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On the localization of electrons in disordered molecular wires

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The aim of this report is to investigate electronic properties of a chain of atoms when its translational symmetry is broken by a topological disorder. The study uses the inverse participant ratio to obtain information on the localization of electrons in phase space.

Key words: *disorder; localization; inverse participant ratio; Husimi function*

1. Introduction

It is well established that electronic processes in low-dimensional systems, such as molecular wires, are determined by the quantum phenomena. One of the most intriguing problems of modern physics is the localization of conduction electrons in low-dimensional topologically disordered systems in the presence of various perturbations, such as magnetic field, temperature, spin-orbit scattering or electron–electron interaction. Localization in low-dimensional disordered systems has been subject to numerous theoretical papers, and we know that all eigenstates in such systems are localized by an arbitrary weak disorder [1–3] for uncorrelated random potentials [4]. On the other hand, localized states play a key role in the optical and transport properties of disordered systems.

In this paper, we use a method based on the phase space representation of quantum mechanics [5–8] to investigate localization. We applied this method to non-interacting electrons in a molecular wire using a one-electron liquid Kronig–Penney model [9, 10] and the Husimi function [11, 12]. The inverse participant ratio in phase space is calculated as a function of the disorder parameter for various wire lengths.

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2. Theoretical model

A one-dimensional wire with topological disorder is described by the liquid Kronig–Penney model [9, 10]. We consider the time-independent Schrödinger equation for a system of non-interacting electrons with effective mass m, moving in a random potential $V(x)$, namely

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

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

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

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

where $F_0 = mV_0b/\hbar^2$, and the parameter b is defined as the width of the square interatomic barriers, with V_0 being their height.

In the case of a system originating from a simple regular lattice (one-dimensional crystal), the locations x_i of the scattering centres in the chain are determined by the formula

$$x_i=(i+\eta r_i)a, \quad i=1, 2, ..., N \tag{3}$$

Equation (3) includes a random number r_i from the range (–1,1); a is the average distance between neighbouring sites, and η is a measure of the strength of disorder. This choice assures a fully periodic situation for η = 0 and an internal disorder proportional to η when we pass from a perfect lattice to a disordered system.

The limit of $V_0 \to 0$ and $b \to 0$ allows us to define a constant strength of the scattering potential, i.e. V_0b = const. Even in the case of a disordered chain we can construct a wave function for electrons that satisfies equation (1) by using the analytical expression for the wave function $\chi_i(x)$ inside the i-th square well

$$\chi_i(x)=C_i\cos(kx+\varphi_i) \tag{4}$$

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

Joining the solutions (4) found at the consecutive ranges gives the wave function $\psi(x)$ which must satisfy the following conditions:

$$\psi(x_i^+)=\psi(x_i^-) \tag{5}$$

$$\frac{d}{dx}\psi(x)\bigg|_{x_i^+}-\frac{d}{dx}\psi(x)\bigg|_{x_i^-}=2F_0\psi(x_i) \tag{6}$$

where the finite discontinuity at the step results from integrating Eq. (1).

Knowledge of the exact form of $\psi(x)$ allows us to construct the Husimi function as follows

$$\rho_H(x,k) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/2} \left| \int dx' \exp\left[-\frac{(x-x')^2}{4\sigma^2} + ikx' \right] \psi(x') \right|^2 \tag{7}$$

where σ^2 is chosen as La/π^2.

3. Results and discussion

In disordered systems, the phase and amplitude of the electronic wave function is changed by spatial fluctuations of potentials. In consequence, the envelope of the wave function decays exponentially from a localization centre ξ. This means that the electronic density $|\psi_n(x)|^2$ will not spread over the entire system, but will remain localized around ξ. This result can be described by the expression [15]

$$\psi_n(x) \propto A(x) \exp\left(-\frac{|x-\xi|}{\ell} \right) \tag{8}$$

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

For a simple regular lattice, the electronic states can be extended over the whole system. As the disorder becomes larger, the localized states get more compressed. More information on the compression of the wave function can be extracted from the inverse participation ratio. This quantity is defined as the second moment of the electronic density and is given in real space by the formula

$$P_x(E_n) = \int dx |\psi_n(x)|^4 \tag{9}$$

and in momentum space by

$$P_k(E_n) = \int dk |\phi_n(k)|^4 \tag{10}$$

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

The inverse participant ratio is inversely proportional to the volume of the part of the system that contributes effectively to eigenfunction normalization [16]. Our calculations indicate that this quantity has a monotonic character and strongly depends on the realization of disorder. In real space, the inverse participant number increases with increasing

