

Dynamical localisation of conduction electrons in one-dimensional disordered systems

View from the phase-space perspective

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Abstract The phase-space approach based on the Wigner distribution function is applied to the description of dynamics of conduction electrons in finite one-dimensional systems with randomly distributed scattering centres. It is shown that the coherent multiple scattering of the carriers in the disordered environment leads to the slowdown of its dynamics due to the weak localisation. This quantum phenomenon can be treated as a source of the subdiffusion of the quantum particles.

Keywords Wigner distribution function · Disordered systems · Localisation

1 Introduction

Many years of studies on transport properties of disordered systems provided the understanding of the mechanisms leading to the slowdown of the conduction electrons dynamics in the diffusive regime of the solid systems. The coherent multiple scattering processes of the carriers on the set of randomly distributed scattering centres lead to the momentum correlations, so that the electronic transport reveals the non-Markovian properties, i.e., successive scatterings of carriers are not independent [1]. One of the main consequences of these correlations is the phase coherence of the carriers. This coherence enhances the classical return probability and leads to the correction to the diffusion process of conduction electrons [2–5]. The processes described by this correction are

responsible for a deviation from the Einstein–Smoluchowski diffusion law. The phenomenon behind the correction is called the weak localisation and it is perceived as a precursor of the Anderson or strong localisation. The latter takes place in the limit of strong disorder when the coherent multiple scattering processes can block the electronic transport in the disordered environment. It is worth noting that both of these phenomena, i.e., weak and strong localisation may also be present in complex media other than the electronic systems [6].

The slowdown of the dynamics of carriers in the weakly disordered environment can be regarded as a manifestation of the process of anomalous diffusion of particles, which can be described by the relation for the mean squared deviation of the displacement,

$$\langle [x(t) - x(t_0)]^2 \rangle = 2D(t)t, \quad (1)$$

where $D(t)$ is the time dependent diffusion coefficient, $x(t)$ is the position of particle at time t , and $x(t_0)$ is the initial location. The relation (1) is often replaced by a more transparent form which enables us to classify the anomalous diffusion processes according to the anomalous diffusion parameter α that is specified by the relation [7]

$$\langle [x(t) - x(t_0)]^2 \rangle = 2D_\alpha t^\alpha, \quad (2)$$

where D_α is the anomalous diffusion coefficient measured in the units of $\text{m}^2\text{s}^{-\alpha}$. In agreement with the relation (2), the anomalous diffusion processes can be classified as follows: $\alpha = 0$ corresponds to the case of the strong localisation, $0 < \alpha < 1$ corresponds to the subdiffusion processes (the weak localisation), $\alpha = 1$ corresponds to the classical diffusion processes, $1 < \alpha < 2$ corresponds to superdiffusion processes, and $\alpha = 2$ corresponds to the ballistic transport.

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The power type dependence of the mean squared deviation of the displacement on time is one of the possible laws describing the anomalous diffusion processes [7]. Therefore we conclude that the relation given by Eq. (1) is more general and it can be extrapolated to the regime of electronic transport where the quantum effects play a vital role.

The coherent multiple scattering processes lead to the subdiffusion of the conduction electrons in the weakly disordered systems. Inclusion of such processes to the description of the transport processes requires some additional quantum considerations because the origin of the existing momentum correlations is a consequence of the quantum interference. One of the possible ways to investigate the influence of the quantum effects on the dynamics of carriers in the framework of the kinetic theory is the phase-space approach proposed by Wigner and further developed by Moyal, Groenewold and others [8,9]. Their approach makes the quantum mechanics resemble the statistical mechanics because of the usage of the quantum version of the distribution functions.

In the present contribution we examine the subdiffusion process of the electronic quantum state represented by a Gaussian wave packet. We discuss its dynamics in the static random potential of the one-dimensional finite system using the phase-space analysis based on the Wigner function and on the equation of motion in the Moyal form [10].

The paper is organised as follows. In Sect. 2, we present some basic theoretical facts about the phase-space formulation of the quantum dynamics, and a model of the disordered system which is used in our calculations. Section 3 contains the results of calculations and their discussion, and the conclusions are contained in Sect. 4.

