Phase Space Description of Localization in Disordered One-Dimensional Systems

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(Received October 17, 2005; revised version July 10, 2006)

The degree of electronic localization in disordered one-dimensional systems is discussed. The model is simplified to a set of Dirac δ -like functions used for the potential in the Schrödinger equation and calculations are carried out for the ground state. The disorder of topological character is introduced by the random shifts of the potential peaks. For comparison, we also discuss two aperiodic systems of the potential peaks: Thue–Morse and Fibonacci sequences. The localization, both in the momentum and the real space, is analyzed for different disorder strengths and sizes of the system. We calculate the localization length, and additionally we express the localization effects in terms of the inverse participation function and also by means of the Husimi quasi-classical distribution function in the phase space of the electron (position, momentum) coordinate system. We present the influence of disorder generated by the random and aperiodic sequences of potential on the energy spectrum.

PACS numbers: 73.21.Hb, 73.20.Fz, 71.23.An

1. Introduction

Low-dimensional systems are promising materials for applications in modern electronics, where the quantum phenomena determine the processes in nano-devices. Therefore, one of the most important questions in this matter is about importance of disorder in such systems, because in the case of quantum wells or wires disorder plays a crucial role and can dramatically change the properties of the system [1, 2]. Besides, the properties of disordered systems strongly depend on the realization of disorder controlled by technological processes [3].

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In general one-dimensional disordered systems can be treated as the superposition of compositional disorder and structural one which is reduced to the topological disorder in this dimension. These limiting cases of disorder can be described by the Anderson model [4, 5] and the Edwards model [6], respectively. The problem of determining the electronic properties of topologically disordered systems has a long history of important issues like for example the metal–insulator transition [7]. The nature of this transition is one of the fascinating problems in condensed matter.

As it is well established, in disordered one-dimensional systems all eigenstates are localized by an arbitrary weak disorder [8–10] for uncorrelated random potentials [11]. This means that the amplitude of the wave function exponentially decays over long distance, as it was pointed by Mott and Twose [12]. The properties of the topologically disordered one-dimensional system of non-interacting electrons are considered. We focus our investigation on the ground state of the system when the disorder is present and assume that the ground state is isolated from the excited states.

Our work was partially stimulated by paper [13], where authors discussed the properties of two lattice models, namely the Anderson model [4] and the Harper model [14], or Aubry–André model [15] in the phase space. The influence of localization on transport properties of disordered one-dimensional wires is presented in papers [16, 17]. In our work we use the same model potential with Dirac- δ scatterers to calculate phase space localization properties for different random or aperiodic sequences.

The paper is organized as follows. Section 2 describes the liquid Kronig–Penney model [18, 19] and its version defined by a sequence which we refer to as the “cosine” sequence. We also use the Thue–Morse [20] and Fibonacci [21] sequences as the examples of aperiodic structures. Section 3 consists of the analysis of ground state properties. We calculate the localization length for all above-mentioned sequences and next we use the inverse participation ratio (IPR) [22, 23] as the measure of the electronic wave function localization in the real space and the momentum space. The influence of disorder on the density of states (DOS) is also investigated. Finally we consider the IPR in the phase space using the Husimi function as an example of distribution function in the phase space [24, 25] for systems with different sizes. In Sect. 4 we discuss our results.

2. Model of disordered wire

The one-dimensional wire with topological disorder is described by the liquid Kronig–Penney model [18, 19], which can be regarded as the realization of the Edwards model in one dimension. We consider the time-independent Schrödinger equation for the system of non-interacting electrons with effective mass m which move in a random potential $V(x)$, namely

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right) \psi(x) = \varepsilon \psi(x), \quad (1)$$

where ε and $\hbar$ have their usual meanings.

In fact, the potential $V(x)$ represents the collection of N elements, e.g. atoms or more complex structural units placed in a chain of size $L = x_N - x_1$. The scattering potentials are assumed well located at random positions x_i ,

$$V(x) = \sum_{i=1}^N F_0 \frac{\hbar^2}{m} \delta(x - x_i), \quad (2)$$

where $F_0 \hbar^2/m$ is the area in the $V(x)$ plot in the vicinity of Dirac- δ function located at x_i , which represents the strength of local $V(x)$. A regular lattice makes a set of equally spaced points with the lattice constant a . An amorphous structure is given as a set of scattering centers in the chain at locations x_i ,

$$x_i = (i + \eta r_i)a, \quad i = 1, 2, \dots, N, \quad (3)$$

where r_i is a random number from the range $(-1, +1)$ and parameter $\eta \geq 0$ is just a measure of disorder. Let us note that $\eta = 0$ yields the crystalline state.