disorder strength. Simultaneously, in momentum space, the inverse participant ratio decreases as the strength of disorder increases and we observe a delocalisation of the wave function [17]. One of the possible phase space representations of the quantum states $|\phi_n\rangle$ is given by the Husimi function ρ_H, defined as in [11, 12]

$$\rho_H(x,k) = \left|\langle x_0, k_0 | \phi_n \rangle\right|^2 \tag{11}$$

where $\langle x_0, k_0|$ corresponds to a state whose uncertainty is minimal around x_0 and k_0 in real and momentum space [7], respectively. The implicit form of the Husimi function when the Gaussian form [8] for $\langle x_0, k_0|$ is used is given by formula (7).

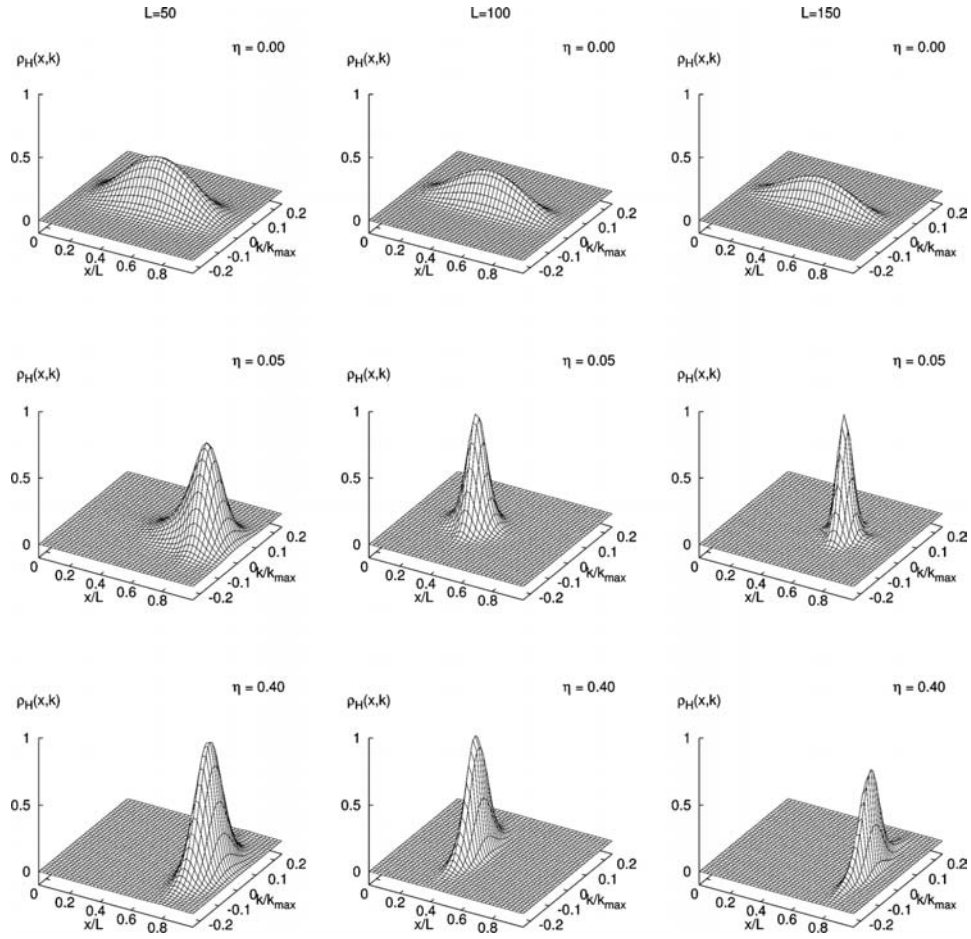

Fig. 1. The Husimi function for a disorder parameter η = 0, 0.05, 0.4 and wire length L = 50, 100, 150; $k_{max} = 2\pi/a$

Figure 1 presents the Husimi functions corresponding to the ground state wave functions for some arbitrarily chosen values of disorder and for different numbers of

atoms: N = 50, 100, and 150. In all cases, the average distance between neighbouring atoms is equal and taken as the unit length for molecular wires. Therefore, the results presented in Fig. 1 correspond to the lengths L = 50, 100 and 150.