2 Phase-space representation of quantum state and its dynamics

The description of the conduction electron’s dynamics in terms of the classical distribution function over the phase space, which satisfies the Liouville or Boltzmann equations is insufficient for the quantum transport phenomena because the interference effects are ignored [11]. Nevertheless, the concept of the phase space can be used to describe the dynamics of the quantum states provided the Heisenberg uncertainty principle for the momentum and position operators is taken into account. The consequences of the principle are twofold. Firstly, the distribution function cannot be localised in an area of the phase space smaller than the reduced Planck’s constant \hbar . Secondly, the observables form the non-commutative algebra [12]. The inclusion of both the aspects to the theoretical description of the electron’s quantum states in the phase space allows us to introduce the Wigner distribution function (WDF), which is defined by the Wigner–Weyl transform of the one-particle density operator [13]

$$f(x, p, t) = \int dx' \rho \left(x - \frac{x'}{2}, x + \frac{x'}{2}, t \right) e^{(i/\hbar)px'}, \quad (3)$$

where $\rho(x, x')$ is the density matrix in the coordinate representation. The WDF is a real and normalised function of the spatial and momentum coordinates. Its marginal distributions in the coordinate space,

$$n(x, t) = \int dp f(x, p, t), \quad (4)$$

and in the momentum space,

$$n(p, t) = \int dx f(x, p, t), \quad (5)$$

represent the time-dependent probability densities in terms of position and momentum, respectively.

In contrast to the classical distribution functions the WDF can take negative values in some regions of the phase-space [14]. The negativity of the WDF is the reason for the non-classical character of this distribution function [15]. This property of the WDF is a consequence of the Wigner–Weyl transform which “forces” the off-diagonal elements of the density matrix to the resulting distribution function. Therefore, the WDF contains the mutually dependent quantum correlations between the momentum and position states of the conduction electrons.

The equation of motion for the WDF can be written in the Moyal form as follows [10]

$$\frac{\partial f(x, p, t)}{\partial t} + \frac{p}{m} \frac{\partial f(x, p, t)}{\partial x} = \{U_W(x), f(x, p, t)\}_\star, \quad (6)$$

where m is the effective mass of the conduction electron, $U_W(x)$ is the Weyl symbol of the potential energy $U(x)$, and $\{U_W(x), f(x, p, t)\}_\star$ represents the Moyal bracket which is defined by the formula

$$\{U_W(x), f(x, p, t)\}_\star = \frac{2}{\hbar} U(x) \sin \left[\frac{\hbar}{2} \left(\overrightarrow{\frac{\partial}{\partial p}} \overleftarrow{\frac{\partial}{\partial x}} - \overleftarrow{\frac{\partial}{\partial x}} \overrightarrow{\frac{\partial}{\partial p}} \right) \right] \times f(x, p, t). \quad (7)$$

The arrows indicate in which direction the derivatives act. The Moyal form of the transport equation is equivalent to the kinetic form of the transport equation [16, 17],

$$\begin{aligned} \frac{\partial f(x, p, t)}{\partial t} + \frac{p}{m} \frac{\partial f(x, p, t)}{\partial x} \\ = \frac{1}{2\pi\hbar} \int dp' V(x, p - p') f(x, p', t), \end{aligned} \quad (8)$$

but the integral kernel (the Wigner potential) represents a non-local potential and its form is given by the formula

$$V(x, p) = \frac{i}{\hbar} \int dx' e^{(i/\hbar)px'} \times \left\{ U\left(x + \frac{1}{2}x'\right) - U\left(x - \frac{1}{2}x'\right) \right\}. \quad (9)$$

Within the presented model, the potential energy $U(x)$ of the conduction electron in the one-dimensional disordered system is represented by the superposition of the non-overlapping short range potentials $u_n(x)$. Each of such scattering centres is described by the power-exponential function, and thus the potential energy takes on the form

$$U(x) = \sum_n u_n(x) = U_0 \sum_n \exp\left[-\left(\frac{x - X_n}{w}\right)^s\right]. \quad (10)$$

The positions of the scattering centres along the system are generated according to the formula [18]

$$X_n = \left(n + \frac{1}{2}\right)a + r_n, \quad n = 0, \pm 1, \pm 2, \dots, \quad (11)$$

where $a = 85$ nm is the period of a reference periodic system, and each r_n is a random number taken independently with uniform probability from the range $[-40, 40]$ nm. Each of the single scatterers is characterised by the same repulsive strength $U_0 = 11.4$ eV, and its shape is described by the parameters $w = 3.2$ nm and $s = 2$.