Another example of amorphous structure used in our calculations is the “cosine” sequence determined by

$$x_{i+1} = x_i + a[(1 - x_c) \cos(2\pi\alpha i^\nu) + 1], \quad (4)$$

where α is an irrational number from the range $(0, 1)$ (in our calculations we take $\alpha = 3/(5\pi)$ as in Ref. [26]), x_c is a cut-off parameter, and ν is a measure of disorder.

The relation given by Eq. (4) with some modification was proposed as a description of disorder in lattice models. More details on this form can be found in Ref. [26] and references therein. Here, we use the distribution of positions x_i which is based on the potential distribution of the original model. We also introduce the cut-off parameter x_c . The role of this parameter will be explained later. The considered sequence is used for comparison with the sequence which is introduced here as a first case. In both cases we can control the degree of disorder in the systems with parameters η and ν , respectively.

For comparison we also consider two types of aperiodic chains which are produced in semiconductor structures. The Thue–Morse sequence (t_n) over $\{0, 1\}$ can be defined recursively for all $n \geq 0$ by

$$t_0 = 0, \quad t_{2n} = t_n, \quad t_{2n+1} = \bar{t}_n,$$

where $\bar{t}_i$ is defined as $\bar{t}_i = 1 - t_i$ for $t_i \in \{0, 1\}$.

That gives the integer sequence

$$01101001100101101001011001101\dots$$

used as a pattern while forming chains. In the same way we can make use of the Fibonacci sequence over $\{0, 1\}$, using the following inflation rule $0 \rightarrow 01$ and $1 \rightarrow 0$. Starting with 0, one obtains the sequence in the form [27]

010010100100101001010010101010...

The both integer sequences are used to form the aperiodic chains. Ones correspond to the scattering potential in the lattice placed at x_i ($i = 1, \dots, N$). Zeros are just empty places in positions where the δ potentials are present in the simple periodic lattice.

The wave function which satisfies Eq. (1) is an analytical expression in between consecutive δ -like peaks, for $x > x_i$ of each i th peak

$$\chi_i(x) = C_i \cos(kx + \varphi_i), \quad (5)$$

where C_i is the amplitude, $k = \sqrt{2m\varepsilon}/\hbar$, and φ_i is the phase.

Stepping over the peaks makes it necessary to adjust a new amplitude C and phase φ , so that the two conditions at each crossing

$$\psi(x_i^+) = \psi(x_i^-), \quad (6)$$

$$\left. \frac{d}{dx} \psi(x) \right|_{x_i^+} - \left. \frac{d}{dx} \psi(x) \right|_{x_i^-} = 2F_0 \psi(x_i), \quad (7)$$

are satisfied. These conditions come directly from the continuity of the wave function and continuity of its first derivative for regular potentials; however for singular potentials of δ -like form, $F_0 \delta(x - x_i)$, the discontinuity in derivative of ψ , as given by Eq. (7), is expected.

The presented method can be successfully applied to numerical calculations for systems which include about 100–200 elements at maximum. For longer systems numerical calculations may become divergent in this simple shooting numerical integrator.

The knowledge of exact form of $\psi(x)$ allows us to find the DOS function $\rho(E)$ from the relation

$$\rho(E) = \frac{dS}{dE}, \quad (8)$$

where $S(E)$ is the number of zeros of the wave function $\psi(x)$, and corresponds to the number of excited states with energy $\varepsilon \leq E$.

3. Results and discussion

The energy spectrum (DOS function) for the reference periodic chain is presented in Fig. 1a. Figure 1b shows DOS for corresponding disordered case $\eta > 0$. By analogy we introduce disorder to the “cosine” system by changing the value of ν parameter — see Figs. 1e and f. In both cases disorder gives the localized states in the energy gap which broaden the bands when disorder becomes larger, and the tails of localized states are shaped. This effect can be interpreted as the smearing off the van Hove singularities at the band edges. The localized and extended states are separated by the mobility edge [28] which represents the critical energy for the metal–insulator transition in the Anderson scenario. The DOS function for aperiodic chains which are formed by the Thue–Morse and Fibonacci sequences

Fig. 1. Density of states $\rho(E)$ calculated for 10^5 sites in (a) periodic system, (b) amorphous system with $\eta = 0.4$, (c) Thue-Morse sequence, (d) Fibonacci sequence and “cosine” sequences with (e) $\nu = 1$, (f) $\nu = 1.1$. Insets contain results for 100 sites.

clearly exhibit an intermediate character between crystal and systems upon amorphization. The appearance of the energy gaps is a consequence of introducing an aperiodic modulations of the scattering centers position. The energy spectrum (DOS) presented in Fig. 1 was calculated for the quite long chains (10^5 elements), because the results obtained for the shortest ones should be treated more carefully from the statistical point of view. On the other hand calculating DOS functions does not lead to numerical difficulties even for very long systems, affecting only time needed for computation and not the accuracy.