We can see that for a medium strength of disorder the Husimi function in phase space has the most localized form. Quantitative information on the degree of localization of the Husimi function in phase space can be extracted from the phase space inverse participant number, which is given by the formula

$$P_{xk} = \frac{1}{2\pi} \int dx dk \rho_H^2 (x,k) \tag{12}$$

This quantity represents the effective volume occupied by the Husimi function in phase space, in analogy with the inverse participant ratio in real or momentum space.

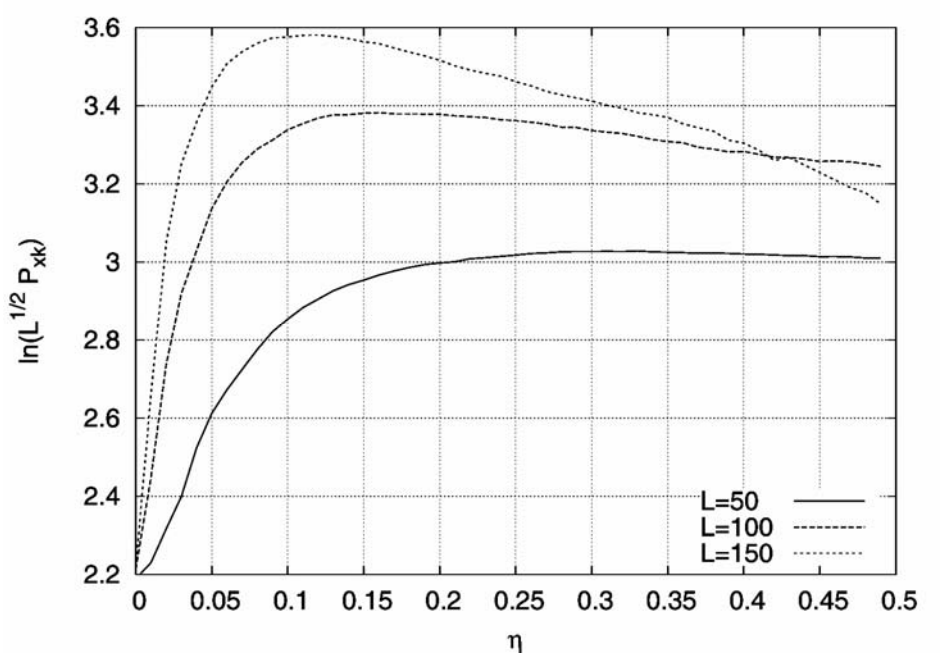

Fig. 2. The inverse participant ratio P_{xk} in phase space scaled with the chain length for L = 50, 100, and 150

The dependence of the inverse participant ratio in phase space on the disorder parameter, as a function of length L, is presented in Fig. 2. For the shortest wires (L = 50), we observe a plateau for moderate and strong disorder. In the remaining cases, a broad maximum is formed in the limit of weak disorder. The electronic wave function for such systems is non-vanishing only for a finite number of atoms. All these results suggest that we should get a peak corresponding to the most squeezed quantum

state in the limit of very long wires. We expect that this hypothesis can be confirmed by numerical calculations based on high performance computing.

4. Numerical procedure

Each wave function of the ground state $\psi_0(x)$ is calculated from the Schrödinger equation for the ground state energy, which has to be determined using the shooting method and assuming the boundary conditions

$$\psi_0\left(x=0\right)=\psi_0\left(x=L\right)=0 \tag{13}$$

The relations between the median values of the inverse participant ratio and η parameters presented in Fig. 2 have been calculated for sets of 200 chains by repeating this procedure for each chain in our input data. From the numerical point of view, we find the P_{xk} parameters and Husimi functions this way mainly by performing simple one- and two-dimensional integrations.

All results included in this paper have been computed for chains consisting of N = 50, 100, or 150 sites, with an average inter-atomic distance of a = 1 in all wires.

5. Conclusion

In conclusion, we have used a one-dimensional version of the liquid Kronig –Penney model to investigate the process of electron localization in molecular wires when the strength of disorder η and wire length L are increased. We calculated the inverse participant ratio in phase space as one of the possible measures of particle localization in disordered media. Additionally, we demonstrate the influence of disorder on the ground state of the system, which is represented by the Husimi function in phase space.

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