One of the advantages of using the WDF is a possibility to use a straightforward method of calculating the expectation values of the dynamical variables. Almost all required expectation values of those variables can be calculated according to the formula [19]

$$\langle A(t) \rangle = \int dx dp A_W(x, p) f(x, p, t). \quad (12)$$

where $A_W(x, p)$ is a real scalar function obtained by the Weyl transform of the hermitian operator which represents dynamical variable.

3 Results and discussion

We have determined the propagation of the WDF through the disordered environment by means of the effective numerical algorithm [20] based on the split-operator approach which was adopted to the Moyal form of the transport equation for the WDF (6). Since this approach is based on the Fast Fourier Transform, it allows to perform simulations in much larger systems and for considerably longer time scales than in the

case of traditional methods based on direct discretisation of the Wigner equation.

For the current calculations, the initial WDF $f(x, p, 0)$ corresponds to the Gaussian wave packet centred in the phase space around the point (x_0, p_0) :

$$f(x, p, 0) = \frac{1}{\pi \hbar} \exp\left\{-\frac{2\delta_x^2(p - p_0)^2}{\hbar^2} - \frac{(x - x_0)^2}{2\delta_x^2}\right\}, \quad (13)$$

where $\delta_x = 0.3[(2\pi\hbar^2)/(mk_B T)]^{1/2} \approx 10$ nm is the initial half-width of the wave packet at $T = 77$ K [21]. For the calculations the following values are also assumed: $x_0 = 0$, $p_0 = 0.15 \hbar \text{ nm}^{-1}$, and the effective mass of carriers $m = 0.067m_0$, where m_0 is the free electron rest mass. All parameters for the computer simulations are taken as typical for the conduction electrons in semiconductor GaAs nanostructures. The phase-space calculations are performed on the computational grid with $N_x = 16384$ mesh points for the x -coordinate, and $N_p = 1024$ mesh points for the x -component of momentum. The averaging procedure is based on 20 realisations of the disordered system.

Because δ_x is less than the minimal distance between any two scattering centres, it entitles us to conclude that we consider the coherent electronic transport in the diffusive regime according to the Ioffe-Regel criterion [1], since the distance between neighbouring scattering centres can be treated as the mean free path for the one-dimensional systems. Therefore we expect to observe a hallmark of the weak localisation effect in the finite disordered samples.

The snapshots of the WDF in the initial ($t = 0$), final ($t = 240$ ps) and two intermediate time instants of the simulation are presented in Fig. 1. Highly non-classical flow of the WDF is clearly visible when negative values of the WDF emerge for $t > 0$ [cf. Fig. 1b,c,d], as a result of the quantum interference phenomena [15]. Figure 2 shows the marginal distributions of the WDF in coordinate and momentum spaces, corresponding to the snapshots presented in the previous figure. The marginal distributions of the WDF in the coordinate space shows that at the end of the simulation, and also at all intermediate steps, the probability density for the conduction electron has a maximum at the initial position $x_0 = 0$. On the other hand, the marginal distributions of the WDF in the momentum space show two maxima of the distribution of momentum placed around $\pm p_0$ (where p_0 is the initial value of the momentum). It seems to be in agreement with the general theory of weak localisation because the multiple scattering processes due to the constructive quantum interference exhibit a narrow backscattered peak [5].

Subsequently, we determine the momentum autocorrelation function to investigate the presence of the momentum correlations for the conduction electrons in the disordered environment. For this purpose, we calculate

Fig. 1 Wigner distribution function $f(x, p)$ for one particular realisation of the disordered potential, at different time instants **a** $t = 0$, **b** $t = 2$ ps, **c** $t = 7$ ps, and **d** $t = 240$ ps

