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Application of Non-Classical Distribution Function to Transport Properties of Semiconductor Nanodevices

P. Wójcik, B.J. Spisak*, M. Wołoszyn and J. Adamowski

Faculty of Physics and Applied Computer Science
AGH University of Science and Technology
al. Mickiewicza 30, 30-059 Kraków, Poland

The non-classical distribution function formalism is used for studying the electron transport in a nanosystem. We calculated the current–voltage characteristics of a triple barrier one-dimensional nanostructure which is connected to three-dimensional (highly doped semiconductor) reservoirs by the ohmic contacts. We also estimated the peak-to-valley ratio for the considered nanostructure and discussed the effect of switching the bias from peak-to-valley and from valley-to-peak voltages.

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1. Introduction

Rapid development of fabrication and measurement techniques in the semiconductor industry allows one to produce electronic devices that are smaller than 50 nm. At this scale the quantum effects fully determine the optical, magnetic as well as transport properties of systems. Among these devices, the semiconductor multilayered nanostructures are very promising artificial structures for application in the new generation of electronic devices. In order to investigate the transport properties of such systems the quantum theory of electronic transport is required. Many theoretical works have been devoted to the problem of electronic transport through the resonant tunnelling diode, i.e. the double barrier systems [1–3] and their natural extension — the triple barrier nanostructures [4, 5]. In the present work, we have applied the non-classical distribution function formalism based on the Wigner distribution function [6, 7] to the triple barrier nanostructure. We have solved numerically the quantum kinetic equation for the Wigner function [8, 9] and determined the current–voltage characteristics and the switching time of the current into nanostructure. The paper is organised as follows. In Sect. 2, we

*corresponding author; e-mail: spisak@novell.ftj.agh.edu.pl

present the theoretical model of the triple barrier nanosystem and briefly discuss the formalism of non-classical distribution function. In Sect. 3 we apply the formalism to quantitative analysis of the electronic transport through the nanosystem. Section 4 contains conclusions.

2. Nanodevice model and formalism

The fabrication of multilayered nanostructures is mainly based on two experimental techniques, namely the molecular beam epitaxy (MBE) and metalorganic chemical vapour deposition (MOCVD) [10, 11]. The obtained structures consist of layers of different semiconductors, in most cases having nearly the same lattice parameters. The electronic properties of such systems depends on the layer thickness and properties of constituent semiconductors. The most common multilayered systems are based on GaAs and $Al_xGa_{1-x}As$ where x varies between 0.1 and 0.4. In such structures, the lattice parameters of both semiconductors are almost the same, therefore, the effect of strain is not significant. On the other hand, the differences in band gaps of GaAs and $Al_xGa_{1-x}As$ lead to discontinuities in conduction and valence bands. These band discontinuities form quantum barriers and quantum wells in the potential energy for conduction electrons and holes, respectively.

In this paper, we consider the triple barrier nanosystem composed of GaAs/$Al_{0.3}Ga_{0.7}As$/GaAs/$Al_{0.3}Ga_{0.7}As$/GaAs layers as it is shown in Fig. 1. In the potential wells, the resonant states with discrete energy levels are formed. Under bias voltage, conduction electrons can tunnel through the triple barrier nanostructure from left to right reservoirs. This process is modified by the gate voltage that allows one to force the resonance condition for tunnelling process in the nanodevice. We describe the electrons in this nanostructure by the single-particle effective-mass Hamiltonian within the 1D approximation. We assume that the triple barrier nanostructure is connected to the three-dimensional highly doped semiconductor reservoirs by the ohmic contacts. Each of the reservoirs (L, R) is characterised by the equilibrium Fermi–Dirac distribution function, with Fermi energy $E_{\mathrm{F}}^{\mathrm{L(R)}}$.

