# ONE-DIMENSIONAL APERIODIC SYSTEMS IN PHASE SPACE*

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We consider the localisation properties of electrons in one-dimensional aperiodic systems. The phase space formalism based on the quasi-distribution functions is applied to the description of such systems. The Wehrl entropy is calculated from the Husimi function and used for reconstructing the localisation properties.

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## 1. Introduction

Electronic properties of a simple perfect crystal are determined by periodicity of the system. The Hamiltonian has the translational symmetry of the system and, therefore, we can classify the solutions of the Schrödinger equation according to the irreducible representation of the symmetry group. This irreducible representation is specified by the wave-vector $k$. The one-electron states in the system are extended, and the wavefunctions of electrons are given by the Bloch functions, $\psi_k(x)$, which are plane waves modulated by a periodic function of position $x$, [1]. The translational symmetry of the system can be broken by an external perturbation (*e.g.* magnetic field, temperature) or disorder that is almost always present in real systems. Other class of systems which do not posses the translational symmetry are aperiodic systems. We expect that the one-electron states in such structures can be localised in a finite range of the configurational space because at the first glance the aperiodic systems look like the disordered ones. It is especially interesting in the context of the metal-insulator transition in one-dimensional systems. According to standard theory of localisation [2–7],

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all one-electron states in one-dimensional system are exponentially localised for any amount of disorder. Meanwhile, numerical experiments performed with the random dimer model [8] show the existence of both extended and localised one-electron states. This unexpected result was confirmed experimentally in semiconductor superlattice a few years later [9].

The aim of this paper is to study the influence of aperiodicity on the electron localisation in quantum wires. Our alternative approach is based on the phase space concepts of non-relativistic quantum mechanics [10, 11]. In this formalism, the quantum state of the system is described by the quasi-distribution function in the phase space [12, 13].

The paper is organised as follows. In Section 2 we describe the theoretical model of quantum wire. As a basis of aperiodic potentials we use four types of aperiodic chains: Fibonacci, Thue–Morse, Rudin–Shapiro, and period-doubling sequences. In Section 3 we introduce the concept of the phase space description of quantum systems and we calculate basic quantities characterising the localisation properties of the systems. In conclusion we summarise presented results.

## 2. Model

The structural disorder is generated by the random positions of single ions in space. In this case the effective potential arises from the superposition of $N$ ionic potentials, *i.e.*

$$V(\boldsymbol{x}) = \sum_{i=1}^{N} v_i(\boldsymbol{x} - \boldsymbol{x}_i)\,, \tag{1}$$

where $v_i(\boldsymbol{x})$ is the potential of a single ion located at $\boldsymbol{x}_i$. The distribution of the ions in $n$-dimensional space may be described by a probability distribution function of positions of single ions, $P[\{\boldsymbol{x}_i\}]$, each of which is characterised by the same repulsive potential ($v_i = v$).

We apply this model to the description of finite aperiodic wires. The quantum wire may be modelled by a one-dimensional chain of length $L$ with well defined positions of short range ion potentials. Therefore, we assume that the effective potential is represented by a set of the Dirac delta functions with strength $v$ and located at the positions $x_i$, such that $x_{i+1} = x_i + a_i$, with $i = 1, 2, \ldots, N$. Note that $a_i = a$ yields the crystal structure. The positions of ions in the aperiodic wire are fully deterministic. This means that the positions of single ions are well defined by appropriate family of two-sided sequences. Here, we consider four types of sequences, namely Fibonacci, Thue–Morse, Rudin–Shapiro and period-doubling ones [14]. We generate these sequences over $\{0, 1\}$, using the following inflation rules [15, 16]

(a) Fibonacci sequence: $0 \to 01$, $1 \to 0$;
(b) Thue–Morse sequence: $0 \to 01$, $1 \to 10$;
(c) Rudin–Shapiro sequence: $00 \to 0001$, $01 \to 0010$, $10 \to 1101$, $11 \to 1110$;
(d) period-doubling sequence: $0 \to 01$, $1 \to 00$.

