One-dimensional tight-binding models with correlated diagonal and off-diagonal disorder

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We study localization properties of electronic states in one-dimensional lattices with nearest-neighbour interaction. Both the site energies and the hopping amplitudes are supposed to be of arbitrary form. A few cases are considered in details. We discuss first the case in which both the diagonal potential and the fluctuating part of the hopping amplitudes are small. In this case we derive a general analytical expression for the localization length, which depends on the pair correlators of the diagonal and off-diagonal matrix elements. The second case we investigate is that of strong uncorrelated disorder, for which approximate analytical estimates are given and compared with numerical data. Finally, we study the model with short-range correlations which constitutes an extension with off-diagonal disorder of the random dimer model.

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I. INTRODUCTION

The studies on the localization of electronic states in disordered solids can be traced back to the seminal paper of P. W. Anderson, where the localization of quantum states was first discussed in connection with transport properties of a random lattice. This is a natural association, since the extended or localized nature of the one-particle wave-functions in a disordered system plays a key role in the determination of the metallic or insulating character of the system itself. As an outstanding example of the link between transport properties and wave-function localization in random media one could cite, for instance, the metal-insulator transition that occurs in disordered three-dimensional samples upon increasing the randomness of the material.

The importance of the Anderson localization, however, far exceeds the limited field of condensed matter physics. That is mainly due to the fact that quantum interference is the fundamental mechanism responsible for the electron localization in a random lattice; as a consequence, analogous localization effects can take place in any phenomenon that involves propagation of waves in a disordered medium. The same conceptual framework thus allows one to understand seemingly heterogeneous phenomena as the localization of water waves, the coherent backscattering of photons, and the universal conductance fluctuations typical of mesoscopic samples (see, for instance, reference).

The basic one-dimensional (1D) Anderson model has proved to be a valuable tool to gain insight in the complex phenomenon of localization. The model is appealing because it is extremely simple and yet retains the capacity to provide a non-trivial description of the localization process. Mathematically, the Anderson model is defined by the tridiagonal Hamiltonian

\[ \hat{H} = \sum_n (|n\rangle \langle n-1| + |n\rangle \langle n+1| + |n\rangle \langle n|) \]  

and disorder is introduced through the site energies \( \delta_n \) which are supposed to be random and independent variables (with an appropriate distribution).

In spite of its undiscussed usefulness, the basic model cannot account for many essential aspects of localization phenomena, such as the metal-insulator transition. The twofold reason of this shortcoming lies in the 1D nature of the system and in the statistical independence of the random site energies \( \delta_n \). As a consequence of these two key features, all eigenfunctions of the Hamiltonian turn out to be localized, even if the disorder is infinitesimally small.

The key role played by dimensionality in the localization processes led at first to the conclusion that only a 3D generalization of the Anderson model could reproduce such basic characteristics of disordered solids as the existence of mobility edges or the metal-insulator transition. The progress in the investigation of 1D systems, however, eventually led to the realization that such models can exhibit a richer behaviour than it was previously thought. In fact, it was discovered that even in one-dimensional lattices there are classes of random potentials which allow for extended states (see, e.g., reference).

In all these 1D systems the disorder exhibits spatial correlations, in contrast to the totally uncorrelated potential of the standard Anderson model. A significant example of a system where the correlations of the site potential can produce delocalized states is given by the so-called ‘random dimer’, which is characterized by a peculiar form of short-range correlations of the potential.

The analysis of models with correlated disorder revived the interest in 1D chains and revealed the essential role of correlations. One must observe, however, that the short-range correlations of the random dimer and similar systems can give rise at best to a discrete set of
extended quantum states: in other words, the localization length diverges only for discrete values of the energy. The situation may change when long-range correlations come into play, as it was recently discovered in [3], where the general case of diagonal disorder with arbitrary correlations was considered and a direct relation between the localization length and the potential pair correlators was established. Using this relation it was shown how to reconstruct a site-potential giving rise to any given form of energy dependence of the localization length [3]. A particular conclusion is that even 1D random lattices can possess a continuum of extended states (and mobility edges), provided the disorder exhibits appropriate long-range correlations.

In the present work we follow an approach similar to that of reference [3] by extending the study to a general case of 1D Anderson model with any kind of diagonal disorder and off-diagonal nearest-neighbour interaction.

This work is organized as follows. The rest of the introduction is devoted to the definition of the model under study. In Section II we analyse the case in which the disorder and off-diagonal nearest-neighbour interaction. In Section III we consider the case of strong correlations. In Section IV we investigate the case of random site- and hopping energies, the study. In Section V we analyse the case in which the on the case of random site- and hopping energies, the numerical data. In Section IV we investigate the case of strong range correlations.

The concluding remarks are exposed in Section V.

A. Definition of the model

We study the localization properties of the following one-dimensional tight-binding Hamiltonian

\[
\hat{H} = \sum_n \left[ \langle n | \gamma_{n-1} | n - 1 \rangle + | n \rangle \gamma_{n+1} \langle n + 1 | + | n \rangle \delta_n \langle n | \right]
\]

(2)

where the site energies \( \delta_n \) and the off-diagonal elements \( \gamma_n \) are arbitrary real variables. From the physical point of view, the Hamiltonian (2) describes an ‘electron’ moving in a discrete 1D lattice. The energies \( \delta_n \) measure the strength of the bond of the electron to the ‘atoms’ of the chain, while the hopping terms \( \gamma_n \) represent the probability amplitudes for an electron localized in a single site to jump to the nearest atoms to the right or to the left.