In disordered systems, the phase and amplitude of the electronic wave function is changed by the spatial fluctuations of potentials and in consequence the envelope of the wave function decays exponentially from a localization center ξ as it is shown in Fig. 2. Moreover, as disorder becomes larger the localized states become more compressed (compare Fig. 2a with b and e with f).

This means that the electronic density $|\psi_n(x)|^2$ will not spread all over the system but will remain localized around ξ . Therefore the wave function can usually be fitted by the expression [12]

$$|\psi_n(x)| = A(x) \exp(|x - \xi|/\lambda), \quad (9)$$

where $A(x)$ is a randomly varying function describing the fluctuations of the amplitude of the wave function $\psi_n(x)$, and λ is the localization length which can be defined as the asymptotic decay length of the envelope.

Fig. 2. Ground state wave function for $L = 100$ and (a) periodic system, (b) amorphous system with $\eta = 0.4$, (c) Thue–Morse sequence, (d) Fibonacci sequence, “cosine” sequence with (e) $\nu = 1$, “cosine” sequence with (f) $\nu = 1.1$.

We compute the localization length λ for the ground state using Eq. (9). The fitting procedure needs to fix the position of maximum amplitude, $A(\xi)$.

Our results for the Thue–Morse and Fibonacci chains as a function of size of the system are presented in Table, and the results for disordered case are presented in Fig. 3. We observe a decay of wave function as disorder is increasing. Here, we turn to the role of the cut-off parameter, x_c . It results from the relation $\lambda(\nu)$ presented in Fig. 4 that the localization length is decreased for increasing value of the cut-off parameter. We presume that the cut-off parameter introduces the

TABLE

IPR values and localization lengths for Thue–Morse and Fibonacci sequences.

	L	$\ln(L^{-1/2}P_x)$	$\ln(L^{-1/2}P_k)$	$\ln(L^{-1/2}P_{xk})$	λ
Thue–Morse	50	−5.145	−3.935	−1.835	17.60
	100	−6.214	−4.317	−2.543	35.76
	150	−6.818	−4.526	−2.940	53.35
Fibonacci	50	−5.230	−3.854	−1.628	14.19
	100	−6.409	−4.120	−2.444	36.63
	150	−6.829	−4.475	−2.666	42.18

Fig. 3. Localization length in amorphous system as a function of disorder parameter η .

Fig. 4. Localization length for “cosine” sequence.

partial ordering in the distribution of scattering centers which is independent of the size of the system. In all presented cases the localization length λ is less than the size of the system L . This allows us to classify the considered systems as the insulators.

More information on the density of probability of finding electron can be extracted from the IPR. This quantity is defined as the second moment of the electronic density and is given by the formula

$$P_x(E_n) = \int dx [|\psi_n(x)|^2]^2 \quad (10)$$

in the real space, and in the momentum space by

$$P_k(E_n) = \int dk [|\phi_n(k)|^2]^2, \quad (11)$$

where the function $\phi_n(k)$ is the Fourier transform of $\psi_n(x)$.

The IPR is inversely proportional to the volume of the part of a system which contributes effectively to eigenfunction normalization [29]. The calculations indicate that the IPR strongly depends on the realization of disorder, therefore, for the amorphous systems we consider the *typical* value of the IPR which is defined as the median of the IPR distribution function [30].

Our attention is focused on the ground state of the disordered wire which is modeled by the Hamiltonian in the form (1) with a suitable distribution function of scattering centers. We use both the position and momentum representations of particle quantum states to investigate the localization of the ground state electronic function using the IPR in these representations.

As it is shown in Figs. 5 and 6, the IPR in the real space for both kinds of systems increases with the growing strength of disorder. Although in the case of the “cosine” system it is not clear because strong fluctuations hide a possible dependence. Therefore, we carefully draw this conclusion there, however the results for $x_c > 0$ help to justify it.

Fig. 5. Inverse participation ratio in the real space (P_x) and momentum space (P_k) calculated for amorphous systems.

Fig. 6. IPR values P_x and P_k for “cosine” sequences.

Each time such dependence corresponds to the squeeze of the ground state wave function in the real space. Simultaneously, in the momentum space, the IPR decreases as the strength of disorder increases and we observe a delocalization of the wave function in this space. Additionally we investigate the influence of the cut-off parameter x_c on the IPR vs. disorder parameter ν . The results presented in Fig. 6 suggest that the cut-off parameter causes the disappearance of fluctuations for a small value of parameter ν . The values of IPR for aperiodic chains are presented in Table for different system sizes ($L = 50, 100, 150$). These results allow us to assert that the Thue–Morse and Fibonacci ones are comparable to a crystal or an amorphous system with a small value of the disorder parameter η .