In our notation zeros correspond to empty sites in the simple crystal lattice, and ones correspond to delta potentials in the lattice.

The eigenfunctions of suitable aperiodic system are given by the solution of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi''(x) + v\sum_{i=1}^{N}\delta(x-x_i)\psi(x) = E\psi(x)\,, \tag{2}$$

with the boundary conditions

$$\begin{bmatrix} \psi(x_i^+) \\ \psi'(x_i^+) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 2v & 1 \end{bmatrix} \begin{bmatrix} \psi(x_i^-) \\ \psi'(x_i^-) \end{bmatrix}. \tag{3}$$

We solve Eq. (2) for the above mentioned family of aperiodic systems. In our calculation, we consider systems which consist of 100 elements. For each system, we numerically calculate eigenfunctions $\psi_n(x)$ with energies $E_n$ using simple shooting method. The numerical method is not appropriate in case of transport properties analysis but here it may be used to investigate localisation properties of the eigenfunctions.

Localised states may be characterised by localisation length $\lambda_n$ defined by the exponential decay of the eigenfunction

$$\psi_n(x) = A_n(x)e^{-|x-x_0|/\lambda_n}\,, \tag{4}$$

where $A_n(x)$ is the amplitude of wavefunction, and $x_0$ is the centre of the localisation.

In fact, the localisation length is not a well defined criterion of localisation for the *finite* aperiodic or disordered systems as it was pointed by Izrailev *et al.* [17]. In this case the localisation properties may be characterised by the inverse participation ratio (IPR) which is defined as the second moment of the eigenfunction local intensity $|\psi_n(x)|^2$ and is given by [18, 19]

$$P_x^{(n)}(E_n) = \int dx\,|\psi_n(x)|^4\,. \tag{5}$$

IPR is proportional to the length of the system part where the eigenfunction is non-zero. For localised states $P_x^{(n)}(E_n) \propto L^0$, and for the extended states, we have $P_x^{(n)}(E_n) \propto L^{-1}$.

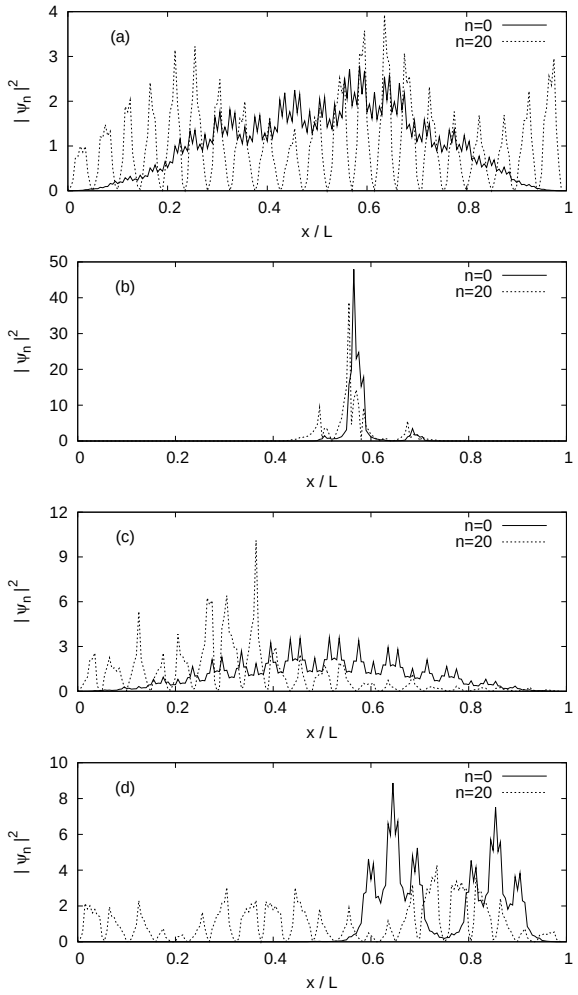


Fig. 1. Eigenfunction local intensity in case of the ground state $n = 0$ and $n = 20$ for (a) Fibonacci, (b) Rudin–Shapiro, (c) Thue–Morse and (d) period-doubling sequences.