Notice that in our model the transition amplitudes

\[ A_{n \rightarrow n \pm 1} = \langle n \pm 1 | H | n \rangle = \gamma_n \]

depend only on the initial state of the electron and not on the final one. This physical feature is connected to the non-Hermitian character of the operator (2). With regard to this point, we stress that, although the operator (2) is not Hermitian, its eigenvalues are real: this allows one to consider it as a physically sound Hamiltonian.

In order to show that the eigenvalues of \( \hat{H} \) are real, let \( E \) be an eigenvalue of the operator (2) and \( |\psi_E\rangle \) the corresponding eigenvector

\[
\hat{H} |\psi_E\rangle = E |\psi_E\rangle.
\]

(3)

Let us now consider the operator \( \hat{H}^T \), i.e. the transpose of \( \hat{H} \) and let us denote with \( |\phi_E\rangle \) the eigenvector of \( \hat{H}^T \) to the eigenvalue \( E \), so that one has

\[
\hat{H}^T |\phi_E\rangle = E |\phi_E\rangle.
\]

(4)

Notice that if \( E \) belongs to the spectrum of \( \hat{H} \), then the same value is also an eigenvalue of \( \hat{H}^T \), since a matrix and its transpose share the same spectrum. Multiplying equation (6) by \( \langle \psi_E | \) one can obtain

\[
E \langle \psi_E | \phi_E \rangle = \langle \psi_E | \hat{H}^T | \phi_E \rangle = \langle \hat{H} \psi_E | \phi_E \rangle = E^* \langle \psi_E | \phi_E \rangle
\]

(5)

where we have used equation (6) and the fact that \( \hat{H} \) is a real matrix (and therefore its transpose coincides with its adjoint). Equation (6) implies that \( E = E^* \), unless one has \( \langle \psi_E | \phi_E \rangle = 0 \). One can rule this last possibility out, however, due to the specific structure of the operator (2). Indeed, for the Hamiltonian (2) one has that

\[
\hat{H}^T = \hat{A}^{-1} \hat{H} \hat{A}
\]

(6)

where \( \hat{A} = \sum_n | n \rangle \frac{1}{\gamma_n} \langle n | \). Relation (6) between \( \hat{H} \) and \( \hat{H}^T \) implies that \( |\phi_E\rangle = \hat{A}^{-1} |\psi_E\rangle \), and this allows one to exclude the possibility that \( |\psi_E\rangle \) and \( |\phi_E\rangle \) are orthogonal. This leads to the conclusion that \( E = E^* \), i.e. that the Hamiltonian (2) has real eigenvalues.

Below, we consider the stationary Schrödinger equation \( \hat{H} |\psi\rangle = E |\psi\rangle \), with eigenvectors

\[
|\psi\rangle = \sum_n \psi_n | n \rangle
\]

Using the explicit form (2) of the Hamiltonian, one can easily see that the Schrödinger equation for the amplitudes \( \psi_n \) takes the form

\[
\gamma_{n+1} \psi_{n+1} + \gamma_{n-1} \psi_{n-1} = (E - \delta_n) \psi_n.
\]

(7)

It is convenient to introduce the new variables

\[
\phi_n = \gamma_n \psi_n
\]

(8)

and

\[
\xi_n (E) = \frac{E - \delta_n}{\gamma_n}.
\]

(9)
so that equation (10) can be cast in the simpler form

\[ \phi_{n+1} + \phi_{n-1} = \xi_n \phi_n. \]  

(10)

The introduction of the amplitudes (8) and of the site-energies (6) thus formally allows one to reduce the problem of determining the eigenstates of model (2) to the equivalent problem of studying the zero-energy eigenstate of the tridiagonal model (11) with diagonal-only disorder. According to this interpretation, for any energy value \( E \) in the original Schrödinger equation there is a corresponding realization \( \{ \xi_n (E) \} \) in (10).

Having thus defined our problem, we proceed to solve it for three distinct physical cases: the limiting case of weak disorder (with arbitrary correlations), the opposite case of strong (uncorrelated) disorder and the case of disorder of arbitrary strength with short-range correlations ('N-mer model'). In the following, we will consider off-diagonal terms of the form

\[ \gamma_n = 1 + \epsilon_n. \]

(11)

The reason for representing the energies \( \gamma_n \) in the form (11) is that in this way we separate two physically distinct contributions to the off-diagonal matrix elements: the first one originates from the kinetic energy term of the Hamiltonian, while the second one, \( \epsilon_n \), represents the fluctuating part of the interaction between nearest neighbours. The latter contribution is the source of randomness for the hopping energies \( \gamma_n \) of our model (3).

II. WEAK CORRELATED DISORDER

A. Localization length

In this Section we consider the general case of weak disorder:

\[ |\epsilon_n| \ll 1 \quad \text{and} \quad |\delta_n| \ll 1 \]

(12)

for any kind of site-energies \( \delta_n \) and interaction \( \epsilon_n \).

Notice that, since the randomness of the hopping terms \( \gamma_n \) comes only from the interaction energies \( \epsilon_n \), the condition of weak disorder for the off-diagonal terms is given by the first of the relations (12) (and not by the condition \( \gamma_n \ll 1 \)). Under the conditions (12) one has

\[ \xi_n \approx E - (E\epsilon_n + \delta_n) \]

so that equation (11) can be approximated by

\[ \phi_{n+1} + \phi_{n-1} = (E - E\epsilon_n - \delta_n) \phi_n. \]

(13)

1. Classical representation of the quantum model

An effective way (14) to study the quantum model (13) consists in representing it in terms of the classical two-dimensional Hamiltonian map

\[
\begin{align*}
    p_{n+1} &= (p_n + A_n x_n) \cos \mu + x_n \sin \mu \\
    x_{n+1} &= - (p_n + A_n x_n) \sin \mu + x_n \cos \mu
\end{align*}
\]

