Homework assignment 6
Basics of semiconducting quantum dots and charge qubits

Semiconducting & Superconducting Quantum Computers

Due: Dec 13th, 2022

Problem 1 - Magical numbers in a circular quantum dot (20 pts / collaboration is encouraged)

In this problem, we numerically solve the eigenvalue problem of a circular quantum dot in GaAs, determine the orbital energies and estimate the charging energy of the dot. From this quantities, we can find the discrete gate voltage values when the dot can support electrical current, i.e. when this single electron transistor is turned on/off.

First, assume that the potential in a circular dot is well approximated by a harmonic potential and the electrons are spinless. If the dot is located in the $x-y$ plane, with its center at the origin, the potential is minimal at the center, while it increases quadratically with the distance from the center of the dot: $V(x,y) = \frac{1}{2}m\omega^2(x^2+y^2)$. Here, ω is determined by the electrostatic environment, and we take it as $\omega = 2\pi 200$ GHz. Although this two-dimensional isotropic harmonic oscillator is a simple model, it is a very good approximation for real dots. Thus, the full Hamiltonian of the circular quantum dot reads as

$$H_{\text{dot}} = -\frac{\hbar^2}{2m}\left(\partial_x^2+\partial_y^2\right) + \frac{1}{2}m\omega^2(x^2+y^2), \tag{1}$$

where m is the mass of the electron in GaAs, which is reduced compared to the free electron mass, $m = 0.063m_e$.

Our goal is to numerically solve this Hamiltonian. Feel free to take a look at the example on Canvas for the case of the square dot with hard walls to get hints. Here, we also go through the main steps of carrying out the numerical calculations. In a numerical approach, we need to introduce a discrete and finite grid in the $x-y$ plane, and solve the Hamiltonian on this grid. The boundaries of the grid for both x and y coordinates are $(-L/2, L/2)$, and we divide this interval to N points, so the distance between the grid points in both directions are $\Delta x = \Delta y = L/N$. For this problem, taking L values of a few hundreds of nanometers is a good choice, because it is a few times bigger than the expected size of the quantum dot. The wavefunctions can be approximated by their discretized version $\psi(x,y) \approx \psi(i,j)$, where $x \approx i\cdot\Delta x$ and $y \approx j\cdot\Delta y$.

a) After introducing the grid, we need to define the operators which act on the wavefunctions. For example, focusing on one dimension of the wavefunction, we can express the derivative operator $\underline{\underline{D_x}}$ as a block-diagonal matrix.

$$\frac{d}{dx}\psi(x) \approx \frac{\psi(x_{i+1})-\psi(x_{i-1})}{2\Delta x} = \underline{\underline{D_x}}\cdot\underline{\psi}, \tag{2}$$

where

$$\underline{\psi} = \begin{pmatrix} \psi(1\cdot\Delta x) \\ \psi(2\cdot\Delta x) \\ \dots \\ \psi(N\cdot\Delta x) \end{pmatrix}.$$

and

$$\underline{\underline{D_x}} = \frac{1}{2\Delta x}\begin{pmatrix} 0 & 1 & 0 & \dots & \dots \\ -1 & 0 & 1 & 0 & \dots \\ 0 & -1 & 0 & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & -1 & 0 \end{pmatrix}.$$

Show that the second derivative operator $\underline{\underline{DD_x}}$ can be approximated also by a block diagonal matrix

$$\frac{d^2}{dx^2}\psi(x) \approx \underline{\underline{DD_x}}\cdot\underline{\psi}, \tag{3}$$

where

$$\underline{\underline{DD_x}} = \frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & \dots & \dots \\ 1 & -2 & 1 & \dots \\ 0 & 1 & -2 & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & 1 & -2 \end{pmatrix}.$$

Note that if we consider the two-dimensional case, the operators acting on the full two-dimensional space are the Kronecker delta products of the operators of the individual coordinates. For example, $\partial_x^2 \leftrightarrow \underline{\underline{DD_x}} \otimes I$, or $\partial_y^2 \leftrightarrow I \otimes \underline{\underline{DD_y}}$, or $x^2 \leftrightarrow \underline{\underline{x^2}} \otimes I$.

