Department of physics, NTNU
TFY4340/FY8909 Quantum transport theory

Exercise set 2

Handed out: 04.03.24
Deadline: 25.03.24

1. **Coulomb honeycomb**

A double single-electron transistor (SET) is shown in Fig. 1. Two metallic islands are coupled to the outside world through tunnel junctions characterized by capacitances $C_{L(R)}$, and through the ideal capacitors with tunable gate voltages $V_{g1(2)}$. The islands are coupled to each other through a tunnel junction characterized by capacitance C_{12}.

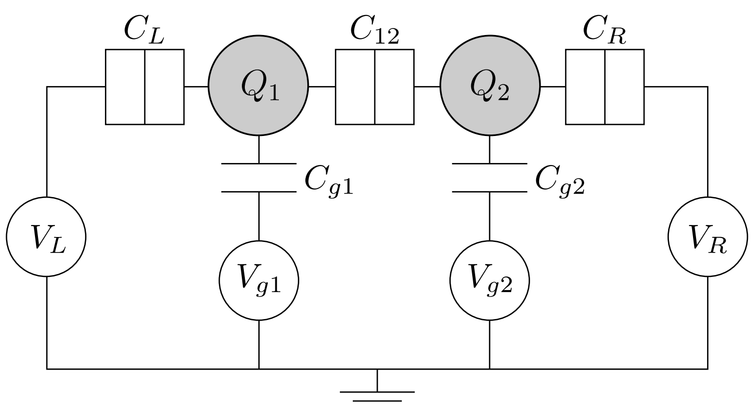

Figure 1: A double single-electron transistor. The gray areas show the two islands on which the quantized charges Q_1 and Q_2 reside.

By tuning the gate voltages, we can change the number of electrons N_1 and N_2 residing on each island, and thus the net charges $Q_1 = -N_1|e|$ and $Q_2 = -N_2|e|$.

In the lecture on Coulomb blockade, we generalized our result for the equilibrium energy of the single SET to

$$U(N_1, N_2) = \sum_{i,j=1,2} E_C^{(i,j)} \left(N_i - \frac{q_i}{e}\right)\left(N_j - \frac{q_j}{e}\right), \tag{1}$$

for the case of the double SET, where $E_C^{(i,j)}$ is the charging energy matrix. Using the notation from Fig. 1, one can derive that

$$E_C = \frac{e^2}{2(C_1C_2 - C_{12}^2)} \begin{pmatrix} C_2 & C_{12} \\ C_{12} & C_1 \end{pmatrix}, \tag{2}$$

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} C_L & C_{g1} & 0 & 0 \\ 0 & 0 & C_{g2} & C_R \end{pmatrix} \begin{pmatrix} V_L \\ V_{g1} \\ V_{g2} \\ V_R \end{pmatrix}, \tag{3}$$

where

$$C_1 = C_L + C_{g1} + C_{12}, \tag{4}$$
$$C_2 = C_R + C_{g2} + C_{12}. \tag{5}$$

Assume that the double SET is not voltage biased, i.e., $V_L = V_R = 0$, such that we can set the chemical potentials of the left and right leads to zero, $\mu_L = \mu_R = 0$.

(a) Using the set of parameters

$$C_L = C_R = 0.2\,\frac{|e|}{\mathrm{mV}}, \quad C_{g1} = C_{g2} = 0.3\,\frac{|e|}{\mathrm{mV}}, \quad C_{12} = 0, \tag{6}$$

and using your favorite software package, plot the boundaries of the region in the plane of (V_{g1}, V_{g2}) where $N_1 = N_2 = 1$ is the ground state. Comment on the shape you found.

(b) Using the same parameters as before, but now including a finite inter-island capacitance $C_{12} = C_L$, plot again the boundaries of the region where $N_1 = N_2 = 1$ is the ground state. Comment on the changes in the shape of the region.

2. **Universal conductance fluctuations**

This task involves a small numerical experiment, simulating the transport through a randomly disordered conductor. The model we are going to use is sketched in Fig. 2(a): We assume that we have a (quasi-)one-dimensional disordered conductor that is connected to a source and a drain reservoir. The disorder manifests itself as a set of randomly placed impurities (which we treat as point scatterers), as indicated by the small black dots. In the end, the goal is to calculate the *total* scattering matrix that relates the N channels on the far left (source) side to the N channels on the far right (drain) side, for a given fixed impurity configuration. From that matrix we can calculate the total conductance of the conductor, for that specific disorder configuration. Finally, repeating the calculation for many random disorder configurations, we can get an idea of the average conductance as well as the typical fluctuations in the conductance.

We will go through this step by step, and do not worry if your code does not fully work in the end, just sketch how you decided to approach the different parts of the problem.