(14)

with

\[ E = 2 \cos \mu \]

(15)

and

\[ A_n = \frac{\delta_n + 2 \epsilon_n \cos \mu}{\sin \mu}. \]

(16)

The map (14) describes the behaviour of a harmonic oscillator subjected to periodic delta kicks of amplitude \( A_n \). The map can in fact be derived by integrating over a period \( T = 1 \) the equations of motion of the kicked oscillator defined by the Hamiltonian

\[ H = \mu \left( \frac{p^2}{2} + \frac{x^2}{2} \right) + \frac{x^2}{2} \sum_{n=-\infty}^{\infty} A_n \delta (t - n). \]

The complete equivalence of the quantum system (13) with the classical one defined by the map (14) can be easily proved by eliminating the \( p \) variable from equations (14). In this way, one obtains the relation

\[ x_{n+1} + x_{n-1} = (2 \cos \mu - A_n \sin \mu) x_n \]

which coincides with equation (13) if one identifies the variable \( x_n \) with the site amplitude \( \phi_n \) and if the parameters of the quantum model (13) and those of the classical map (14) are related by the equations (14) and (16). Therefore it becomes possible to analyse the solutions of equation (13) in terms of ‘trajectories’ in the phase-space of the map (14). In such an approach, localized quantum states correspond to unbounded trajectories in the classical phase-space, while extended quantum states are represented by bounded trajectories (see details in [10]).

It is convenient to express the map (14) in polar coordinates \((r, \theta)\) introduced via standard relations \( p = r \cos \theta \) and \( x = r \sin \theta \). The substitution in equation (14) gives

\[
\begin{align*}
    \cos \theta_{n+1} &= \frac{1}{D_n} \left[ \cos (\theta_n - \mu) + A_n \sin \theta_n \cos \mu \right] \\
    \sin \theta_{n+1} &= \frac{1}{D_n} \left[ \sin (\theta_n - \mu) - A_n \sin \theta_n \sin \mu \right]
\end{align*}
\]

where

\[ D_n = \frac{x_{n+1}}{r_n} = \sqrt{1 + A_n \sin (2 \theta_n) + A_n^2 \sin^2 \theta_n}. \]

Using this approach, the inverse localization length \( l^{-1} \) (or Lyapunov exponent \( \lambda \)) can be expressed as

\[ l^{-1} = \lambda = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \log \frac{x_{n+1}}{x_n} \]

(17)
Except that at the band edge (i.e. for $|E| \to 2$), expression (17) can be safely reduced to

$$
\lambda = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \log \left( \frac{r_{n+1}}{r_{n}} \right) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \log D_{n}
$$

(18)

(see [1] for details).

For weak disorder, the logarithm in (18) can be expanded and to the second order of perturbation theory one gets

$$
\lambda = \frac{1}{8} \langle A_{n}^{2} \rangle + \frac{1}{2} \langle A_{n} \sin (2\theta_{n}) \rangle
$$

(19)

where the symbol $\langle \cdots \rangle$ stands for the ‘time’-average, $\langle x_{n} \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} x_{n}$.

2. Computation of the noise-angle correlator

To compute the correlator $\langle A_{n} \sin (2\theta_{n}) \rangle$ with second-order accuracy we follow the approach of [9]. We define the noise-angle $a_{k}$ and the noise-noise $q_{k}$ correlators as follows,

$$
a_{k} = -\frac{2i}{\sigma_{A}^{2}} e^{2i\mu} \langle A_{n} e^{2i\delta_{n-k}} \rangle
$$

(20)

and

$$
q_{k} = \frac{1}{\sigma_{A}^{2}} \langle A_{n} A_{n-k} \rangle = \frac{E^{2}(\epsilon_{n} \epsilon_{n-k}) + 2E(\epsilon_{n} \delta_{n-k}) + \langle \delta_{n} \delta_{n-k} \rangle}{E^{2}(\epsilon_{n}^{2}) + 2E(\epsilon_{n} \delta_{n}) + \langle \delta_{n}^{2} \rangle}
$$

(21)

where $\sigma_{A}^{2}$ is the ‘noise’-variance

$$
\sigma_{A}^{2} = \langle A_{n}^{2} \rangle = \frac{E^{2}(\epsilon_{n}^{2}) + 2E(\epsilon_{n} \delta_{n}) + \langle \delta_{n}^{2} \rangle}{1 - E^{2}/4}.
$$

The terms (20) measure the ‘temporal’ correlations of the noise $A_{n}$ with the angle variable $\theta_{n}$, while equation (21) defines the normalized autocorrelation function for the noise variable (14). Notice that, since the noise strength (16) is a function both of random terms $\epsilon_{n}$ and $\delta_{n}$ and of the energy $E = 2 \cos \mu$, the noise-noise correlator (21) depends on the energy $E$ as well as on the (spatial) correlators of the random variables $\delta_{n}$ and $\epsilon_{n}$.

From the definitions (20), (21) it follows that

$$
\langle A_{n} \sin (2\theta_{n}) \rangle = \text{Re} \left( \frac{\sigma_{A}^{2}}{2} e^{-2i\mu} a_{0} \right).
$$

(22)

As in reference [9] it can be shown that the correlators $a_{k}$ satisfy the relations

$$
a_{k-1} = e^{-2i\mu} a_{k} + q_{k}, \quad \text{for } k = 1, 2, 3, \ldots
$$

which in turn imply that

$$
a_{0} = \sum_{k=1}^{\infty} q_{k} e^{-2i\mu(k-1)}.
$$

(23)

Substituting (23) into (22), one can write

$$
\langle A_{n} \sin (2\theta_{n}) \rangle = \frac{\sigma_{A}^{2}}{2} \sum_{k=1}^{\infty} q_{k} \cos (2\mu k)
$$

so that the Lyapunov exponent (19) takes the form

$$
\lambda = \lambda_{0} \varphi (\mu)
$$

(24)

where

$$
\lambda_{0} (E) = \frac{\sigma_{A}^{2}}{8} \left( \langle \delta_{n}^{2} \rangle + 2E(\epsilon_{n} \delta_{n}) + E^{2}(\epsilon_{n}^{2}) \right)
$$

(25)

and

$$
\varphi (\mu) = 1 + 2 \sum_{k=1}^{\infty} q_{k} (\mu) \cos (2\mu k)
$$

(26)

while the parameter $\mu$ is related to the energy $E$ through equation (15).