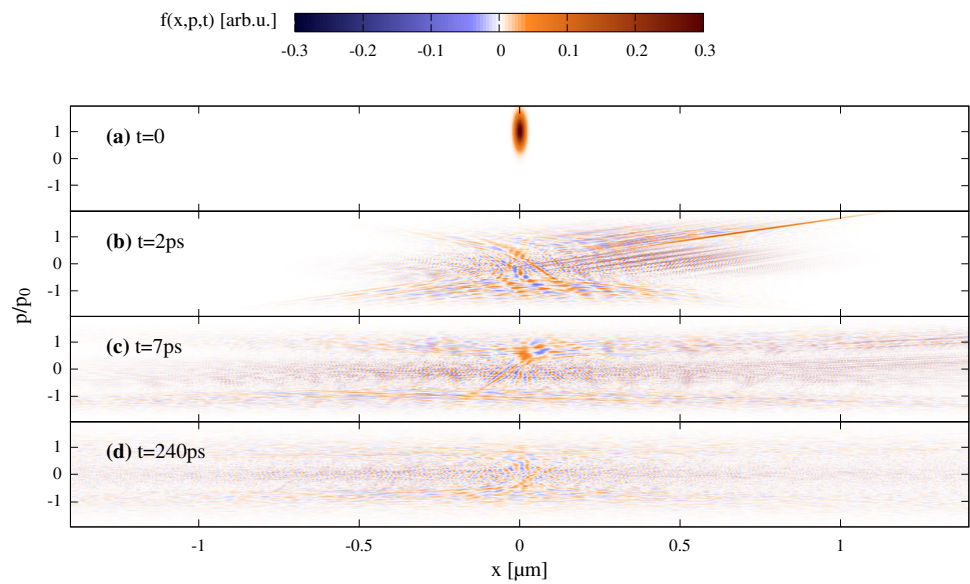
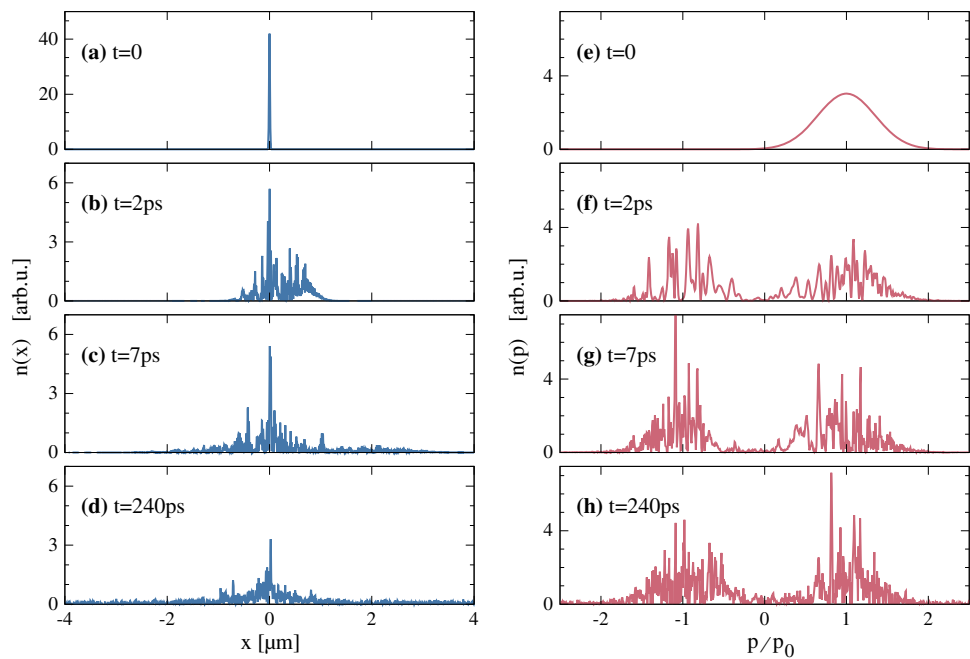


Fig. 2 Marginal distributions of the WDF in **a–d** coordinate and **e–h** momentum space, at time instants corresponding to the results presented in Fig. 1



$$C_p(\Delta t) = \overline{\langle p(t) \rangle \langle p(t + \Delta t) \rangle} \tag{14}$$

where $\langle p(t) \rangle$ is the expectation value of the momentum calculated according to the formula (12), and the bar symbol denotes the time-average. The results are presented in Fig. 3. The decay time of the momentum correlations is $\Delta t \approx 9$ ps and it is nearly three times greater than the scattering time $\tau = \langle \Delta X \rangle / v_0 \approx 3$ ps, where $\langle \Delta X \rangle$ is the mean distance between scattering centres, and v_0 is the velocity of the carriers. It implies that the successive collisions with the scatterers cannot be perceived as the independent events. Hence we can conclude that in the considered one-dimensional disordered

