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# Phase-Space Approach to the Position-Momentum Correlations of the Conduction Electron States in a Double-Barrier Resonant Nanosystem

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The phase-space formulation of quantum mechanics based on the Wigner distribution function is applied to investigate the influence of the scattering processes on the electronic position-momentum correlations in the resonant-tunnelling nanosystem.

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## 1. Introduction

The phase-space formulation of the electron dynamics in the condensed matter is well established kinetic method describing transport phenomena in the systems [1]. Originally this method was based on the classical equations of statistical physics, and their applications depend on an actual physical situation. However, none of these equations is suitable for a description of the transport properties of nanoscale nanodevices in which the quantum phenomena play primary role. In some sense, the nanosystems can be regarded as a training ground for an observation these phenomena and testing a variety of concepts associated with them. To meet these expectations, the quantum generalisation of the kinetic method can be based on the density operator and its equation of motion in the mixed position-momentum representation proposed by Weyl and Wigner [2]. In this representation, the phase space acquires new properties which lead to a loss of the commutative property, and the dynamical variables defined over the space form the non-commutative algebra. This observation suggests that the position and momentum are mutually dependent variables.

In this report we present results of our studies concerning the position-momentum correlations of the conduction electrons in a simple resonant-tunelling nanosystem. We investigate the influence of the scattering processes which destroys the phase coherence of the tunelling electrons through the double-barrier nanostructure on the considered correlations between these two dynamical variables. For this purpose, we solve the quantum kinetic equation for the Wigner distribution function (WDF) within the relaxation time approximation and determine the symmetrical correlation function of the first order as a function of the relaxation time for different points at the current–voltage characteristics.

## 2. Theory

The Weyl transform of the electronic density operator $\rho(x,x')$ defines the Wigner function [2]:

$$f(x,p)=\frac{1}{2\pi\hbar}\int \mathrm{d}x'\rho\left(x-\frac{x'}{2},\ x+\frac{x'}{2}\right)\mathrm{e}^{(\mathrm{i}/\hbar)px'},\quad(1)$$

which is commonly called the quasi-distribution function. In contrast to the classical distribution functions, this function can take negative values in some regions of the phase-space. We emphasize that the coarse graining procedure of the WDF over cells $\Delta x\Delta p \gg 2\pi\hbar$ in the phase-space diminishes the negative values and the classical distribution function $f_{\mathrm{cl}}(x,p)$ is recovered [3]:

$$\int_{\Delta x\Delta p}\mathrm{d}x\,\mathrm{d}p\,f(x,p)=\int_{\Delta x\Delta p}\mathrm{d}x\,\mathrm{d}p\,f_{\mathrm{cl}}(x,p)$$
$$+O\left(\frac{2\pi\hbar}{\Delta x\Delta p}\right)^2.\quad(2)$$

From the mathematical point of view, the negative values of the WDF can be regarded as a consequence of the Weyl transform which “forces” the off-diagonal elements of the density matrix to the resulting distribution function [4]. On the other hand, this property of the WDF can be also explained in terms of the quantum interference between correlated pieces of the WDF which occupy different regions of the phase space [5]. Hence, we can conclude that the WDF comprises the mutually dependent quantum correlations between the momentum and position states of the electrons. In spite of the fact that the WDF can be negative, the expectation value of any dynamical variable can be calculated in the same manner as the average value in the classical statistical mechanics,

$$\langle A\rangle=\int \mathrm{d}x\,\mathrm{d}pA_W(x,p)f(x,p),\quad(3)$$

where $A_W(x,p)$ is a real function obtained by the Weyl transform of the operator that represents a dynamical variable. According to Eq. (3), we can introduce a general formula for a quantitative measure of the extent of the correlation of the two dynamical variables [6]:

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$$C_{nm} = \langle x^n p^m \rangle - \langle x \rangle^n \langle p \rangle^m . \tag{4}$$

In the particular case when $n = m = 1$, the quantity given by Eq. (4) is reduced to the symmetrical correlation function of the first order that is the main subject of our interest.