3. Discussion of the results

Expression (24), together with equations (23) and (20), gives the localization length as a function of the energy and of the diagonal and off-diagonal potential correlators. Notice that this is a very general result, because its validity rests exclusively on the weak disorder assumption (14) and does not depend on the particular form of the variables $\delta_{n}$ and $\epsilon_{n}$. Equation (24) can therefore be applied to a broad variety of specific problems.

A simple examination of formula (24) also reveals that the inverse localization length $\lambda$ is the product of two factors, $\lambda_{0}$ and $\varphi (\mu)$, defined respectively by equation (25) and (26). This factorization is physically meaningful, because $\lambda_{0}$ represents the Lyapunov exponent for the case of totally uncorrelated disorder (i.e. when $q_{k} = 0$ for $k \geq 1$), while the function $\varphi (\mu)$ describes the correction introduced by the spatial correlations both in diagonal and off-diagonal terms.

Let us now analyse separately the two factors (23) and (26). As was indicated, the first one gives the inverse localization length when no correlations exist among the matrix elements of the Hamiltonian (4). This system corresponds to a simple generalization of the Anderson model, in which not only the site energies but also nearest-neighbour hopping energies are independent random variables. From this point of view, the expression (23) can be seen as an extension of the known formula for the standard Anderson model,

$$
\lambda = \frac{W^{2}}{96 (1 - E^{2}/4)}.
$$

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Indeed the inverse localization length (25) reduces to this form if one assumes that there is no off-diagonal disorder (i.e. \( \langle \epsilon_n^2 \rangle = 0 \) and \( \langle \epsilon_n \delta_n \rangle = 0 \)) and that the variance of the site energies is the one fixed by the Anderson distribution (i.e. \( \langle \delta_n^2 \rangle = W^2/12 \)). Expression (25), however, also shows that the introduction of off-diagonal randomness modifies in a non-trivial way the energy dependence of the Lyapunov exponent with respect to the standard diagonal case. In particular, extended states can arise for specific values of the energy. If, for instance, the diagonal case.

In particular, extended states can arise for specific values of the energy. If, for instance, the diagonal case.

The factor (26) accounts for the modifications generated by the correlations both in the diagonal and off-diagonal terms. One should stress that this factor depends both on the correlations and energy. This is a key feature, because it implies that, as an effect of the correlations, the sample can become more or less transparent for specific values of the energy. As can be seen from equation (24), if \( \varphi (\mu ) > 1 \), the Lyapunov exponent is increased with respect to the uncorrelated case, meaning that correlations make the sample more opaque. On the contrary, when \( \varphi (\mu ) < 1 \), the chain becomes more transparent. Thus, if the function (26) goes to zero in a certain energy range, the states of the system will be extended inside that region and localized outside of it: this shows how mobility edges can arise even in 1D systems, provided that the potential has the proper correlations.

Once the statistical properties of the potential are known, formulas (24), (25) and (26) exactly determine the Lyapunov exponent as a function of the energy. They can be used, however, also to solve the inverse problem, i.e. to specify what the correlations of the disorder must be for the Lyapunov exponent to exhibit a given energy dependence. This is a problem of practical interest because of the relevance of its potential technological applications: knowing what particular disorder generates a specific energy dependence of the Lyapunov exponent might lead to the construction of superlattices with the required transport properties.

Let us now write explicit relations between statistical properties of the disorder and the Lyapunov exponent for the case when the diagonal disorder is independent from the off-diagonal one (\( \langle \epsilon_n \delta_{n-k} \rangle = 0 \). For this we write the function \( \varphi (\mu ) \) in Fourier series,

\[
\varphi (\mu ) = \sum_{k=-\infty}^{+\infty} \varphi_k e^{i2\mu k}
\]

where the expansion coefficients are defined by the relation

\[
\varphi_k = \frac{1}{\pi} \int_{-1}^{+1} \varphi (\mu ) e^{-i2\mu k} d\mu.
\]

Inserting (27) and (21) in equation (26) one obtains the relations

\[
\langle \delta_n^2 \rangle \varphi_k + \langle \epsilon_n^2 \rangle (\varphi_{k-1} + 2\varphi_k + \varphi_{k+1}) = \langle \delta_n \delta_{n-k} \rangle + 2\langle \epsilon_n \epsilon_{n-k-1} \rangle + 2\langle \epsilon_n \epsilon_{n-k} \rangle + \langle \epsilon_n \epsilon_{n-k+1} \rangle
\]

which constitute the explicit link between the Fourier components of \( \varphi (\mu ) \) and the disorder correlators \( \langle \delta_n \delta_{n-k} \rangle \) and \( \langle \epsilon_n \epsilon_{n-k} \rangle \). Once the Lyapunov exponent (and hence the factor \( \varphi (\mu ) \)) is known, the relations (28) set a constraint on the statistical properties of \( \delta_n \) and \( \epsilon_n \). Notice that, in contrast to the purely diagonal case discussed in [9], here the interplay of diagonal and off-diagonal disorder does not allow a complete specification of the correlators from the knowledge of the localization length.