Selected eigenfunction local intensities of the discussed aperiodic systems are shown in Fig. 1. Fig. 1(a) shows the ground state ($n = 0$) and one of the excited states ($n = 20$) for the Fibonacci sequence with IPR values $P_x^{(0)}(E_0) = 0.015$ and $P_x^{(20)}(E_{20}) = 0.017$, respectively. In Fig. 1(b) we show the results for Rudin–Shapiro sequence. In this case the IPR values are $P_x^{(0)}(E_0) = 0.235$ and $P_x^{(20)}(E_{20}) = 0.135$. Fig. 1(c) shows the same states for the Thue–Morse sequence with $P_x^{(0)}(E_0) = 0.017$ and $P_x^{(20)}(E_{20}) = 0.032$. Fig. 1(d) shows the same states for the period-doubling sequence with

$P_x^{(0)}(E_0) = 0.041$ and $P_x^{(20)}(E_{20}) = 0.019$. A similar analysis of the IPR parameter can be performed in the momentum space but it is not important for the present investigation and will be omitted.

The other the commonly used quantity in this case is the entropic localisation length, defined through the Shannon entropy of eigenstates [17]. We use this concept in the next section where we consider the phase space structure of the eigenfunctions of the aperiodic systems.

## 3. Phase space description of quantum system

The usage of the phase space formulation of quantum mechanics allows us to include simultaneously position and momentum representations in the description of quantum state. It is very useful for visualising correlated position and momentum properties of quantum state. This formulation of quantum mechanics is based on Wigner's quasi-distribution function [20] and Weyl's correspondence between an arbitrary physical quantity in classical mechanics and quantum-mechanical operators in the Hilbert space [21]. For a quantum system in a pure state, Wigner function carries the same information as the wavefunction. In general, the Wigner function

$$\rho_n^{\mathrm{W}}(x,k) = \int dx' \, \langle x - \tfrac{1}{2}\, x'|\psi_n\rangle\langle\psi_n|x + \tfrac{1}{2}\, x'\rangle e^{ikx'} \,, \tag{6}$$

is normalised and real with its marginal distributions being the probability densities. However, the Wigner function can take negative values in some subregions of the phase space and, therefore, cannot be identified with a probability distribution.

In the phase space, there exists an infinite family of quasi-distribution functions which can be defined by taking different quantisation rules. A special place in the formulation belongs to the Husimi function representing a general class of non-negative quasi-distribution functions. The Husimi function for the individual quantum eigenstates $|\psi_n\rangle$ is defined as a Gaussian smoothing of the Wigner function and is given by the formula [12, 13]

$$\rho_n^{\mathrm{H}}(x,k) = |\langle x,k|\psi_n\rangle|^2 \,, \tag{7}$$

where $|x,k\rangle$ is the minimal uncertainty state centred around the position $x$ and momentum $k$ in the phase space.

The smoothing is realised over a domain with size not smaller than $\hbar/2$. This process assures that the resulting function is positive defined [22]. In Fig. 2, we show the Husimi function (7) of the ground states and the 20-th excited states for the all aperiodic systems that are considered here. In all cases, the Husimi function is located in the regular region of the phase

