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Wigner distribution function description of a multilayered nanostructure with magnetic impurities

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Abstract. The Wigner distribution function formalism is applied to the description of transport properties of spintronic multilayer nanodevice. The central layer of the nanodevice is doped with magnetic impurities. The current-voltage characteristics and the spin polarisation of current are calculated.

1. Introduction
The high precision of techniques based on semiconductor technology enables the construction of semiconductor heterostructure on a nanometre scale. On this length scale, quantum effects determine the basic characteristics of the nanodevice, and the nonclassical behaviour is utilised to design a new generation of digital elements and circuits [1]. The current trends in designing nanodevices are focused on the use and manipulation of the electron charge as well as the spin degree of freedom to enhance the performance of nanodevices. One of the simplest examples of spintronic nanodevices based on the hybrid semiconductor technology is a trilayer nanostructure where two dilute ferromagnetic semiconductors (DMS) are separated by a nonmagnetic semiconductor (NMS) layer [1].

In this report we analyse the transport properties of a simple model of the spintronic nanostructure DMS/NMS/DMS assuming that the NMS region of nanodevice contains magnetic impurities. Our analysis is based on the quantum kinetic equation for the Wigner distribution function because of its intrinsic interesting description of quantum mechanics and its potential usefulness in the simulation of nanodevice.

2. The Model nanodevice and method of calculation
The structure and the potential profile of the simulated spintronic nanostructure is shown in Fig. 2. The total length of the nanodevice is 16 nm with a 4 nm nonmagnetic semiconductor layer of GaN that is separated from the dilute magnetic semiconductor layers of GaMnN by spin-dependent potential barriers made from AlGaN. The existence of the spin-dependent barriers results from the difference between majority and minority spin electron states at the Fermi level in GaMnN [2].

We assume the same magnetisation axis for both GaMnN layers and the exchange splitting energy $\Delta_{\sigma}^{DMS}$. The magnetic elements (Mn) in the clean layer of GaN are a consequence of the fabrication process. The concentration of impurities is low, and assumed to be smeared out.
The impurities can be characterised by a splitting parameter $\Delta_{\sigma}^{\text{NMS}}$, according to [3] such that $\Delta_{\sigma}^{\text{NMS}} < \Delta_{\sigma}^{\text{DMS}}$. The impurities in the NMS lead to loss of phase coherence after a time $\tau_{\varphi}$ [4].

When a small bias voltage is applied the spin-polarised electrons are in a nonequilibrium state and the spin-polarised current density can be evaluated by the formula

$$j_{\sigma}(x) = \frac{e}{2\pi} \int \frac{dk}{m} \rho_{\sigma}(x, k),$$

where $m$ is the effective mass of conduction electrons, and $\rho_{\sigma}(x, k)$ is the Wigner distribution function for electrons with spin $\sigma$ for a 1-D system. We model the nanostructure in this fashion on the grounds that the system is translationally invariant in the $y$ and $z$ direction.

The Wigner distribution function, $\rho_{\sigma}(x, k)$ can be found by the solution of the simplified version of the quantum kinetic equation [5, 6], namely

$$\frac{\partial \rho_{\sigma}(x, k, t)}{\partial t} + \frac{\hbar k}{m} \frac{\partial \rho_{\sigma}(x, k, t)}{\partial x} + \frac{1}{2\pi i\hbar} \int dk' \mathcal{U}(x, k - k') \rho_{\sigma}(x, k', t)$$

$$= -\frac{\rho_{\sigma}(x, k, t) - \rho_{\sigma}^0(x, k, t)}{\tau_{\varphi}},$$

where $\rho_{\sigma}^0(x, k, t)$ is the equilibrium distribution function for electrons with spin $\sigma$, and the integral kernel $\mathcal{U}(x, k - k')$ represents the non-local potential energy. The form of the integral

**Figure 1.** Potential energy profile in the spintronic nanodevice for zero bias voltage $V_b$ between contacts and parallel magnetisation in the DMS layers. Energy scale relative to the Fermi level.
kernel can be found in [7]. The non-local potential energy includes the band offset, and the smeared impurity potential.

We solve the quantum kinetic equation for the Wigner distribution function \( f_{\sigma}(k) \) using the open boundary conditions in the form [8]

\[
\rho_\sigma(0, k) \bigg|_{k>0} = f^L_\sigma(k),
\]
\[
\rho_\sigma(L, k) \bigg|_{k<0} = f^R_\sigma(k),
\]

where \( f^L_\sigma(k) \) is chosen to be the semiclassical form

\[
f^L_\sigma(k) = \frac{mk_BT}{\pi \hbar^2} \ln \left\{ 1 + \exp \left[ -\frac{1}{k_BT} \left( \frac{\hbar^2 k^2}{2m} - \mu_L^{(R)}(k) \right) \right] \right\},
\]

where \( T \) is the temperature and \( \mu_L^{(R)} = E_F \pm \Delta_{DMS}^{\sigma} \) is the electrochemical potential of the left (right) DMS.

The numerical calculations were carried out using the computational grid with \( N_x = 116 \) mesh points for the position \( x \) and \( N_k = 314 \) for the wave vector \( k \). We assume that the conduction electrons are described by the conduction band effective mass of GaN, i.e. \( m = 0.228 m_0 \).

3. Results and discussion

When the amount of dopants inside the NMS increases, the maximum current density is decreasing in case of the majority carriers by about 15 %. At the same time the maximum value is slightly shifted towards higher voltages for positive values of \( \Delta_{NMS}^{\sigma} \), and toward lower voltages for negative values of \( \Delta_{NMS}^{\sigma} \). Similar shifts are observed for the minority carriers, but with rather insignificant changes of the current density values (less than 2 %).

One of the most important transport characteristics of spintronic nanodevice is the polarisation of the current density that is defined as follows [9]

\[
P_\sigma(V_b) = \frac{j_\uparrow(V_b) - j_\downarrow(V_b)}{j_\uparrow(V_b) + j_\downarrow(V_b)}.
\]

Figure 2 presents the polarisation of the current density as a function of the parameter \( \Delta_{NMS}^{\sigma} \) for several different values of the bias voltage \( V_b \). Degree of the polarisation depends on the applied bias voltage. For example at 0.18 V the current density polarisation slightly decreases from 98 % at \( \Delta_{NMS}^{\sigma} = -4 \) meV to 90 % at \( \Delta_{NMS}^{\sigma} = 4 \) meV. When the bias voltage is increased to 0.20 V the polarisation virtually does not depend on \( \Delta_{NMS}^{\sigma} \) and is about 85 %. After a further increase of the bias voltage polarisation is decreasing. At \( V_b = 0.22 \) V it is an increasing function of \( \Delta_{NMS}^{\sigma} \), from zero at -4 meV to about 65 % at 4 meV.

4. Concluding remarks

Using the Wigner distribution function formalism, we investigated the influence of magnetic impurities on the transport characteristics of the spintronic nanodevice DMS/NMS/DMS. We find that the polarisation of the current density is very sensitive to the magnetic impurities which leads to the conclusion that the purity of the non magnetic layer influences the basic transport characteristics of nanodevice.

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Figure 2. Polarisation of the current density for various values of the bias voltage. The dephasing time $\tau_\varphi$ is 100 fs.

References