The relations (28) admit a particularly simple solution for the case in which the diagonal and off-diagonal disorder are statistically independent (i.e. \( \langle \epsilon_n \delta_{n-k} \rangle = 0 \)), but share the same statistical properties (so that their auto-correlation functions are equal: \( \langle \delta_n \delta_{n-k} \rangle = \langle \epsilon_n \epsilon_{n-k} \rangle \)). In this peculiar case, the relations (28) do determine the disorder correlators: indeed, one has

\[
\frac{\langle \delta_n \delta_{n-k} \rangle}{\langle \delta_n^2 \rangle} = \frac{\langle \epsilon_n \epsilon_{n-k} \rangle}{\langle \epsilon_n^2 \rangle} = \varphi_k.
\]

This result can be understood from the observation that in this special case the noise-noise correlators (21) take the form \( q_k = \langle \delta_n \delta_{n-k} \rangle / \langle \delta_n^2 \rangle \) and no longer depend on the energy, so that they can be interpreted as Fourier coefficients of the series (26).

### B. Numerical data

We checked numerically the validity of (24) using the classical map approach for the computation of the Lyapunov exponent. We consider the map

\[
\begin{pmatrix}
P_{n+1} \\
X_{n+1}
\end{pmatrix} = M_n \begin{pmatrix}
P_n \\
X_n
\end{pmatrix}
\]

with

\[
M_n = \begin{pmatrix}
\cos \mu & A_n \cos \mu + \gamma_n \sin \mu \\
\frac{1}{\gamma_{n+1}} \sin \mu & -\frac{1}{\gamma_{n+1}} (\gamma_n \cos \mu - A_n \sin \mu)
\end{pmatrix}
\]

which is exactly equivalent to the original Schrödinger equation (10), provided the parameters \( E \) and \( A_n \) of the matrix (30) are defined by the relations (15) and (16). This means that, if (17) and (14) are fulfilled, then the values of the \( X \) coordinate at the time steps \( n - 1 \), \( n \) and \( n + 1 \) obey the same relation expressed by (18) for the probability amplitudes \( \psi_n \).

It should be pointed out that the determinant of the single time-step map (30) is not unitary, det \( M_n = \gamma_n / \gamma_{n+1} \) and, therefore, the determinant oscillates around the unit value as a function of \( n \). This does not mean, however, that the map (30) does not conserve the total flux. Indeed, the disordered sample represented by...
the Hamiltonian \( (2) \) cannot actually be infinite; therefore some kind of boundary conditions have to be imposed. A typical boundary condition is the periodic one: in this case one assumes that the disordered sample is a closed chain made up of \( N \) ‘atoms’ so that the site- and hopping-energies obey the equations: \( \delta_{N+1} = \delta_1 \) and \( \gamma_{N+1} = \gamma_1 \). Consequently, one has

\[
\prod_{k=1}^{N} \det M_k = \frac{\gamma_1}{\gamma_2} \frac{\gamma_2}{\gamma_3} \ldots \frac{\gamma_{N-1}}{\gamma_N} \frac{\gamma_N}{\gamma_{N+1}} = \frac{\gamma_1}{\gamma_{N+1}} = 1
\]

so that the total determinant across the sample is exactly equal to one. A more physical boundary condition arises if the disordered sample is embedded between two perfect leads. This physical condition translates in the mathematical requirements \( \delta_n = 0 \) and \( \gamma_n = 1 \) for \( n > N \) or \( n \leq 1 \), which, in turn, lead again to the condition (31) for the total determinant of the map through the whole sample.

Let us now see how the map \( (29) \) can be effectively used for the computation of the Lyapunov exponent. As was shown above, it is convenient to introduce the polar coordinates \( X = r \sin \theta \) and \( Y = r \cos \theta \) and cast the map \( (29) \) in the form

\[
\begin{align*}
\cos \theta_{n+1} &= \frac{r_{n+1}}{r_n} \cos (\theta_n - \mu) + (A_n \cos \mu + \epsilon_n \sin \mu) \sin \theta_n \\
\sin \theta_{n+1} &= \frac{r_{n+1}}{r_n} \frac{1}{1 + \epsilon_n} \sin (\theta_n - \mu) + (A_n \sin \mu + \epsilon_n \cos \mu) \sin \theta_n
\end{align*}
\]

which allows an easy computation of the expression (18) for the Lyapunov exponent. In this way, we tested the validity of the formula \( (24) \) for the special case in which the hopping energies \( \epsilon_n \) are independent random variables with a common distribution, while the site-energies are defined by the relation

\[
\delta_n = \alpha \epsilon_n \quad \text{with} \quad |\alpha| < 2.
\]

Taking into account Eqs. (33) and (11), the Schrödinger equation \( (7) \) can be written as

\[
(1 + \epsilon_{n+1}) \psi_{n+1} + (1 + \epsilon_{n-1}) \psi_{n-1} = (E - \alpha \epsilon_n) \psi_n.
\]

The box distribution

\[
p(\epsilon_n) = \frac{1}{2W} \theta \left( \frac{W}{2} - |\epsilon_n| \right)
\]

of width \( W \) was chosen for the variables \( \epsilon_n \). For this particular model the general expression \( (24) \) reduces to the following form:

\[
\lambda = \frac{W^2 (E + \alpha)^2}{96 (1 - E^2/4)}.
\]