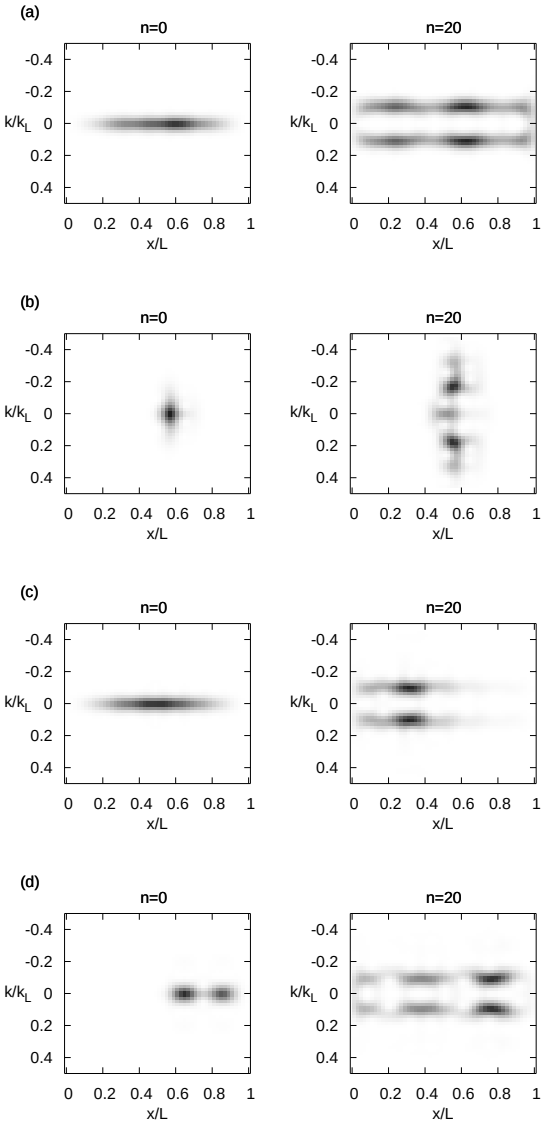


Fig. 2. Husimi function for $n = 0$, $n = 20$ and for (a) Fibonacci, (b) Rudin–Shapiro, (c) Thue–Morse and (d) period-doubling sequences (darker shade indicates larger values).

space. For the Fibonacci (Fig. 2(a)), Thue–Morse (Fig. 2(c)) chains, the Husimi functions $\rho_0^{\mathrm{H}}(x,k)$ and $\rho_{20}^{\mathrm{H}}(x,k)$ are extended in the real space (line or double line is parallel to the position axis). In fact, these quantum states are very weakly localised in phase space. The most intriguing properties

are displayed by the Husimi functions of the states in the Rudin–Shapiro chain (Fig. 2(b)). The ground state is very well localised in both variables, and the 20-th excited state is slightly extended in momentum space but it remains localised in the real space. Similar properties of Husimi function are observed in the limit of very strong disorder where the Husimi function is given by a line parallel to the momentum axis [23]. The Husimi functions for the period-doubling chain (Fig. 2(d)) exhibit intermediate properties, namely the ground state is localised in finite region of real space and the excited states are localised along the position axis.

Using the definition of the Husimi function we can introduce the phase space IPR as a measure of effective volume occupied by the Husimi function in the phase space, *e.g.* [24, 25]. However, we consider Wehrl entropy instead of the phase space IPR as an alternative measure of localisation of the quantum state. The Wehrl entropy of individual eigenstates $|\psi_n\rangle$ in the phase space is defined as follows [26, 27]

$$S_n^{\mathrm{W}} = -\frac{1}{2\pi}\int dx\, dk\, \rho_n^{\mathrm{H}}(x,k)\ln\rho_n^{\mathrm{H}}(x,k)\,. \tag{8}$$

This quantity is small for eigenstates that are localised in the phase space and large for the extended eigenstates.

Formally we can relate the Wehrl entropy (8) to the localisation length $\lambda_n^{\mathrm{W}}$ in the phase space by the formula

$$\lambda_n^{\mathrm{W}} = L\exp\left[S_n^{\mathrm{W}} - S^{\mathrm{ref}}\right], \tag{9}$$

where quantity $S^{\mathrm{ref}} = \ln(2L) - 1$ is the normalisation factor chosen according to Ref. [17, 28]. In this definition the localisation length is normalised to the length of the system.

