The Wigner function approach to spin-dependent electronic transport in presence of magnetic impurities

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The transport of spin-polarised electrons through the ferromagnetic/non-magnetic/ferromagnetic tri-layer nanostructure is considered. The non-magnetic metal layer contains the magnetic impurities. The calculations of a spin-dependent current density for different spin configurations of magnetic impurities are performed using the simplified version of the quantum kinetic equation for the Wigner distribution function.

Theoretical model

The device consists of a non-magnetic metallic layer between two non-interacting ferromagnetic leads both made of the same material. The layer is doped with two magnetic impurities.

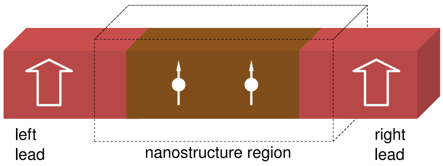

Figure 1. *Schematic view of the investigated ferromagnetic/ non-magnetic/ ferromagnetic structure.*

The simplified version of the quantum kinetic equation for the Wigner distribution function $\rho_\sigma(x,k)$ has the form [1, 2]

$$\frac{\hbar k}{m}\frac{\partial \rho_\sigma(x,k)}{\partial x} = \frac{i}{2\pi\hbar}\int dk'\, U_w(x,k-k')\rho_\sigma(x,k'),$$

where m is the conduction band effective mass, and the non-local integral kernel is defined as

$$U_w(x,k-k') = \int dx' \left[U(x+\frac{x'}{2}) - U(x-\frac{x'}{2})\right] e^{-i(k-k')x'},$$

The total electrostatic potential energy of the electron $U(x)$ is given by the sum of band potential $U_B(x)$ and magnetic impurity potential $U^\sigma_{imp}(x)$, namely

$$U_B(x) = \sum_{i=1}^{2} U_i \Theta(x-x_i)\Theta(x_{i+1}-x),$$

where x_i is the position of interface, i.e., $|x_{i+1}-x_i|$ determines the thickness of the barrier region, and U_i is the height of the i-th barrier.

$$U^\sigma_{imp}(x) = \sum_{k=1}^{2} J_0 S_z(X_k) s_z(x)\delta(x-X_k)$$

where J_0 is the coupling constant, $S_z(X_k)$ is the z-component of impurity spin localised in the positions X_k, and $s_z(x)$ is the z-component of conduction electron spin.

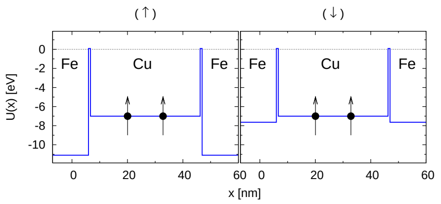

Figure 2. *The model potential energy in case of the parallel spin configurations of impurities and without bias voltage applied. Energy scale relative to electrochemical potential.*

Results

Numerical calculations were performed for Fe/Cu/Fe system at 77 K using the computational grid of $(N_x = 4000) \times (N_k = 274)$ points. The magnetisations of both ferromagnetic leads are parallel. The quantum kinetic equation for the Wigner distribution function is solved with the open boundary conditions in the form [3]

$$\rho_\sigma(0,k)\Big|_{k>0} = f^L(k)\ ;\ \rho_\sigma(L,k)\Big|_{k<0} = f^R(k)$$

where $f^{L(R)}(k)$ is the supply function for electrons in the left (right) reservoir:

$$f^{L(R)}(k) = \frac{mk_BT}{\pi\hbar^2}\ln\left(1+e^{-\frac{\frac{\hbar^2k^2}{2m}-\mu_{L(R)}}{k_BT}}\right)$$

T – temperature, $\mu_{L(R)}$ – electrochemical potential of the left (right) reservoir.

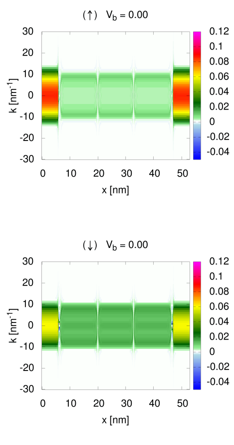

Figure 3. *The Wigner distribution function calculated for for parallel (↑↑) configuration of magnetic impurities and* $V_b = 0$.

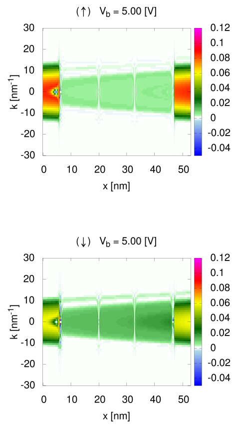

Figure 3. *The Wigner distribution function calculated for for parallel (↑↑) configuration of magnetic impurities and* $V_b = 5$ *V.*

The first moment of the Wigner distribution function corresponds to the spin-dependent current density, namely [1]

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

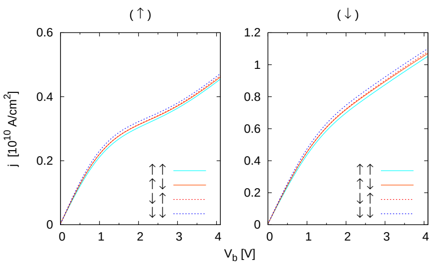

Figure 4. *Current density calculated from the Wigner distribution functions obtained for various configurations of impurities.*

For a fixed spin state of impurities the spin polarisation of the current density has the form [4]:

$$P_j(V_b) = \frac{j_\uparrow(V_b) - j_\downarrow(V_b)}{j_\uparrow(V_b) + j_\downarrow(V_b)}$$

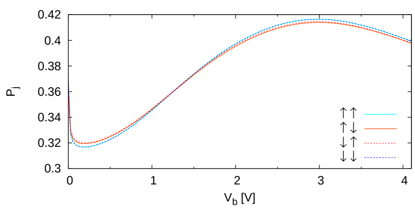

Figure 5. *Polarisation of the current density.*

Conclusions

- The spin-polarised current depends weakly on the spin configuration of magnetic impurities in the non-magnetic region.
- The current polarisation is determined by the height of the barriers at the interfaces.
- Effects of small number of magnetic impurities on transport characteristics of the FM/NM/FM is insignificant.

References

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