" $\varepsilon(n)$. This program was partially implemented in Ref. [1], where the one-dimensional tight-binding Schrödinger equation with two kind of spectra (absolutely continuous and point) and Gauss distribution of the site potential was examined. However, it is known [12], that in the general case the space of states can be decomposed into the direct sum of subspaces with the wave functions belonging to the point, singular continuous and absolutely continuous parts of spectra. This statement is closely connected with a possibility for presenting an integrated density of states, as for any monotone function, in the sum of three functions: the stepwise, singular and absolutely continuous ones. Here we point to a general method, which is the extension of that used in Ref. [1], and construct a particular example of 1D system having all three above-mentioned types of spectra [13].

To this end we use a new instrument of constructing the related sequence of $\varepsilon(n)$ with a given correlation function $K(r)$ using an additive Markov chain [14, 15]. Here we give a short description of this method.

Consider a homogeneous binary sequence of symbols, $\varepsilon(i) = \{\varepsilon_0, \varepsilon_1\}$, $i \in \mathbb{Z} = \ldots, -2, -1, 0, 1, 2, \ldots$. To determine the $N$-step Markov chain we have to introduce the conditional probability function $P(\varepsilon(i) \mid \varepsilon(i-N), \varepsilon(i-N+1), \ldots, \varepsilon(i-1))$. It is a probability of occurring the definite symbol $\varepsilon_i$ (for example, $\varepsilon(i) = \varepsilon_1$) after $N$-word $T_{N,i}$, where $T_{N,i}$ stands for the sequence of symbols $\varepsilon(i-N), \varepsilon(i-N+10), \ldots, \varepsilon(i-1)$. The additive Markov chain is characterized by the conditional probability function of the form

$$P(\varepsilon(i) = \varepsilon_1 \mid T_{N,i}) = p_1 + \sum_{r=1}^{N} F(r)(\varepsilon(i-r) - < \varepsilon >). \quad (6)$$

We refer to the amount $F(r)$ (introduced first in Ref. [16]) as the memory function. It describes the strength of influence of previous symbol $\varepsilon(i-r)$ ($r = 1, ..., N$) upon a generated one, $\varepsilon(i)$. Here $p_1$ is the relative part of
symbols \( \varepsilon_1 \) among the total number of symbols in the whole sequence \( (p_1 \text{ is not necessarily equal to } 1/2) \). There is a single-valued relation between the memory function \( F(r) \) and the correlation function \( K(r) \) of the Markov chain, see Ref. \[16, 17\].

\[
K(r) = (\varepsilon_1 - \varepsilon_0) \sum_{r'=1}^{N} F(r) K(r-r'), \quad r \geq 1.
\]  

(7)

This equation allows finding the memory function \( F(r) \) and effective constructing the Markov chain with the obtained conditional probability \( P(\cdot | .) \) introduced in Eq. \(6\).

Let us present a "Recipe" and enumerate the consecutive steps of the general method for constructing the correlated sequence of \( \varepsilon_n \) with desired spectra:

1. Dividing the interval of energy \( E \) (or, that is the same, of the wave number \( k \)) to the regions where we want to have different types of spectra.

2. Prescribing \( \Lambda \) or/and \( \tilde{K}(2k) \) in these intervals, we construct "by hand" the total Fourier transform of correlation function \( \tilde{K}(2k) \) for all values of \( k \in [-\pi, \pi] \).

3. Calculating \( K(r) \) as inverse transform of \( \tilde{K}(2k) \).

4. Solving Eq. \(7\), we determine the memory function \( F(r) \) and the conditional probability function \( P(\cdot | .) \).

5. Constructing sequence of \( \varepsilon_0 \) and \( \varepsilon_1 \) with obtained function \( P(\cdot | .) \).

![FIG. 1: The line \( y = \phi x + \xi \) "generates" the Fibonacci sequence (9). The strip bounded by two lines \( y = \phi x \) and \( y = \phi x + 1 \) corresponds to an ensemble of all possible Fibonacci sequences with \( 0 \leq \xi < 1 \). The line \( y = \phi x + \xi \) intersects a horizontal line \( y = 1 \) between 0 and 1 (and so does another line \( y \) between \( r \) and \( r+1 \)) at point \( a \) (and \( b \)) and gives \( \Phi_\xi(0) = 1 \) (and \( \Phi_\xi(r) = 1 \)). Such values of \( \xi \) give a nonzero contribution to the integral (12).](image)

To construct the total correlation function \( K(r) \) we have to calculate the "patrial" ones. Let us present here some simple examples of the correlation functions corresponding to the above-mentioned sequences exhibiting the pure spectra of periodic, random and quasi-periodic chains.