The quantum kinetic equation within the relaxation time approximation satisfied by the WDF has the Boltzmann-*like* form, namely

$$\frac{\hbar k}{m^*}\frac{\partial f(x,k)}{\partial x} + \frac{1}{2\pi \mathrm{i}\hbar}\int \mathrm{d}k'\, W(x,k-k') f(x,k') = -\frac{f(x,k) - f^0(x,k)}{\tau}, \tag{5}$$

where the wave vector $k$ is related to the momentum $p$ via the de Broglie formula: $p = \hbar k$, $m^*$ is the effective mass of conduction electron, $f^0(x,k)$ is the equilibrium WDF, and $\tau$ is the relaxation time due to the scattering processes taking place inside the nanodevice. In turn, the drift term in Eq. (5) has the non-local form, and the integral kernel $W(x,k)$ is given by the formula

$$W(x,k) = \int \mathrm{d}x' \left( U\left(x + \frac{x'}{2}\right) - U\left(x - \frac{x'}{2}\right)\right) \mathrm{e}^{-\mathrm{i}kx'}, \tag{6}$$

where $U(x)$ is the total potential energy of the conduction electrons. It is interesting to note that the first order expansion of the total potential energy into the Taylor series around $x$ reduces Eq. (5) to the Boltzmann equation.

Because the equation for the WDF contains the first order derivative with respect to the position variable, the inflow boundary conditions proposed by Frensley are applied [7]:

$$\begin{cases} f(0,k)\Big|_{k>0} = f^L(k) \\ f(L,k)\Big|_{k<0} = f^R(k), \end{cases} \tag{7}$$

where the supply function $f^{L(R)}(k)$ is taken in the following form [8]:

$$f^{L(R)}(k) = \frac{m^* k_B T}{\pi \hbar^2} \times \ln\left(1 + \exp\left(-\frac{E(k) - \mu^{L(R)}}{k_B T}\right)\right), \tag{8}$$

and $E(k)$ is the quadratic dispersion relation, $T$ is the temperature, $\mu^{L(R)}$ is the electrochemical potential of the left ($L$) or right ($R$) contact, and the contacts are separated by a distance of $L_x$. The difference between electrochemical potential of the contacts, $eV = \mu^L - \mu^R$, generates an uniform electric field $E = V/L_x$ along the nanostructure. As a result the electronic current flowing through the nanosystem depends on the scattering mechanisms which are specified by the relaxation times. The values of the current are determined as the first moment of the WDF, according to the formula

$$j(V) = \frac{e}{2\pi}\frac{1}{L_x}\int \mathrm{d}x \int \mathrm{d}k \frac{\hbar k}{m^*} f(x,k), \tag{9}$$

which stems from the general expression for the expectation value (3).

## 3. Results and discussion

In the first step of our studies, Eq. (5) with the given boundary conditions (7) is numerically solved for the nanosystem displayed in Fig. 1 at the temperature $T = 77$ K. The computational grid with $N_x = 133$ mesh points for the space coordinate $x$, and $N_k = 150$ points for the wave vector $k$ is used, chosen accordingly to the restrictions on the minimum momentum resolution imposed by the uncertainty principle [9].

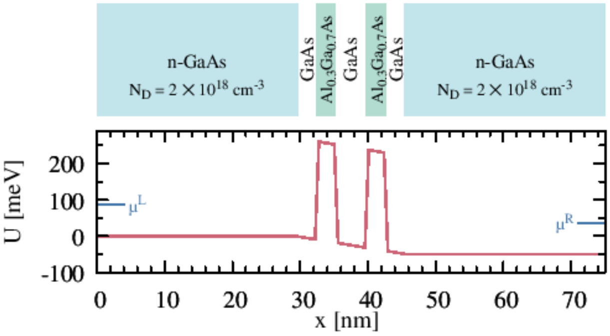

Fig. 1. The potential energy profile in the double-barrier resonant tunneling nanosystem under the bias voltage. Coordinate $x$ is measured along the growth axis of the layers. The contacts doped with donors are separated by the GaAs spacer layers from the nanosystem which consists of the quantum well with GaAs layer sandwiched between two $\mathrm{Al_{0.3}Ga_{0.7}As}$ barrier layers.

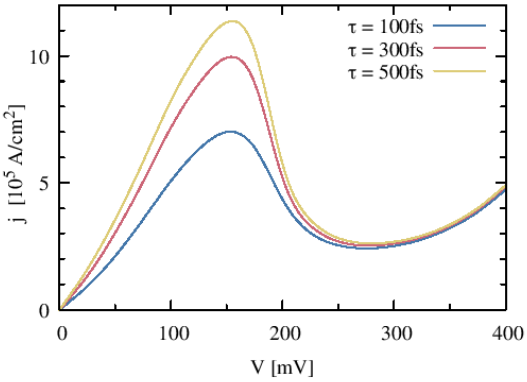

Fig. 2. The current–voltage characteristics of the double-barrier resonant tunneling diode for three different values of the relaxation time.

