Introduction to spintronics – spin transistor

P. Wójcik, A. Mrenca-Kolasinska

February 20, 2025; last update February 24, 2025

1 Introduction

Using the KWANT package we will perform simulations of a spin transistor prototype proposed in the recent years. Its architecture uses the spin-orbit coupling for spin control in the conducting channel, and the control parameter is electric field.

In quantum mechanics the equation describing electron taking spin into account is called Pauli equation, and in 2D it takes the form

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 + \frac{1}{2}g\mu_B\mathbf{B}\cdot\boldsymbol{\sigma} + \alpha(k_y\sigma_x - k_x\sigma_y)\right)\Psi(x,y) = E\Psi(x,y), \tag{1}$$

where m^* is the effective mass, g is Lande factor, μ_B is Bohr magneton, $\mathbf{B} = (B_x, B_y, B_z)$ is magnetic field vector, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is Pauli matrix vector, $k_{x(y)} = -i\partial/\partial x(y)$ are momentum (wave vector) operators, and α is the spin-orbit coupling constant.

The terms in Hamiltonian (1) are called: kinetic term, Zeeman interaction, and spin-orbit (SO) interaction. The Pauli matrices are 2×2 matrices taking the form

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2}$$

So, the Pauli equation in the matrix form is

$$\begin{pmatrix} -\frac{\hbar^2}{2m^*}\nabla^2 + \frac{1}{2}g\mu_B B_z & \frac{1}{2}g\mu_B(B_x - iB_y) + \alpha(k_y + ik_x) \\ \frac{1}{2}g\mu_B(B_x + iB_y) + \alpha(k_y - ik_x) & -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{1}{2}g\mu_B B_z \end{pmatrix} \begin{pmatrix} \psi^{\uparrow}(x,y) \\ \psi^{\downarrow}(x,y) \end{pmatrix} = E \begin{pmatrix} \psi^{\uparrow}(x,y) \\ \psi^{\downarrow}(x,y) \end{pmatrix}. \tag{3}$$

Discretizing equation (1) on a square lattice (i,j) with $\Delta x = \Delta y$, and using the three-point approximation of the second derivative and the central form of the first derivative, we get

$$\begin{aligned} &t\mathbb{I}_{2\times 2}(4\Psi_{i,j} - \Psi_{i+1,j} - \Psi_{i-1,j} - \Psi_{i,j+1} - \Psi_{i,j-1}) + \frac{1}{2}g\mu_B(B_x\sigma_x + B_y\sigma_y + B_z\sigma_z)\Psi_{i,j} \\ &+ it_{SO}\sigma_y(\Psi_{i+1,j} - \Psi_{i-1,j}) - it_{SO}\sigma_x(\Psi_{i,j+1} - \Psi_{i,j-1}) = E\Psi_{ij} \end{aligned} \tag{4}$$

where $t = \frac{\hbar^2}{2m^*\Delta x^2}$, $t_{SO} = \frac{\alpha}{2\Delta x}$, $\Psi_{i,j} = \Psi(x_i, y_j) = (\psi^{\uparrow}(x_i, y_j), \psi^{\downarrow}(x_i, y_j))^T$, and $\mathbb{I}_{2\times 2}$ is a 2×2 identity matrix. Assuming $\Psi_{i,j} = |\Psi_{i,j}\rangle$ and multiplying by $\langle\Psi_{ij}|$, we get the equation

$$\begin{aligned} &t\mathbb{I}_{2\times 2}(4|\Psi_{i,j}\rangle\langle\Psi_{i,j}| - |\Psi_{i+1,j}\rangle\langle\Psi_{i,j}| - |\Psi_{i-1,j}\rangle\langle\Psi_{i,j}| - |\Psi_{i,j+1}\rangle\langle\Psi_{i,j}| - |\Psi_{i,j-1}\rangle\langle\Psi_{i,j}|) \\ &+ \frac{1}{2}\mu_B g(B_x\sigma_x + B_y\sigma_y + B_z\sigma_z)|\Psi_{i,j}\rangle\langle\Psi_{i,j}| \\ &+ it_{SO}\sigma_y(|\Psi_{i+1,j}\rangle\langle\Psi_{i,j}| - |\Psi_{i-1,j}\rangle\langle\Psi_{i,j}|) - it_{SO}\sigma_x(|\Psi_{i,j+1}\rangle\langle\Psi_{i,j}| - |\Psi_{i,j-1}\rangle\langle\Psi_{i,j}|) = E|\Psi_{i,j}\rangle\langle\Psi_{i,j}|, \end{aligned} \tag{5}$$

that contains the on-site and nearest-neighbor hopping energies. In this case they have a form of 2×2 matrices.