We expect that the information about the squeeze of the wave function resulting from the IPR in the phase space should be richer than the one from the real and momentum spaces [31]. One of the possible phase space representations of the quantum states $|\phi_n\rangle$ is given by the Husimi function ρ_H which is defined as [24, 25]

$$\rho_H(x, k) = |\langle x_0, k_0 | \phi_n \rangle|^2, \quad (12)$$

where $\langle x_0, k_0 |$ corresponds to a state whose uncertainty is minimal around x_0 and k_0 in real and momentum spaces [32], respectively.

The implicit form of the Husimi function, when the Gaussian form [33] for the state $\langle x_0, k_0 |$ is used, is given by

$$\rho_H(x, k) = \left(\frac{1}{2\pi\sigma^2} \right)^{1/2} \left| \int dx' \exp \left(-\frac{(x-x')^2}{4\sigma^2} + ikx' \right) \psi(x') \right|^2, \quad (13)$$

where σ^2 is chosen as La/π .

Figure 7 presents the Husimi functions corresponding to the ground state wave functions for some arbitrarily chosen values of disorder. We can see that for the medium strength of disorder the Husimi function in the phase space has the most localized form (Figs. 7a and b). In the remaining cases the Husimi function is spread in the phase space. The quantitative information on the degree of localization of the Husimi function in the phase space can be given by the Wehrl entropy [34]

$$S = -\frac{1}{2\pi} \int dx dk \rho_H(x, k) \ln(\rho_H(x, k)), \quad (14)$$

which is a measure of the phase space volume occupied by the quantum state. Instead of the Wehrl entropy we consider the phase space IPR as alternative measure of localization of the quantum state. In fact, both methods give similar results. The definition of the phase space IPR is given by the formula

$$P_{xk} = \frac{1}{2\pi} \int dx dk \rho_H^2(x, k). \quad (15)$$

This quantity represents the effective volume occupied by the Husimi function in the phase space. In Figs. 8 and 9 we present the IPR in the phase space for the

Fig. 7. Husimi function obtained for 100 sites and (a–c) amorphous system, (d) Thue–Morse sequence, (e) Fibonacci sequence, (f–h) “cosine” sequence.

Fig. 8. Inverse participation ratio P_{xk} in the phase space, results for amorphous systems.

considered systems. In both cases we observe non-monotonic character of the IPR as a function of the strength of disorder η and parameter ν .

The results for amorphous system are different from the curves representing the IPRs in the real and momentum spaces, where we observe the monotonic

Fig. 9. P_{xk} for “cosine” sequences.

characteristic of these quantities. This suggests that the information about the squeeze of the ground state given by the phase space IPR cannot be treated as a simple superposition of information included in the proper spaces IPRs.

For the “cosine” systems situation becomes more complicated because we observe strong fluctuations there again. Notably if non-zero cut-off parameter x_c is considered then the IPR calculated in the phase space for small values of parameter $\nu \leq 1.15$ may be compared to the amorphous case.

The presented method of investigation of the localization in the phase space and the method based on the Wehrl entropy can be regarded as a special cases of the generalized Rényi–Wehrl entropies that are given by the formula [33, 35]

$$R_q = \frac{1}{1-q} \ln \left(\frac{1}{2\pi} \int dx dk (h\rho_H(x, k))^q \right), \quad (16)$$

where q is the Rényi index, and h is the Planck constant.

A detailed discussion of entropic measures of localization in the phase space for some aperiodic quantum systems will be presented in forthcoming work.

4. Conclusions

In this paper we have studied a localization of the electronic wave function in wires when disorder is introduced to systems with different sizes. The comparison of the localization length to the size of the system justifies to classify wires as insulators. If, however, we also account for the excited states and we change the degree of disorder or include external field, the localization length may be comparable to the size of the system. In this case we expect the crossover between the insulating and the metallic regime. We intend to study such cases (when surface contribution is significant) more in detail in forthcoming publications. The results of the present calculations show that the energy spectrum changes, with respect to the crystal case, if the disorder is introduced, then new localized states appear. For the description of the localization effect in the random disordered systems we use the typical value of the inverse participant ratio which is defined as the median of the IPR distribution function.

Disorder leads to interference of the wave function with itself such that it is no longer extended over the whole system but it is confined to a small region of the wire. The size of this region is determined by the strength of disorder. Therefore, the localization can be regarded as the quantum effect due to quantum interference. The use of the concept of Husimi function allows us to present the alternative description of the localization effect which is more appealing from the classical point of view. The phase space representation helps to see the nature of localization in the nanosystems, where the understanding of the properties of such systems also needs some theoretical interpretation.

Acknowledgment

This paper has been partly supported by the Ministry of Scientific Research and Information Technology (Poland) in the framework of the solicited grant PBZ-MIN-008/P03/2003. A part of these calculations was carried out at the Academic Computer Centre CYFRONET-KRAKÓW.

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