In Fig. 3 we present the results of our calculations. We plot the localisation length as a function of the quantum number $n$ for the considered aperiodic systems. In general, the localisation length is increasing with the quantum number $n$. It results from the fact that the Husimi function for individual states occupy a bigger region of the phase space. For shorter ($N = 50$) and longer sequences ($N = 150$) the same relations are observed and the values of $\lambda^{\mathrm{W}}$ do not reveal any significant dependence on the system size which is a consequence of the eigenfunctions and the Husimi functions having very similar characteristics regardless of the above mentioned values of $N$.

Points in Fig. 3 showing local minima of the localisation length (*e.g.* for $n = 60$, Fig. 3(a)) correspond to the states, which energies are placed near the edges of energy bands. That fact was confirmed by independent calculations of the density of states function [29].

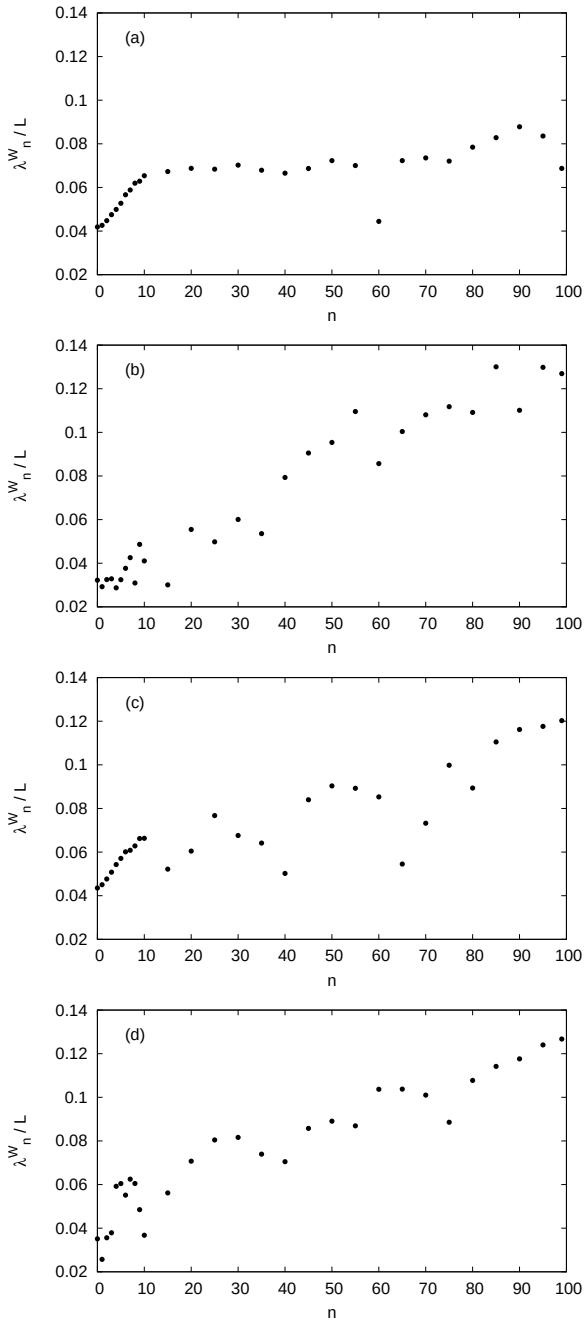


Fig. 3. Localisation length in the phase space: $n = 0, 20$ for (a) Fibonacci, (b) Rudin–Shapiro, (c) Thue–Morse and (d) period-doubling sequences.

## 4. Conclusions

In summary, we have studied the effect of potential aperiodicity on the localisation properties for some one-dimensional isolated systems, considering four types of potential sequences: Fibonacci, Thue–Morse, Rudin–Shapiro and "period-doubling". In the first part of our study, we have obtained the eigenfunctions and energies of Eq. (2). Localisation properties of the eigenfunctions are characterised by the inverse participation ratio in the real space. In the second part, we focus our attention on the phase space description of the quantum states. The individual states are represented by the Husimi function. Using the definition of the Husimi function we calculate the entropic localisation length based on the Wehrl entropy for all aperiodic systems that are considered in this study.

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