2 Implementation in KWANT

For our implementation of the system in KWANT we should assume that:

1. the functions onsite() and hopping() return matrices of size 2×2, which are the hopping energies,

2. we use a square lattice with spacing $\Delta x = \Delta y$. The form of the Hamiltonian (3) indicates that in this case there are two orbitals on each node: one corresponding to spin up electron, and the other one to spin down electron. In order to take it into account, when defining the system we should set $norbs = 2$:

```
lat=kwant.lattice.square(dx, norbs=2)
```

3. if we want to distinguish the two degenerate states in the contact (in our case the spin-degenerate states), and the form of the Hamiltonian allows it (it has a block matrix form), in each contact we can define a parameter called *conservation_law*. We set it to be a square matrix with the dimension equal to the number of orbitals per node, and eigenvalues differing for different separable blocks (orbitals). In the case considered here, the Hamiltonian of the lead will have a block structure if there is no spin-orbit coupling or magnetic field or in the lead[1] (or there is only B_z component),

```
left_lead=kwant.Builder(kwant.TranslationalSymmetry((-dx, 0)),conservation_law=sigma_law)
```

where the matrix *sigma_law* can have the form (to be commented on during the class)

$$sigma\_law = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}.$$

4. if we define the *conservation_law* variable in the leads, for the transmission calculation we can not only refer to the contact number, but also to the orbital number. The example code

```
sys=make_system(nw)
smatrix = kwant.smatrix(sys, energy)
tup_down=smatrix.transmission((1,1), (0,0))
```

calculates the transmission coefficient for the spin up electron injected to the system from the contact number 0 to the contact number 1 and spin down, where in the notation (i, j), i is the contact number, and j is the orbital number.

5. when we calculate the electron density or current in the specified orbital, we use, respectively, the functions *kwant.operator.Density*() and *kwant.operator.Current*(). An example for the calculation of spin up and down electron density, and the sum of the two is shown below

```
sys = make_system(nw)
wave_f=kwant.wave_function(sys,nw.energy)(0)

density_up=tinyarray.array([[1,0],\
                            [0,0]])

density_down=tinyarray.array([[0,0],\
                            [0,1]])

density_both=tinyarray.array([[1,0],\
                            [0,1]])


density_up_op=kwant.operator.Density(sys,density_up)
density_down_op=kwant.operator.Density(sys,density_down)
density_both_op=kwant.operator.Density(sys,density_both)
```

[1]When we set nonzero magnetic field or the SO coupling **only** inside the system, we should define a separate function onsite_lead() or hopping_lead() for the leads.

```
density_up_map=density_up_op(wave_f[0])
density_down_map=density_down_op(wave_f[0])
density_both_map=density_both_op(wave_f[0])
```

3 Spin precession in external magnetic field

Consider a 2D nanowire of length L and width W in external magnetic field $\mathbf{B} = (B_x, B_y, B_z)$.

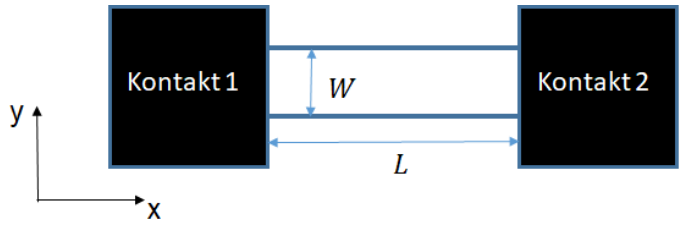

Figure 1: Schematic of the nanowire.

For this system:

1. calculate the dispersion relation $E(k)$ in the lead without magnetic field,
2. calculate the dispersion relation $E(k)$ in the contact for $B = 1$ T, assuming that magnetic field is applied either in the direction x, y and z. Does the observed Zeeman splitting depend on the direction of magnetic field?
3. apply $\mathbf{B} = (0, 0, B_z)$ field in the system, with $B_z = 1$ T, and calculate the conductance as a function of incident electron energy,
4. apply $\mathbf{B} = (0, B_y, B_z)$ field in the system, with $B_z = 0.1$ T applied in the entire device (including leads), and B_y field applied only in the region $[0.2, 0.8]$ L. For the Fermi energy corresponding to the lowest subband (for both spins, $E = 5$ meV) calculate the transmission coefficients $T_{up\leftarrow up}$, $T_{down\leftarrow up}$, $T_{up\leftarrow down}$ and $T_{down\leftarrow down}$ as a function of magnetic field $B_y \in [0, 1]$ T,
5. for the system from 4. plot the charge density for spin up and spin down for electron injected in the lowest subband and $B_y = 0.6$ T,
6. for the system from 4. plot the spin s_x, s_y, s_z density for electron injected in the lowest subband and $B_y = 0.6$ T.

Perform the calculation for $L = 2000$ nm, $W = 100$ nm, $g = -50$, $m^* = 0.014$ and $\Delta x = 4$ nm. In atomic units, Bohr magneton is $\mu_B = 0.5$ a.u.

4 Spin transistor based on the spin-orbit coupling

As we can see, spin can be controlled by external magnetic field. However, in practice it is inconvenient to use magnetic field in transistors; for example, the device would be large. Therefore, other methods of spin control are required. One of them is based on spin-orbit coupling of the Rashba type, which occurs in semiconducting materials. The Rashba SO interaction Hamiltonian has the form

$$H_{RSO} = \alpha(k_y\sigma_x - k_x\sigma_y) = (\alpha k_y, -\alpha k_x) \cdot (\sigma_x, \sigma_y). \tag{6}$$

Note that the form of H_{RSO} resembles the Zeeman effect, with the effective magnetic field $B_{RSO} = (\alpha k_y, -\alpha k_x)$, so, similarly to the magnetic field, we should observe spin precession around the effective field B_{RSO} perpendicular to the direction of electron propagation. Interestingly, the parameter α can be controlled by external electric field, that can be induced by gate electrodes.