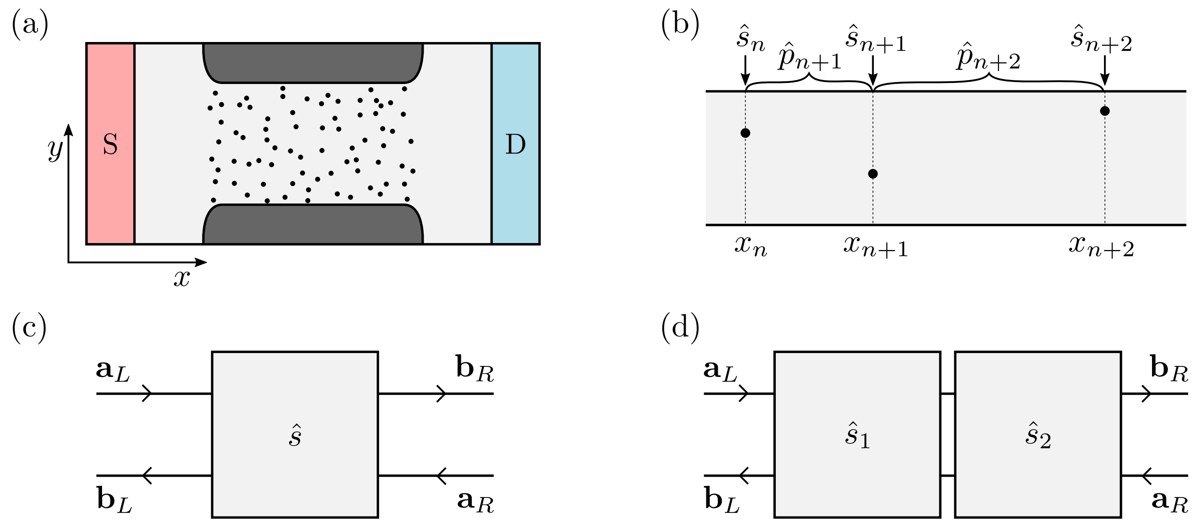

Figure 2: (a) Cartoon of the model we are using: An otherwise perfect one-dimensional conductor with N transmission channels contains a randomly configured set of point scatterers. (b) Zooming in on the conductor, we split the system into parts where the electrons propagate freely and points where they meet an impurity. (c) Illustration of the labeling of the incoming and outgoing amplitudes we will use. (d) Visualization of how two neighboring scatterers with $\hat{s}_1$ and $\hat{s}_2$ could be jointly described with a single scattering matrix that connects the incoming and outgoing amplitudes at the far left and right.

(a) In Fig. 2(b) we zoom in on a very short part of the conductor, only containing a few impurities, located at positions x_n, x_{n+1}, etc. Our approach will be to divide the conductor into a large number of segments, such that we can write down the scattering matrix for each segment:

   i. For each impurity we will use a scattering matrix $\hat{s}_n$ that transmits an incoming electron in channel m to the same outgoing channel m with large probability, or scatters it into any of the other outgoing channels with small but equal probabilities. For simplicity we will use the same scattering matrix for all impurities.

   ii. The "clean parts" in between impurities are modeled using scattering matrices that describe free propagation, $\hat{p}_n$, where an electron with wave number k_m acquires a phase factor $\exp\{ik_m(x_n - x_{n-1})\}$, which depends on the distance between the two neighboring impurities.

   To find the total scattering matrix for the conductor, we thus need to combine a large number of scattering matrices in series. The most convenient matrix structure to work with (for numerical reasons) is

$$\begin{pmatrix} \mathbf{b}_R \\ \mathbf{b}_L \end{pmatrix} = \begin{pmatrix} t & r' \\ r & t' \end{pmatrix} \begin{pmatrix} \mathbf{a}_L \\ \mathbf{a}_R \end{pmatrix}, \tag{7}$$

   which connects incoming and outgoing amplitudes such as illustrated in Fig. 2(c) (note that the structure is very similar, but slightly different from what I used in the lectures). Because this matrix connects *incoming* to *outgoing* modes and not modes on the *left* and *right* side of the scattering region, we cannot combine serial scattering regions by applying matrix multiplication: If we would want to find the matrix that connects the **a**'s and **b**'s in Fig. 2(d), it is *not* simply $\hat{s}_{\text{tot}} = \hat{s}_1\hat{s}_2$.

Find the right relation between the total scattering matrix $\hat{s}_{\text{tot}}$ and the blocks describing transmission and reflection in the two separate matrices $\hat{s}_{1,2}$, i.e., express the $N \times N$ matrices t_{tot}, r'_{tot}, r_{tot} and t'_{tot} in terms of the $N \times N$ matrices t_1, t_2, r'_1, r'_2, r_1, r_2, t'_1 and t'_2 such that the total matrix correctly connects the **a**'s and **b**'s such as sketched in Fig. 2(d).