The conduction electrons are described by the non-classical distribution function $\rho_w(x,k,t)$ which satisfies the integro-differential equation [2, 8, 9]:

$$\frac{\partial \rho_w(x,k,t)}{\partial t} + \frac{\hbar k}{m}\frac{\partial \rho_w(x,k,t)}{\partial x} = \frac{\mathrm{i}}{2\pi\hbar}\int \mathrm{d}k'\; U_w(x,k-k')\rho_w(x,k'), \tag{1}$$

where the integral kernel $U_w(x,k-k')$ represents the non-local potential which takes into account a modification of confining potential $U(x)$ by the external static electric field. The form of the non-local potential is given by

$$U_w(x,k-k') = \int \mathrm{d}x'\; \big[U(x+x'/2) - U(x-x'/2)\big] \exp\big(-\mathrm{i}(k-k')x'\big). \tag{2}$$

The non-classical distribution function $\rho_w(x,k,t)$ is defined as the Wigner–Weyl transform of the one-particle density matrix and is called the Wigner distribution

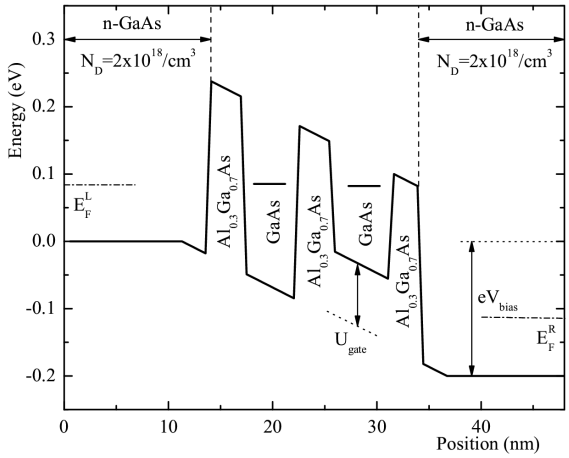

Fig. 1. Energy band diagram of a triple barrier system under bias voltage. The potential of the gate U_{gate} is defined as the difference between left and right quantum-well potentials.

function [6, 7]. From the mathematical standpoint, the Wigner function does not satisfy all the necessary conditions for classical distribution functions, namely it can take negative values in some regions of the phase-space. This feature makes it impossible to interpret the Wigner function as a classical probability distribution function. Nevertheless, the Wigner function is a very useful tool for the quantum modelling of electron transport in nanodevices because the moments of the Wigner function have simple physical interpretation, namely, the zero moment gives the electron density [9],

$$n(x,t) = \frac{e}{2\pi}\int \mathrm{d}k \rho_w(x,k,t), \tag{3}$$

and the first moment represents the flux current

$$j(x,t) = \frac{e}{2\pi}\int \mathrm{d}k \frac{\hbar k}{m}\rho_w(x,k,t). \tag{4}$$

The Wigner function can be determined by solving the steady-state form of Eq. (1) with the open boundary conditions having the form [12]:

$$\begin{aligned} \rho_w(0,k)\Big|_{k>0} &= f^{\mathrm{L}}(k), \\ \rho_w(L,k)\Big|_{k<0} &= f^{\mathrm{R}}(k), \end{aligned} \tag{5}$$

where $f^{\mathrm{L(R)}}(k)$ is given by

$$f^{\mathrm{L(R)}}(k) = \frac{mk_{\mathrm{B}}T}{\pi\hbar^2}\ln\left(1+\exp\left(-\frac{1}{k_{\mathrm{B}}T}\left(\frac{\hbar^2k^2}{2m}-E_{\mathrm{F}}^{\mathrm{L(R)}}\right)\right)\right), \tag{6}$$

where T is temperature, m is the effective mass, and all other symbols have the usual meanings.

3. Results and discussion

We have applied the formalism presented in Sect. 2 to the problem of resonant tunnelling through the triple barrier nanostructure at $T = 77$ K. In our calculation we assume that the effective mass of conduction electron is constant in the entire region of nanodevice. The material parameters of the device are presented in Fig. 1. The calculated current–voltage characteristics of the triple barrier nanodevice for two different gate potentials are shown in Fig. 2. For the zero gate potential, $U_{\mathrm{gate}} = 0$ eV, the I–V characteristic shows four broad maxima peaked around $U_{\mathrm{bias}} = 0.05$, 0.13, 0.2, and 0.35 V, respectively. On the contrary, for the gate potential equal to $U_{\mathrm{gate}} = 0.1$ eV there is only one current peak with higher magnitude and one maximum. These two characteristics coincide in the region of higher voltages (above 0.6 V).