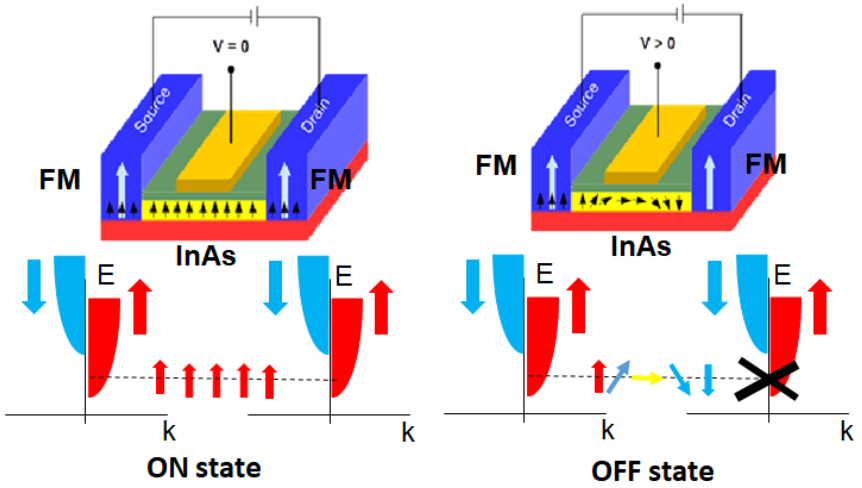

Figure 2: Schematic of the spin transistor based on spin-orbit interaction. A spin polarized electron from a ferromagnetic source is injected to a semiconducting channel. Its spin is controlled by external electric field from a gate electrode through SO interaction. Depending on the spin state of the electron on exit, the system is in the high resistance or low resistance state.

Using this phenomenon, in 1990 Datta and Das [Appl. Phys. Lett. 56, 665 (1990)] proposed a new idea of transistor based on SO interaction for spin control – see fig. 2. In this device, spin polarized electrons from the ferromagnetic contact are injected to a semiconducting channel with strong SO interaction. Applying the right voltage to the gate electrode, we adjust the electric field in the channel, and thus the value of α. Thanks to the spin-orbit interaction, in the region with strong electric field, the electron starts to precess around the effective field B_{RSO}. The number of rotations the electron spin performs depends on the strength of this field, and thus on the α parameter, that's controlled by the gate voltage. If the electron performs an integer number of rotations, it exits the channel with the same spin and can be absorbed by the ferromagnetic drain. On the other hand, if it performs an odd number of half-rotations, it exits the channel with an opposite spin. Then, it cannot be absorbed by the ferromagnetic drain because there are no electron states for spin down electrons in the ferromagnetic. In this way, tuning the gate voltage we control the parameter α, and we can switch the state between the low resistance state (with current allowed to flow) and the high resistance state (with current blocked), obtaining a transistor.
The total current flowing through the nanodevice is the sum of currents of the two opposite spins

$$G = \frac{1+P}{2} G^{up} + \frac{1-P}{2} G^{down}, \tag{7}$$

where P is the polarization of contacts $P \in [0,1]$, and

$$G^{up} = \frac{e^2}{\hbar} \left(\frac{1+P}{2} T_{up \leftarrow up} + \frac{1-P}{2} T_{up \leftarrow down} \right), \tag{8}$$

$$G^{down} = \frac{e^2}{\hbar} \left(\frac{1+P}{2} T_{down \leftarrow up} + \frac{1-P}{2} T_{down \leftarrow down} \right). \tag{9}$$

Consider a nanowire of length L and width W, and calculate the following quantities:

1. dispersion relation in the contacts $E(k)$, assuming that SO interaction is present in the entire device (including contacts),
2. conductance as a function of incident electron energy, assuming that SO interaction is present in the entire device (including contacts),
3. transmission coefficients $T_{up \leftarrow up}$, $T_{down \leftarrow up}$, $T_{up \leftarrow down}$ and $T_{down \leftarrow down}$ as a function of α, assuming that SO interaction is present in the region $[0.2, 0.8]$ L, and that electron is injected in the lowest subband ($E = 5$ meV), sweep the parametr α in the range $[0, 50]$ meVnm,

4. for the system from 3., calculate the conductance G, G^{up} and G^{down} as a function of α for electron injected in the lowest subband, assuming $P = 0.2, 0.4, 1$,

5. for the system from 3., calculate the density of spin up and spin down electrons, and the spin s_x, s_y, s_z density in the nanodevice for electron injected in the lowest subband and α corresponding to a full spin rotation.

Perform the calculations for the following parameters: $L = 800$ nm, $W = 100$ nm, $\Delta x = 4$ nm, $m^* = 0.014$, $g = -50$, $\alpha = 50$ meVnm (α given for task 1. and 2.).