It follows from definition (2) that the correlation function of a chain of alternating potentials \( \varepsilon(n) = \ldots \varepsilon_0 \varepsilon_1 \varepsilon_0 \varepsilon_1 \ldots \) has the form:

\[
C_{a,2}(r) = \frac{(-1)^r}{4} (\varepsilon_1 - \varepsilon_0)^2.
\]  

(8)

It follows from the same definition (2) that the correlation function of the sequence with the same potentials \( \varepsilon(n) = \ldots \varepsilon_0 \varepsilon_0 \varepsilon_0 \ldots \) is equal to zero for all distances \( r \). Nevertheless, the ratio \( C(r)/C(0) = K(r) \) should be defined as unity. Only in this case Eq. \(4\) gives the correct value of the Lyapunov exponent.

The correlation function of the non-biased non-correlated random sequence of \( \varepsilon_n \) is

\[
C_p(r) = (\varepsilon_1 - \varepsilon_0)^2 \left\{ \begin{array}{ll}
1/4, & r = 0 \\
0, & r \neq 0.
\end{array} \right.
\]  

(9)
Let us derive the correlation function of the quasi-periodic chain of potentials $\varepsilon_n$ constructed using the Fibonacci chain, 

$$\Phi_\xi(r) = [(r + 1)\varphi + \xi] - [r\varphi + \xi].$$

(10)

as,

$$\varepsilon_r(\xi) = \varepsilon_0 + (\varepsilon_1 - \varepsilon_0)\Phi_\xi(r), \quad \xi \in [0, 1),$$

(11)

Here $\varphi$ is the so-called golden number, $\varphi = (\sqrt{5} - 1)/2$, and $\xi$ selects some concrete sequence from among all possible Fibonacci sequences. The geometrical meaning of this construction is explained in Fig. 1. To determine the correlation function of this sequence it is convenient to use an ergodic theorem [18] about the homogeneity of distribution of $y_n = n\varphi - \lfloor n\varphi \rfloor$ on the interval $0 \leq y < 1$ for any irrational number $\varphi$ and calculate correlation function $C(r)$ using ensemble average $< \cdot >_a$ instead of space average (2),

$$C(r) = <\varepsilon_n\varepsilon_{n+r}>_a - <\varepsilon_n>^2_a < f(\varepsilon_n) >_a = \int_0^1 f(\varepsilon_n(\xi)) d\xi.$$  

(12)

From a simple geometric consideration, see explanation in Fig. 1, we obtain the following result,

$$C_s(r) = (\varepsilon_1 - \varepsilon_0)^2 \left\{ \begin{array}{ll} 2\varphi - 1 - \{\varphi r\}, & \{\varphi r\} \leq 1 - \varphi, \\ 3\varphi - 2, & 1 - \varphi \leq \{\varphi r\} < \varphi,
\end{array} \right.$$  

(13)

Here $\{x\}$ is the fractional part of $x$. The function $K_s(r) = C_s(r)/C_s(0)$ of continuous argument $r$ is shown in Fig. 2. Actually, the correlation function is defined for the integer arguments, which values are incommensurable with the period $1/\varphi$ of function $C_s(r)$. The function $C_s(r)$ of the discrete argument is shown in Fig. 3. Numerical calculations of $C_s(r)$ carried out using spatial averaging exhibit a good agreement with the analytical one. Below we construct an example of the sequence with a prescribed spectral property. Let us suppose that the Schrödinger Eq. has all three kind of spectra. Let $k_{i1}$ and $k_{i2}$ be the wave vectors corresponding to the top and bottom edges of the bands where the singularly continuous, $i = s$, absolutely continuous, $i = a$, and point (discrete), $i = p$, spectra take place. In fact, we do not need to calculate Fourier transforms $\tilde{K}(k)$ of the correlation function as it is indicated above in the paragraph 3 of the “Recipe”. We can calculate the Fourier transform of the composed correlation function $K(r)$ presented in $k$-space via characteristic functions $\chi_{[k_{i1}, k_{i2}]}(k)$ of the intervals $[k_{i1}, k_{i2}]$, 

$$\tilde{K}(k) = \sum_{i = (a, s, p)} \chi_{[k_{i1}, k_{i2}]}(k)\tilde{K}_i(k).$$

(14)
FIG. 3: The correlation function $K_s(r) = C_s(r)/C_s(0)$ of the Fibonacci chain for $\varepsilon_0 = 0$, $\varepsilon_1 = 1$.  