systems the momentum coherence length L_p is greater than the mean free path $\ell = \langle \Delta X \rangle$. This observation allows us to establish the fundamental length-scale hierarchy for the considered system as follows: $\delta_x < \ell < L_p < L$. In these inequalities we can recognise the condition for the coherent propagation of conduction electrons in the disordered environment [1]. Moreover, the value of the dimensionless transport parameter $k_0 \ell$ is approximately equal to 13, and according to the Ioffe-Regel criterion ($k_0 \ell \gg 1$) it determines the diffusion regime of the electronic transport. The combination of these issues leads to the conclusion that the electronic transport in the diffusion regime contains the coherent part

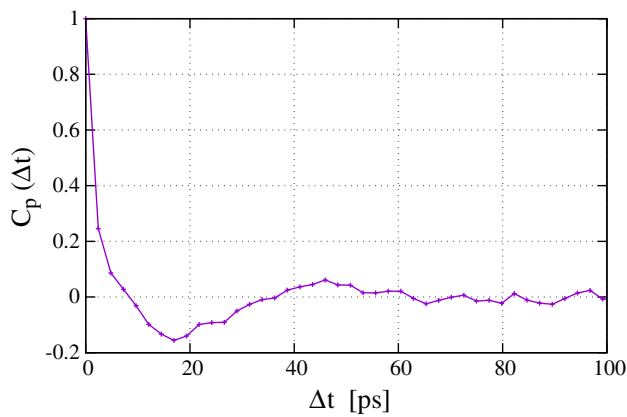


Fig. 3 Normalised autocorrelation function of the momentum expectation value

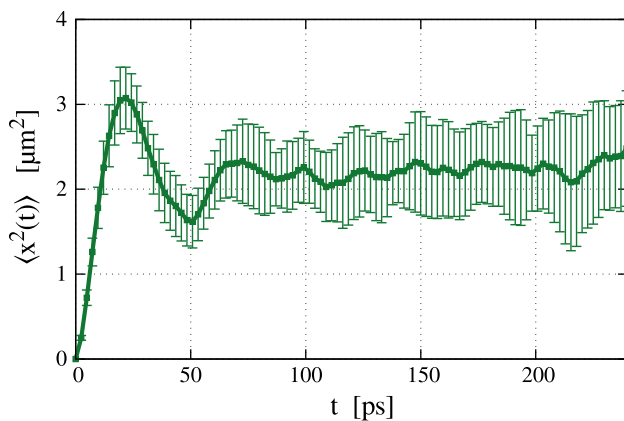


Fig. 4 Expectation value of the mean squared displacement as a function of time, averaged over 20 realisations of the disordered potential. Error bars correspond to the sample standard deviation

responsible for the weak localisation which causes the slowdown of electron's dynamics. Additionally, it can be seen in Fig. 3 that the momentum autocorrelation function displays slowly varying fluctuations that persist in the long-time tail which further enhances our conclusions about the existence of the momentum correlations because it causes a further increase of the momentum coherence length.

Finally, we performed calculations of the mean squared displacement as a function of time using the formula

$$\langle x^2(t) \rangle = \int dx dp x^2 f(x, p, t). \quad (15)$$

The results of the calculations presented in Fig. 4 show that the mean squared displacement fluctuates around the value $2.2 \mu\text{m}^2$, which reveals confinement of the electron density in some finite region of the disordered system. Moreover, the presented calculations suggest a possibility of disappearance of the diffusion coefficient in the limit of $T \rightarrow \infty$, as it was noticed by Anderson [22].

4 Conclusions

In the present paper, we have applied the quantum transport equation in the Moyal form for the Wigner distribution function in the phase space to investigate the dynamics of the conduction electrons in the finite one-dimensional system with the structural disorder. We have shown that the electronic transport in such systems can be seen as the subdiffusion process because of the multiple scattering processes which are coherent due to the correlation of the momentum. It leads to the weak localisation of conduction electrons, and consequently to the slowdown of carriers dynamics in the diffusive regime of the disordered environment which is determined by the fundamental length-scale hierarchy. We have supported this conclusions by the calculation of the momentum autocorrelation function and we have found that the mean squared displacement as a function of time fluctuates around the constant value if longer times of time simulation are considered, which suggests the strong localisation effect.

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