The KWANT package – electron transport simulations in magnetic field

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1 Introduction

In this laboratory, we will get familiar with the Kwant package for the electron transport simulations in nanoscopic devices, based on the tight binding method. The full documentation of the Kwant package with many examples can be found on the official website https://kwant-project.org/doc/dev/.

Before we start the today's task, let us analyze briefly a simple example of a nanowire of width $2W$ and length L – see fig. 1.

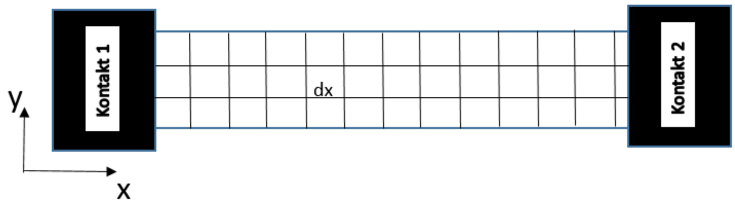

Figure 1: Schematic of the nanowire.

The numerical calculations will be done on a square lattice with the spacing dx. The equation describing the electron transport in this system is the Schrödinger equation

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y)+V(x,y)\psi(x,y)=E\psi(x,y), \tag{1}$$

that, upon discretization on a lattice $(x_i, y_j) \rightarrow (i, j)$, takes the form

$$t(4\psi_{i,j}-\psi_{i-1,j}-\psi_{i+1,j}-\psi_{i,j-1}-\psi_{i,j+1})+V_{i,j}\psi_{i,j}=E\psi_{i,j}, \tag{2}$$

where $t=\frac{\hbar^2}{2m^*dx^2}$.

As shown in the previous lab, this equation has to be solved assuming the proper boundary conditions in the form of plane waves incoming and outgoing from the system, which leads to the so called scattering matrix. KWANT allows us to fill the main matrix and calculate the scattering matrix with the transmission coefficients in a very simple and efficient way. To this end, we should write the discrete equation in a matrix form, assuming (as in the tight-binding approximation (TBA) model), that ψ_{ij} corresponds to the orbital localized on site (i, j). Then

$$t\big(4|\psi_{i,j}\rangle\langle\psi_{i,j}|-|\psi_{i-1,j}\rangle\langle\psi_{i,j}|-|\psi_{i+1,j}\rangle\langle\psi_{i,j}|-|\psi_{i,j-1}\rangle\langle\psi_{i,j}|-|\psi_{i,j+1}\rangle\langle\psi_{i,j}|\big)+V_{i,j}|\psi_{i,j}\rangle\langle\psi_{i,j}|=E|\psi_{i,j}\rangle\langle\psi_{i,j}|, \tag{3}$$

has a matrix form, whose elements correspond to the energy needed to hop between neighbor sites, or hop to the same site – see fig. 2. As an example please analyze the script nanowire.ipynb.

2 Scattering by the potential

Tasks:

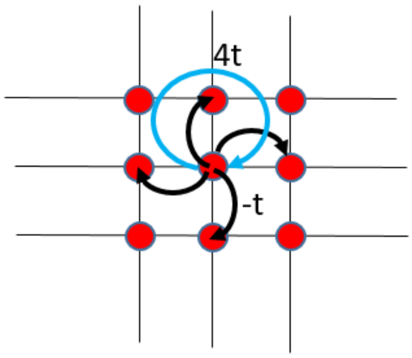

Figure 2: On-site and inter-site energies.

1. Using the example in the nanowire.ipynb file, add scattering potential to the system, with the form of a Gaussian centered in the middle of the nanowire
$$V(x,y) = V_0 \exp\left(\frac{-(x-x_0)^2 - (y-y_0)^2}{\sigma^2}\right), \tag{4}$$
assuming $V_0 = 50$ meV and $\sigma = 10$ nm.

2. Next, calculate the conductance as a function of energy, and the wave functions and current density at the incident electron energy $E = 30,\ 50,\ 100$ meV.