This formula, among other things, shows that for the above-defined model the state corresponding to the energy value \( E = -\alpha \) is always extended, regardless of the noise strength fixed by the parameter \( W \). In particular, when \( \alpha = 0 \) (i.e. there is no diagonal disorder), the model \( (34) \) exhibits an extended state at the band centre, i.e. for \( E = 0 \). The value \( \alpha = 1 \) corresponds to the case, cited in the previous Subsection, in which the binding and hopping energies are equal \( (\epsilon_n = \delta_n) \) and one has a transparent state for \( E = -1 \). The comparison with numerical data revealed an excellent agreement between the theoretical prediction \( (36) \) and the actual behaviour of the Lyapunov exponent \( \lambda \), as can be seen from Fig. 1 and Fig. 2 which represent \( \lambda \) as a function of the energy \( E \) for two values of the parameter \( \alpha \).
III. STRONG (UNCORRELATED) DISORDER

A. Analytical estimates for the localization length

For the strong disorder case we consider the model \( \tilde{H} \) with diagonal terms of the form (33), i.e. \( \delta_n = \alpha \epsilon_n \) with \( |\alpha| < 2 \). The Schrödinger equation is then given by (34) and the model is completely defined once statistical properties of the random variables \( \epsilon_n \) are specified. Throughout this Section we assume that the energies \( \epsilon_n \) are independent random variables with a common probability distribution given by the box distribution (35) of width \( W \). The case of strong disorder is then defined by the condition \( W \gg 1 \).

Again, by introducing the rescaled amplitudes (38) and the binding energies (33), we can reduce the Schrödinger equation (34) to the form (40) with only diagonal disorder. In the latter model the site-energies (38) take now the form

\[
\xi_n = \frac{E - \alpha \epsilon_n}{1 + \epsilon_n}
\]

and are independent random variables whose distribution \( \tilde{p}(\xi_n) \) is related to the probability \( p(\epsilon_n) \) of the original variables \( \epsilon_n \) by

\[
\tilde{p}(\xi_n) = \frac{|\alpha + E|}{(\alpha + \xi_n)^2} p\left(\frac{E - \xi_n}{\alpha + \xi_n}\right).
\]

In explicit form, when \( p(\epsilon_n) \) is the Anderson distribution (35), the corresponding probability for the variables \( \xi_n \) reads

\[
\tilde{p}(\xi_n) = \begin{cases} 
\frac{|\alpha + E|}{(\alpha + \xi_n)^2} \frac{1}{W} & \text{if } \xi_n < \xi^{(1)} \text{ or } \xi^{(2)} < \xi_n \\
0 & \text{if } \xi^{(1)} < \xi_n < \xi^{(2)}
\end{cases}
\]

where

\[
\xi^{(1)} = \min \left\{ \frac{2E + \alpha W}{2 - W} , \frac{2E - \alpha W}{2 + W} \right\}
\]

and

\[
\xi^{(2)} = \max \left\{ \frac{2E + \alpha W}{2 - W} , \frac{2E - \alpha W}{2 + W} \right\}.
\]

Following the Hamiltonian map approach already used in the previous Section, we can cast equation (40) in the form of the two-dimensional map

\[
\begin{pmatrix} 
\phi_{n+1} \\
\phi_n
\end{pmatrix} = \mathbf{T}_n \begin{pmatrix} 
\phi_n \\
\phi_{n-1}
\end{pmatrix},
\]

where \( \mathbf{T}_n \) is the transfer matrix

\[
\mathbf{T}_n = \begin{pmatrix} 
\xi_n & -1 \\
1 & 0
\end{pmatrix}.
\]

By introducing polar coordinates through the relations \( \phi_n = r_n \cos \theta_n \) and \( \phi_{n-1} = r_n \sin \theta_n \), one can write the map (40) in the form

\[
\begin{cases}
\cos \theta_{n+1} = \frac{1}{D_n} \sin \theta_n \\
\sin \theta_{n+1} = -\frac{1}{D_n} [\cos \theta_n + \xi_n \sin \theta_n]
\end{cases}
\]

where

\[
D_n = \frac{r_{n+1}}{r_n} = \sqrt{1 + \xi_n \sin(2\theta_n) + \xi_n^2 \sin^2 \theta_n}.
\]

As before, the Lyapunov exponent is given by the relation (18) and can, therefore, be expressed by the integral

\[
\lambda = \int d\xi \tilde{p}(\xi) \int d\theta \rho_\xi(\theta) \log D(\xi, \theta)
\]

where the symbol \( \rho_\xi(\theta) \) stands for the invariant measure of the variable \( \theta \) of the map (42), and the subscript \( \xi \) stands in order to stress that such a measure depends on the noise distribution \( \tilde{p}(\xi_n) \).

B. Decomposition of the invariant measure

The integral (18) can be separated in two parts, \( \lambda = I_+ + I_- \) with

\[
I_\pm = \int d\xi \tilde{p}_\pm(\xi) \int d\theta \rho_\pm(\theta) \log D(\xi, \theta).
\]

Here \( \tilde{p}_\pm(\xi) \) are the noise distributions

\[
\tilde{p}_+(\xi) = \begin{cases} 
\tilde{p}(\xi) & \text{for } |\xi| > 2 \\
0 & \text{elsewhere}
\end{cases}
\]

and

\[
\tilde{p}_-(\xi) = \begin{cases} 
\tilde{p}(\xi) & \text{for } |\xi| < 2 \\
0 & \text{elsewhere}
\end{cases}
\]

while \( \rho_+(\theta) \) and \( \rho_-(\theta) \) are the corresponding invariant measures. This decomposition is meaningful because numerical computations have shown that, upon increasing the noise strength \( W \), the invariant measure \( \rho_- (\theta) \) becomes more and more sharply peaked around the single values \( \theta = \pi k \) with \( k \) integer (as can be clearly seen from the Fig. 3).
As a consequence, the integral $I_-$ becomes negligible for strong disorder. The formula (43) can therefore be approximated by
\[
\lambda \simeq \int_{|\xi|>2} d\xi \hat{p}(\xi) \int d\theta \rho_+ (\theta) \log D(\xi, \theta).
\] (44)