As a result of these computations, the typical $I$–$V$ characteristics of the double-barrier resonant tunneling diode was obtained, cf. Fig. 2.

In this way, we demonstrated that an increase of the intensity of the scattering processes causes a decrease of the electronic current in the first positive differential resistance region and the negative differential resistance one where the quantum phenomena, i.e., tunnelling and quantum interference give the main contribution to the $I$–$V$ characteristics. Hence we conclude that the position-momentum correlations are stronger in these two regions of the characteristics than in the second positive differential resistance region which is determined by the thermal transport over the barriers. Therefore we decided to investigate the influence of the relaxation time on the symmetrical correlation function $C_{11}(\tau)$ at the first positive differential resistance region of the $I$–$V$ characteristics. Based on the results shown in Fig. 3, we conclude that the increase of the intensity of the scattering processes reduces the initial position-momentum correlations of the electronic states in the considered nanosystem. This observation is closely related to the crossover from the non-Markovian to the Markovian regime of the electronic transport. The decrease of the position-momentum correlations significantly influences the quantum interference, and the phase coherence of the conduction electrons decays.

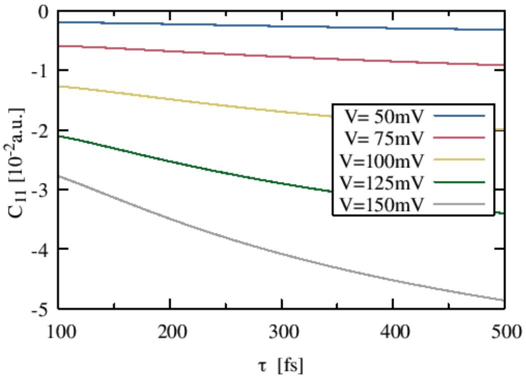

Fig. 3. The relaxation time dependence of the symmetrical correlation function of the first order at selected points of the current–voltage characteristics.

Apart from the symmetrical correlation function $C_{11}(\tau)$, we also determine the phase portrait of the double-barrier resonant nanosystem in the phase space driven by the bias voltage for the selected values of the relaxation time. The result is presented in Fig. 4. The pairs of expectation values of the electron position $\langle x \rangle$ and the wave vector $\langle k \rangle$, calculated for the subsequent voltage values form characteristic loops in the phase space. Starting from $V = 0$, the momentum increases reaching a maximum, then begins to decrease and finally starts increasing again. Such loop-like trajectory is in agreement with the $I$–$V$ characteristics from Fig. 2, since the current and momentum are directly proportional. The area of loops increases for longer relaxation times, because in the positive differential resistance region $\langle x \rangle$ increases slower for larger $\tau$.

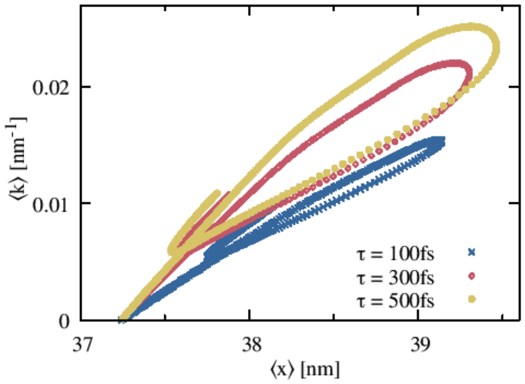

Fig. 4. The phase portrait obtained from the expectation values $\langle x \rangle$ and $\langle k \rangle$ found for subsequent values of the applied bias voltage for several different relaxation times.

## 4. Conclusions

We have applied the phase-space quantum mechanics based on the Wigner distribution function to the study of the position-momentum correlations of the electronic states in the double-barrier resonant nanosystem. We have demonstrated that the symmetrical correlation function of the first order, which is the simplest measure of the considered correlations, is a negative definite monotonically decreasing function of the relaxation time that depends on the differential resistance region in the current–voltage characteristics.

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