3 External magnetic field/Quantum Hall effect

Let us add transverse magnetic field to the system: $B = (0,0,B_z)$. Then, classically, the electron feels the Lorentz force, which is perpendicular to its velocity vector and the magnetic field vector, bending the electron trajectory. From the point of view of electrodynamics, the orbital effect from the magnetic field can be introduced in the equation replacing momentum by the so called canonical momentum

$$p \to \Pi = p - q\mathbf{A},$$

where $\mathbf{A}$ is the vector potential that satisfies

$$rot(\mathbf{A}) = \mathbf{B}.$$

The choice of the potential $\mathbf{A}$ is arbitrary (gauge invariance), so let us assume non-symmetric gauge in the form

$$\mathbf{A} = (-yB, 0, 0).$$

The Schrödinger equation takes the form

$$\frac{1}{2m^*}\left(\left(-i\hbar\frac{\partial}{\partial x} - eyB\right)^2 - \hbar^2\frac{\partial^2}{\partial y^2}\right)\psi(x,y) + V(x,y)\psi(x,y) = E\psi(x,y). \tag{5}$$

We could directly discretize this equation. However, a much better approach is to use the fact that the field introduces a phase factor to the solution, which depends on the vector potential and the path:

$$\psi(x,y) \to \psi(x,y)\exp\left(i\frac{e}{\hbar}\int_0^{\mathbf{r}} \mathbf{A}(\mathbf{r}')d\mathbf{r}'\right).$$

Thus, if we want to keep the equation (3) valid in the presence of external magnetic field, we need to multiply each matrix element by a phase factor, in the literature named the Peierls phase

$$t_{nm} \to t_{nm}\exp\left(i\frac{e}{\hbar}\int_{\mathbf{r}_n}^{\mathbf{r}_m} \mathbf{A}(\mathbf{r}')d\mathbf{r}'\right).$$

Tasks:

1. Derive the Peierls phase for the non-symmetric gauge in the form $\mathbf{A} = (-yB_z, 0, 0)$
2. Input the Peierls phase into the program (multiply the hopping terms by the correct factor).
3. In the system without any scattering potential plot the dispersion relation $E(k)$ in the left contact at $B_z = 2$ T, assuming the width of the nanowire $2W = 80, 200$ nm. What can you see? How to interpret it?
4. At $B_z = 2$ T and $2W = 200$ nm plot the conductance as a function of energy.
5. Show (by plotting) the wave function of the lowest state (energy slightly above the first step), when the electron is input from the left and right contact.

4 Y-shaped junction

As mentioned in the previous section, electron flowing through the nanodevice feels the Lorentz force. We can design a device, which allows us to steer the electrons with magnetic field to a selected output. To this end, we will study a Y-shaped junction (Fig. 3).

Tasks:

1. Using the KWANT documentation [click here] define a nanodevice in a shape of a Y-junction, as presented in Fig. 3, with the dimensions $R_1 = 60$ nm $R_2 = 120$ nm, $W = 60$ nm , $L = 100$ nm.

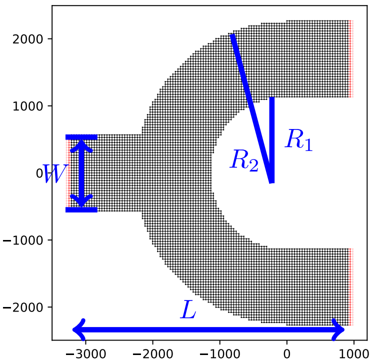

Figure 3: Scheme of the Y-junction.

2. Calculate the dispersion relation in the left channel at $B = 0$.
3. With the incident electron energy within the third subband ($E \approx 0.1$ eV), plot the conductance from the left lead to the upper and lower right lead as a function of magnetic field B_z, at field range $[0, 10]$ T. What do you observe?
4. At selected magnetic field (corresponding to the smooth conductance range as well as the plateau) calculate the current density. Do electron follow the Lorentz force action?