The analysis of this expression reveals the simple dependence $\lambda \propto 1/W$ of the Lyapunov exponent on the noise strength. In fact, in (44) the $W$-dependence of the integral is introduced in a twofold way, through the functional $1/W$ dependence of the noise distribution (37) and through the integration range for the $\xi$-variable. For large enough $W$, the integration range is simply determined by the condition $|\xi| > 2$ because the limits (38) and (39) of the interval where the distribution (37) is zero are located inside the interval $|\xi| < 2$. Therefore, for the integral (44) the only dependence left on the noise strength is the one due to the factor $1/W$ contained in the integrand. Physically, this means that, for strong disorder, the localization length grows linearly with the noise intensity. In contrast to the standard Anderson model, therefore, an increase of the lattice disorder reduces the localization of the electronic wave-functions instead of enhancing it.

C. Another approach for the computation of $\lambda$

Although formula (44) allows one to predict the relation of inverse proportionality between $\lambda$ and $W$ without carrying out any explicit calculations, the determination of the proportionality constant requires a direct evaluation of the integral. Unfortunately, the analytical computation of integral (44) is out of reach, since there is no way to determine the invariant measure $\rho_+(\theta)$. One can overcome this difficulty using a different approach successfully used in [11] for an analogous problem.

Once more, we make use of the fact that the Schrödinger equation (10) is exactly equivalent to the 2D map (11) whose eigenvalues are
\[
\lambda_n^{(1,2)} = \xi_n \pm \sqrt{\xi_n^2 - 2}. \tag{45}
\]

For $|\xi_n| < 2$ the eigenvalues (45) take the form $\lambda_n^{(1,2)} = e^{\pm i\mu_n}$ with $\xi_n = 2 \cos \mu_n$, so that, at each step, the evolution dictated by the map (11) results in a simple rotation in the two-dimensional phase-space. For $|\xi_n| > 2$, however, both eigenvalues of the map (11) are real and this consideration allows one to compute the Lyapunov exponent (14) using the approximated expression
\[
\lambda = \langle \log |\Lambda| \rangle = \int d\xi \hat{p}_+ (\xi) \log \Lambda(\xi), \tag{46}
\]

where $\Lambda = \max \{|\lambda^{(1)}|, |\lambda^{(2)}|\}$. The evaluation of integral (46) leads to the formula
\[
\lambda = \gamma (\alpha) \frac{|E + \alpha|}{W}, \tag{47}
\]

where
\[
\gamma (\alpha) = 2 \int_2^{\infty} d\xi \frac{\alpha^2 + \xi^2}{(\alpha^2 - \xi^2)^2} \log \left( \frac{\xi + \sqrt{\xi^2 - 4}}{2} \right).
\]

The validity of the formula (47) was numerically checked; the computations showed a good agreement between the theoretical prediction and the actual behaviour of the Lyapunov exponent, as can be seen, for instance, from Fig. 4 and Fig. 5.

FIG. 3. Invariant measure $\rho_-(\theta)$ for various noise strengths (data refer to the energy value $E=0.01$ and $\alpha = 0$)

FIG. 4. Lyapunov exponent vs. energy for various noise strengths with $\alpha = 0$
Notice that the Lyapunov exponent (47) exhibits the expected \(1/W\) dependence on the noise strength. As we explained, this is a consequence of the fact that the region \(\xi^{(1)} < \xi < \xi^{(2)}\) where the integrand of formula (49) is zero lies outside the integration domain \(|\xi| > 2\). In passing we remark that, if the condition \(|\alpha| < 2\) were not fulfilled, this conclusion would not be true. Therefore, for \(|\alpha| > 2\) the integral (46) would depend on \(W\) not only through the integrand but also through the limits of the integration domain. The computation of the integral remains possible also in this case, but then the result is no longer as simple as the one expressed by formula (47). That is why we chose to restrict the range of the parameter \(\alpha\) to the interval \(|\alpha| < 2\).

IV. DISORDER WITH SHORT-RANGE CORRELATIONS

In this Section we focus our attention to the case in which the diagonal and off-diagonal disorder in the general model (2) exhibit short-range correlations. More precisely, we consider the model defined by assuming that the couples of random variables \(\zeta_n = (\delta_n, \epsilon_n)\) in the Schrödinger equation (7) fulfill the following conditions:

1. The energies \(\zeta_n\) can take only two values: \(\zeta_+ = (\delta_+, \epsilon_+)\) or \(\zeta_- = (\delta_-, \epsilon_-)\).

2. In every succession \(\{\zeta_n\}\) the values \(\zeta_+\) and \(\zeta_-\) appear in \(N\)-uples made of \(N\) consecutive identical terms.

3. The \(N\)-uples \((\zeta_+, \ldots, \zeta_+)\) and \((\zeta-, \ldots, \zeta-)\) appear at random with equal frequency along the succession \(\{\zeta_n\}\).

If \(N = 2\), the pairs \((\zeta_+, \zeta_+)\) and \((\zeta-, \zeta-)\) are called dimers; for \(N = 3\) the corresponding triplets are named trimers, while for generic \(N\) one speaks of \('N\)-mers'.

Making use of the amplitudes (4) and the energies (2) as in the previous cases, one can write the Schrödinger equation (7) in the form (11) where the diagonal energies (4) now take two values

\[
\xi_{\pm} = \frac{E - \delta_{\pm}}{1 + \epsilon_{\pm}}
\]  

(48)

and appear in equiprobable \(\text{-}\text{uples randomly positioned along the succession \(\{\xi_n\}\). In other words, the model (2), with both diagonal and off-diagonal disorder specified by the preceding 1), 2), and 3) conditions, can be associated with the \(N\)-mer model already studied in the literature (see (10) and references quoted therein).