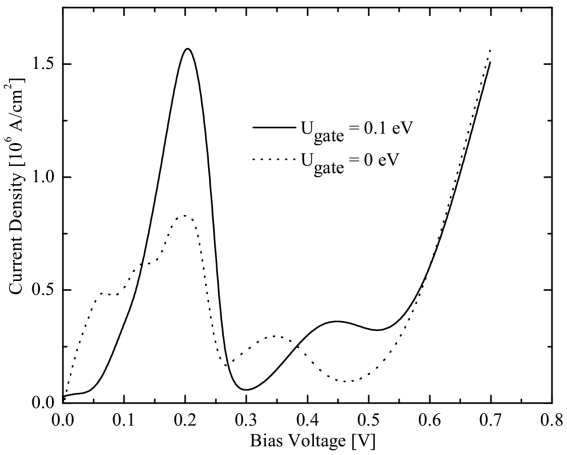

Fig. 2. I–V characteristics of triple barrier resonant tunnelling system.

Here we present the qualitative explanation of the results. The free electrons are injected to the triple barrier nanosystem with energies approximately equal to the Fermi level in the left reservoir. The bias voltage shifts the resonant states in the nanosystem and the electrons with energies close to the resonances can pass through the nanosystem to the right reservoir with high probability. It means that the maximum current is achieved if the resonant-state energy is equal to the Fermi energy of the left reservoir. The application of the gate voltage to one of the wells (right potential well in Fig. 1) allows to manipulate the resonant states in the right well with respect to the left quantum well. The manipulation of the depth of the one of wells is realised experimentally (cf. [13]). The current peak in Fig. 2 corresponds to the situation when the appropriate resonant levels in both wells coincide with the Fermi energy of the left reservoir. In this case, the maximum tunnelling current flows through the nanodevice.

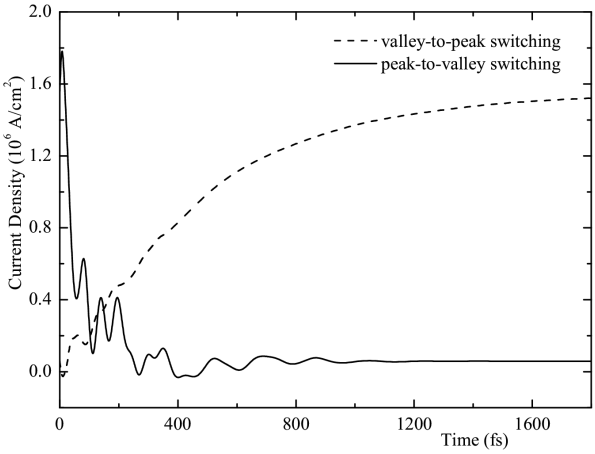

Fig. 3. The time dependence of the current density for peak-to-valley and valley-to--peak switching of the bias voltage.

One of the most important technological parameters characterising the nanodevice is the peak-to-valley ratio that gives the indirect measure of the negative differential resistance. It results from our calculations that the peak-to-valley ratio is equal to 27. This high value suggests that such nanodevice can be used as a logic element in nanoelectronics.

We have also determined the bias switching time from peak to valley and valley to peak. We can extract these parameters from the time dependence of current density. For this purpose we have performed time dependent simulations based on Eq. (1). The initial condition has been chosen in the form of a function which corresponds to the steady-state Wigner function for the current peak and the steady-state Wigner function for the current valley with $U_{\mathrm{gate}} = 0.1$ eV, respectively [14]. In computer simulations, the bias voltage is suddenly raised from 0.2 V (the peak voltage V_{p}) to 0.3 V (the valley voltage V_{v}). Next, the bias was rapidly lowered from V_{v} to V_{p}. Figure 3 shows the results of simulations. For the peak-to-valley switching, the steady-state current is reached after a time of 1000 fs, while for the valley-to-peak switching, the steady-state current stabilises after 2000 fs. The results of our calculation of the switching time are comparable to the experimental data for the resonant-tunnelling nanodevices [15].

4. Conclusions

In summary, we have applied the non-classical distribution function formalism based on the Wigner distribution function to the triple barrier nanodevice. We have calculated the basic characteristics of such nanosystem and have shown that the nanosystem exhibits a resonantly enhanced negative resistance. We have demonstrated that the triple barrier nanodevice controlled by the gate has the short switching time.

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