where characteristic function $\chi_{[k_1, k_2]}(k)$ is equal to 1 if $k \in [k_1, k_2]$ and equals 0 otherwise. Straightforward calculations yield:

$$K(r) = \sum_i \left[ \frac{k_{i2} - k_{i1}}{\pi} K_i(r) + \frac{1}{\pi} \sum_{r' = 1}^{\infty} [K_i(r + r') + K_i(r - r')] \frac{\sin r'k_{i2} - \sin r'k_{i1}}{r'} \right].$$  \hspace{1cm} (15)

Here the functions $(\sin r'k_{i2} - \sin r'k_{i1})/r'$ are the Fourier transforms of the characteristic functions. In the case $i = p$, the contribution of the point spectrum to Eq. (15) is reduced to one term only,

$$[...] = \begin{cases} 
\sin r'k_{p2} - \sin r'k_{p1}, & r \neq 0, \\
\frac{k_{i2} - k_{i1}}{\pi}, & r = 0.
\end{cases}$$  \hspace{1cm} (16)

Note that in deriving Eq. (15) we did not use the concrete form of correlation functions Eqs. (8), (9) and (13). In Fig. 4 the result of numerical simulation of the normalized Lyapunov exponent $\Lambda'(E) = 32 \sin^2(k) \Lambda(E)/(\varepsilon_1 - \varepsilon_0)^2$ is presented for the system exhibiting two types of spectrum, namely, absolutely continuous with $\Lambda' = 0$ at $0 < E < 1$ and point spectrum $\Lambda' = 1.5$ at $1 < E < 2$.  

FIG. 4: The "normalized" Lyapunov exponent $\Lambda'$ of the binary correlated system vs. the energy $E$. The solid line is the prescribed characteristic of system with the stepwise Lyapunov exponent $\Lambda'$. The dots are the result from the calculation of the Lyapunov exponent of the sequence $\varepsilon(n)$ constructed by means of the memory function $F(r)$ obtained by numerical solution of Eq. (7) for the correlation function $K(r) = \sin(\pi r/3)/(\pi r/3)$, corresponding to the stepwise Lyapunov exponent.

Thus, we have proposed a method for constructing 1D sequences of sites $\varepsilon(n)$ with a correlated disorder exhibiting
a hybrid spectrum with three different spectral components ordered in any predefined manner in the region of energy $E$ and/or wave number $k$.

Authors are grateful to L. A. Pastur for the discussion which was helpful in the formulation of the problem under study. We thank S. A. Gredeskul, A. A. Krokhin, and F. M. Izrailev for useful and enlightening discussions.

[1] F. M. Izrailev and A. A. Krokhin, Phys. Rev. Lett. 82, 4062 (1998).
[2] L. Tesieri, J. Phys. A.: Math. Gen. 35, 9585 (2002).
[3] F. M. Izrailev and N. N. Makarov, J. Phys. A.: Math. Gen. to be published.
[4] P. W. Anderson, Phys. Rev. 109, 1492-1505 (1958).
[5] J. C. Flores, J. Phys. Condens. Matter 1, 8471 (1989).
[6] A. Bovier, J. Phys. A 25, 1021 (1992).
[7] P. Carpena, P. Bernaola-Galván, P. Ch. Ivanov, and E. Stanley, Nature 418, 955 (2002).
[8] P. Carpena, P. Bernaola-Galván, P. Ch. Ivanov, and E. Stanley, Nature 421, 764 (2003).
[9] D. J. Thouless, J. Phys. C 6, L49 (1973).
[10] M. Griniasty and S. Fishman, Phys. Rev. Lett. 60, 1334 (1998).
[11] J. M. Luck, Phys. Rev. B 39, 5834 (1989).
[12] M. Reed and B. Simon, Methods of Modern Mathematical Physics (Academic Press, New York, London, 1978).
[13] In the frame of the theory of perturbation one cannot pretend that in each domain of energy the spectrum contains only one pure component. We can claim only that in each energetic region there dominate one of spectral component.
[14] O. V. Usatenko and V. A. Yampol’skii, Phys. Rev. Lett. 90, 110601 (2003).
[15] O. V. Usatenko, V. A. Yampol’skii, K. E. Kechedzhy and S. S. Mel’nyk, Phys. Rev. E 68, 06117 (2003).
[16] S. S. Melnyk, O. V. Usatenko, V. A. Yampol’skii, arXiv:physics/0412169 to appear in Physica A.
[17] S. S. Melnyk, O. V. Usatenko, V. A. Yampol’skii, and V. A. Golick, Phys. Rev. E 72 (2), 026140 (2005).
[18] V. I. Arnold and A. Avez, Ergodic Problems in Classical Mechanics (Benjamin, New York, 1968).
[19] The Lyapunov exponents are equal to zero for both regions of singular and absolutely continuous spectra and do not distinguish them. The numerical study of three types of spectra demands more sophisticated tools such as participation ratio or fractal dimension and will be carried out elsewhere.