As in reference [11], we can use the equivalence of the model (10) with the map (11) and study the solutions of the Schrödinger equation (10) in terms of the trajectories of the map (11). With this interpretation in mind, we can address the problem of extended states for the model (10) by considering a single \(N\)-mer of type \(\zeta_+\) embedded in an infinite chain of \(\zeta_-\) \(N\)-mers. In this case the orbits of the map (11) are not affected by the single \(\zeta_+\) \(N\)-mer provided that the total transfer matrix through the \(N\)-mer is equal to the identity matrix (apart from a plus/minus factor). In other words, one must have

\[
\mathbf{T}_+^N = \pm \mathbf{E}
\]  

(49)

where \(\mathbf{T}_+\) is the transfer matrix (11) (with \(\xi_n = \xi_+\)) and \(\mathbf{E}\) is the unit matrix.

The ‘transparency’ condition (49) can be satisfied provided that the stability condition \(|\xi_+| < 2\) for the map (11) is fulfilled. In this case the eigenvalues of the matrix \(\mathbf{T}_+\) have the form \(e^{\pm \mu_+}\) (with \(\xi_+ = 2 \cos \mu_+\)) and the equation (13) is equivalent to \(\exp(\mu_+ N) = \pm 1\) which in turn leads to \(\mu_+ = \pi k/N\) with \(k\) integer. On the other hand, the stability condition \(|\xi_+| < 2\) requires to discard the \(k\) values \(k = m \cdot N\) with \(m\) integer. Using (45) and the relation \(\xi_+ = 2 \cos \mu_+\), we come to the conclusion that the \(N\)-mer is transparent for the following energy values

\[
E = \delta_+ + 2 (1 + \epsilon_+) \cos \left(\frac{\pi k}{N}\right)
\]

with \(k = 1, 2, \ldots, N - 1\).

The study of the single \(N\)-mer case allows one to understand that, in the general case of a chain where \(\text{-}\text{mers of type } \zeta_+ \text{ and } \zeta_- \text{ randomly alternate}, the model (2) with disorder correlated by \(\text{-}\text{uples has extended states when the energy takes the values}

\[
E = \begin{cases} 
\delta_+ + 2 (1 + \epsilon_+) \cos \left(\frac{\pi k}{N}\right) \\
\delta_- + 2 (1 + \epsilon_-) \cos \left(\frac{\pi k}{N}\right)
\end{cases}
\]  

(50)

where \(k = 1, 2, \ldots, N - 1\). In the particular case when the diagonal and off-diagonal disorder are related by the linear equation \(\delta_n = \alpha \mu_n\), one should add the special value \(E = -\alpha\) to the list (60), because in this case the
variables take the single value $\xi_n = -\alpha$ and disorder disappears from equation (4).

The theoretical prediction was checked by numerically computing the Lyapunov exponent for the system with dimer- and trimer-correlated disorder as a function of the energy. Numerical experiments have confirmed the validity of formula (50), specifically, the Lyapunov exponent vanishes whenever the energy takes one of the values (50), see Figs. 6, 7.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig6}
\caption{Lyapunov exponent for dimer-correlated disorder with $\delta_{\pm} = 0$, $\epsilon_+ = 0$, $\epsilon_- = 0.5$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig7}
\caption{Lyapunov exponent for trimer-correlated disorder with $\delta_{\pm} = 0$, $\epsilon_+ = 0$, $\epsilon_- = 0.5$.}
\end{figure}

V. CONCLUDING REMARKS

In this paper we have studied the 1D tight-binding model described by the Hamiltonian which has both diagonal and off-diagonal variable matrix elements. The main object of this study is the analysis of the localization length and its dependence on underlying correlations in the diagonal and off-diagonal potential. By making use of the reduction of the quantum model to a proper classical Hamiltonian map, we have considered a few most interesting cases of the interplay between diagonal and off-diagonal correlated disorder.

The first case which has been analysed in details is the model with a weak site-potential and a weak fluctuating part in the off-diagonal matrix elements. In this case we have derived a general analytical expression for the localization length valid for any kind of randomness in the potential. More specifically, the localization length is expressed in terms of pair correlators for the diagonal and off-diagonal matrix elements. Using this expression, one can consider any kind of correlated disorder, as well as deterministic potential and hopping off-diagonal amplitudes. The expression obtained for the localization length allows to reveal how this latter quantity is influenced by pair correlations. A few specific cases of correlated disorder have been discussed to illustrate the role of the correlations. One of the most interesting results is that if the diagonal and off-diagonal disorder are proportional to each other, there is a specific value of the energy for which the eigenstates are extended. For finite sample, therefore, there is a region where all states are fully transparent as in the dimer models with short-range correlations.

Another case studied in this paper is that of strong disorder (both diagonal and off-diagonal). In this case we have been able to obtain an approximate analytical expression for the localization length which shows that, when lattice randomness increases, localization effects weaken. This feature contrasts with the behaviour of the standard 1D Anderson model (with only diagonal disorder) and is a non-trivial consequence of the interaction of the site-potential with the off-diagonal hopping energies.

Very recently [12] an analytical expression for the invariant density $\rho_\xi(\theta)$ in the strong disorder case has been obtained in a different context.

Finally we have examined the case of disorder with short-range correlation, focusing our attention on the specific $N$-mer model, where disorder correlations are introduced by assigning the same value of the site- and hopping-energies to $N$ consecutive chain sites. For this case we have showed how correlations give rise to a discrete set of extended states.

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