b) Write down the Hamiltonian in a numerical form (preferable in Python). Note that it is a good idea to use sparse matrices since most of the values of the matrix are zeros. See the example on Canvas for syntax. (Of course, you can use other platforms than Python if you prefer.)

c) Find the eigenvalues and eigentstates of the Hamiltonian. Plot the first few eigenstates in a 2D plot, and the eigenenergies as a function of the state index (upto level 25). At which states do you get degeneracies? These states corresponds to filling up the same shell of the artificial atom. With this, we calculated the orbital energies of the dot.

d) Now we estimate the charging energy of the dot. First, assume that the dot size corresponds to the radius which contains 99.9% of the amplitude square of the ground state wavefunction. What is this radius? Then, for simplicity, we consider a case when the gate electrode is 10 nm below the dot in GaAs ($\epsilon_r = 12.9$), and has the same diameter as the dot, so we can assume that the capacitance of the dot comes from this parallel plate capacitance with area of the dot size, and plate distance of 10 nm. What is the capacitive energy of the dot in meV?

e) Now, we can calculate the chemical potential μ for the dot as a function of the number of electrons N. Plot $\mu(N)$ for the first 25 electrons.

f) To better visualize the structure of the chemical potential, it is helpful to calculate the difference between the chemical potentials of neighboring states, and define the addition energy as $E_{\rm add}(N) = \mu(N+1) - \mu(N)$. This quantity corresponds to the voltage increments that is required to add electrons to the dot. When we fill the same shell in the dot, $E_{\rm add}(N)$ is constant as we need to pay only the constant charging energy and constant orbital energy for adding an electron to the dot. When $E_{\rm add}(N)$ has a jump, it indicates that the electron was placed at a higher shelf (we need to pay both the charging energy and a higher orbital energy). The electron numbers where these jumps happen are the magical numbers. What are the magical numbers in this dot?

Problem 2 - Simulating a non-adiabatic gate in the charge qubit (20 pts / collaboration is encouraged)

In a charge qubit, which is realized in a capacitively coupled double quantum dot system at certain gate voltages, the energy levels of the qubit can be described by the following Hamiltonian:

$$H_{\rm qubit} = -\epsilon\sigma_z + t\sigma_x, \tag{4}$$

where ϵ is an effective gate voltage, t is the (negative) tunneling amplitude, and σ_i are the Pauli matrices in the basis of having the electron sitting in the left ($|L\rangle$) or the right dot ($|R\rangle$). Here, we define the qubit at the gate voltages of $\epsilon = 10t$.

a) Find the eigenstates of the qubit in the basis of $\{|L\rangle, |R\rangle\}$, when $\epsilon = 10t$. How good approximation is it that $|0\rangle = |L\rangle$ and $|1\rangle = |R\rangle$? Regardless, we will take this approximation for the rest of the problem.

b) Assuming that we initialized the qubit in the $|0\rangle = |L\rangle$ state, we move the gate very quickly from the initial $\epsilon = 10t$ to $\epsilon = \delta$ value, and we keep the gate voltages fixed for the time t_p. In this case the Hamiltonian describing the evolution of the qubit is

$$H_{\rm gate} = -\delta\sigma_z + t\sigma_x. \tag{5}$$

So we have an initial state $|0\rangle = |L\rangle$, a Hamiltonian $H_{\rm gate}$, and a time t_p while the Hamiltonian influences the behavior of the qubit. Using QuTip, create a two-dimensional plot that shows the expectation value of finding the qubit in the excited $|1\rangle = |R\rangle$ state as a function of δ and t_p. The parameters are $t = -2\pi \cdot 0.5$ GHz, $\delta = -2\pi \cdot 5$ GHz... $+ 2\pi \cdot 5$ GHz (101 points), and $t_p = 0$ ns...2 ns (101 points). *Hint:* This Hamiltonian is identical to a Rabi Hamiltonian in the RWA-approximation, a problem that we already solved numerically before in QuTip. You might find it helpful to look at previous examples for qubit evolution on Canvas.

c) Carry out the simulation in the presence of decay and pure dephasing (T_1=1 ns, T_ϕ=1 ns).

Alternative Homework
(35 pts / no collaboration, instead of solving Problems 1-2)

1. Explain the idea behind the semiconducting quantum dots, charge qubits, spin qubits and their control. (3 pages, single spaced).