Note: The paths "in between" $\hat{s}_1$ and $\hat{s}_2$ in this formalism are of zero length, so the outgoing amplitudes on the right side of $\hat{s}_1$ are *exactly* equal to the incoming amplitudes on the left side of $\hat{s}_2$. The regions of free propagation between the impurities we will describe with their own scattering matrices $\hat{p}_n$, as mentioned above, where the word "scattering" now might be slightly confusing because the $\hat{p}_n$ do not describe any actual scattering, only free propagation.

We will use the notation

$$\hat{s}_{\text{tot}} = \hat{s}_1 \otimes \hat{s}_2, \tag{8}$$

for this relation between these matrices. Note that $\otimes$ in this notation does *not* mean a regular tensor product; it is just short-hand for "form the correct total scattering matrix that describes scattering through $\hat{s}_1$ and $\hat{s}_2$ in series."

Hint: To make this exercise a bit more foolproof: The correct answer for the upper left block is

$$t_{\text{tot}} = t_2(1 - r'_1 r_2)^{-1} t_1,$$

so if this is what you found, then you are doing it right.

(b) Now that we found the right way to "glue" scattering matrices together, we can investigate the separate components. Write down $\hat{p}_n$ in terms of the k_m (the channel-dependent wave number of the electrons contributing to the current) and the set of coordinates $\{x_n\}$.

(c) For all $\hat{s}_n$ we will use $\hat{s} = e^{i\alpha D}$ with D a $2N \times 2N$ matrix where all elements are 1 and α is a small real number. What does the limit $\alpha \to 0$ correspond to? Explain why this choice for $\hat{s}$ guarantees unitarity of the scattering matrix for any α.

(d) Now we are in business. Assuming $N = 30$ channels present and hard-wall (inifite-well) boundary conditions for the transverse part of the wave function (along y), I propose to use

$$k_m = C\sqrt{(30.5)^2 - m^2}, \tag{9}$$

where $1 \le m \le 30$ and C is an unimportant prefactor with dimensions m^{-1}, which we will set to 1 in the following. Explain how this choice for k_m is consistent with the hard-wall boundary conditions and with $N = 30$.

(e) Generate a set of 600 coordinates $\{x_n\}$ for impurity locations picked randomly from a uniform distribution ranging from $x = 0$ to $x = 60\,000$. This will make the average spacing between the impurities approximately 100 (in units of $1/C$ to be precise). Transform this to a set of 601 lengths of "clean" regions, that will enter the $\hat{p}_n$.

(f) Now you can construct the 601 matrices $\hat{p}_n$ and, after choosing α, the matrix $\hat{s}$. Set $\alpha = 0$ and calculate numerically the total scattering matrix

$$\hat{s}_{\text{tot}} = \hat{p}_1 \otimes (\hat{s} \otimes (\hat{p}_2 \otimes (\hat{s} \otimes (\cdots \otimes (\hat{p}_{600} \otimes (\hat{s} \otimes \hat{p}_{601})))))). \tag{10}$$

The parentheses are included to avoid suggesting that the operator $\otimes$ is associative, which it is not. If this remark confuses you, think again about what you solved in part (a) and how you should treat the solution.

Extract the total transmission probability from $\hat{s}_{\text{tot}}$; look at Eq. (7) to remind yourself of the structure of the scattering matrices in this exercise. What do you find for the conductance of the conductor? Can you explain the value you found?

(g) Now set $\alpha = 0.035$ and repeat the calculation 200 times, every time using a different random disorder configuration [see part (e)]. Plot the resulting conductances (simply a scatter plot of the 200 conductances as a "function" of disorder configuration number). Show the plot and give the average conductance and the variance in the conductance.

(h) Finally, we will do the same calculation, but now assuming *incoherent* transport. We implement the absence of quantum coherence by using pure *probability* scattering matrices $\hat{S}$ and $\hat{P}_n$ that are defined as

$$[\hat{S}]_{k,l} = |[\hat{s}]_{k,l}|^2 \quad \text{and} \quad [\hat{P}_n]_{k,l} = |[\hat{p}_n]_{k,l}|^2, \tag{11}$$

i.e., all matrix elements are replaced by their magnitude squared, thus throwing out all information about the phase of the electronic wave functions traveling through the conductor. Obviously, now we find for all propagator matrices $\hat{P}_n = 1$, so the total probability scattering matrix is now

$$\hat{S}_{\text{tot}} = \hat{S} \otimes (\hat{S} \otimes (\cdots \otimes \hat{S})) = (\hat{S})^{\otimes 600}, \tag{12}$$

assuming that you understand my creative notation at the end.

Calculate the conductance using this total probability matrix for $\alpha = 0.035$.

Hint: Pay attention in the last step, when extracting the total transmission probability from $\hat{S}_{\text{tot}}$.

(i) Compare the numbers you found in (g) and (h) and explain how they (hopefully) agree with the conclusions of lecture 8. (If in doubt what I mean, look at the last slide of lecture 8.)

(j) Include the code you wrote (this will not be graded, but it could help me, for instance, in seeing that you got the point of the exercise but just got stuck in bugs or so).