Computational Essay: "Quantum dot" charge qubits in semiconductors

Introduction

The goal of this assignment is to build your computational skill set by numerically solving the Schrodinger equation and to build up an understanding of semiconductor charge qubits based on your simulations. In addition to writing/modifying Python code, you have to assess the quality of your solutions, identify numerical artifacts that affect your solution, make your own decisions about relevant parameter ranges to explore, and finally relate your solution to the physics of qubits. Another important goal of the task is to develop your ability to communicate your results in writing for a scientific community. A set of sub-tasks are listed below to guide you through the basics of this assignment.

Task description

Mathematical Model: A quantum bit or qubit is a two-level quantum system that forms the basis states for computation. You can represent them as a '0' and a '1' in analogy to a classical bit, and associate these with two energy levels and their corresponding wavefunctions. Distinct from a classical bit that can assume a '0' or a '1' state at a time, a qubit, on the other hand, can simultaneously assume both states, a property known as "superposition" in quantum mechanics. Mathematically, this means a qubit state $|\psi\rangle$ assumes a form $|\psi\rangle = a|0\rangle + b|1\rangle$, where a, b are complex numbers such that $\sqrt{|a|^2 + |b|^2} = 1$ (normalized). A measurement on this state should be able to distinguish between $|0\rangle$ and $|1\rangle$, and will obtain a $|0\rangle$ outcome with probability $|a|^2$ and $|1\rangle$ with $|b|^2$. A quantum logic gate/operation controls the superposition between $|0\rangle$ and $|1\rangle$ in a desired manner. For example, a quantum X operation on $|\psi\rangle$ flips the state of the qubit resulting in $a|1\rangle + b|0\rangle$ (like classical NOT operation), while a quantum phase gate (S) generates a phase θ between $|0\rangle$ and $|1\rangle$, such that $S|\psi\rangle = a|0\rangle + be^{i\theta}|1\rangle$. For example, the Pauli-X matrix, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, can denote an X-gate operation, as $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} b \\ a \end{pmatrix}$.

A two-level quantum system mapped to the qubit can be modelled by the Hamiltonian, $H = \begin{bmatrix} E & t \\ t^* & -E \end{bmatrix}$, where E and t are parameters that will depend on the physical system. This can be generated from linear combinations of Pauli matrices

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

Part A

Either analytically or numerically, solve the eigenvalues (E_1 & E_2) and eigenvectors (ψ_1 & ψ_2) of the above 2×2 qubit Hamiltonian H. Plot or sketch the two energy levels (eigenvalues) as a function of the variable E (for some reasonable choices of E & t, you may assume that t is a real number). What is the minimum value of $E_2 - E_1$ (in terms of t)? Plot/Sketch the probability of measuring '0' and that of '1' for the two wavefunctions (eigenvectors) as a function of E. Note, for a normalized eigenvector $\psi_1 = c_1|0\rangle + c_2|1\rangle$, and $\psi_2 = c_3|0\rangle + c_4|1\rangle$, you should plot the 4 probabilities and label them appropriately. For example, the probability of measuring a '0' in the state ψ_1 is $|c_1(E,t)|^2 = |\langle\psi_1|0\rangle|^2$. Note, t in this part does not represent time.

Now, let us try to engineer this Hamiltonian in a real system, such as a metal-oxide-semiconductor (MOS) device used in silicon quantum computing (shown in Figure 1). The electrostatic potential of

each metal gate (G_1, G_2) traps an electron in 3D near the surface of silicon (^{28}Si) and forms what is called a "quantum dot" (QD), which can also be thought of as an "artificial atom". Using the discrete quantum states of the trapped electron, qubits can be implemented in a number of ways. Choosing a basis of '0' and '1' means we need to select two energy levels and be able to control their superposition. We also need to make sure these levels are sufficiently isolated from other energy levels in the system. Leakage into other states outside these two basis states may cause decoherence & relaxation (the loss of quantum information), which is detrimental to quantum computing.

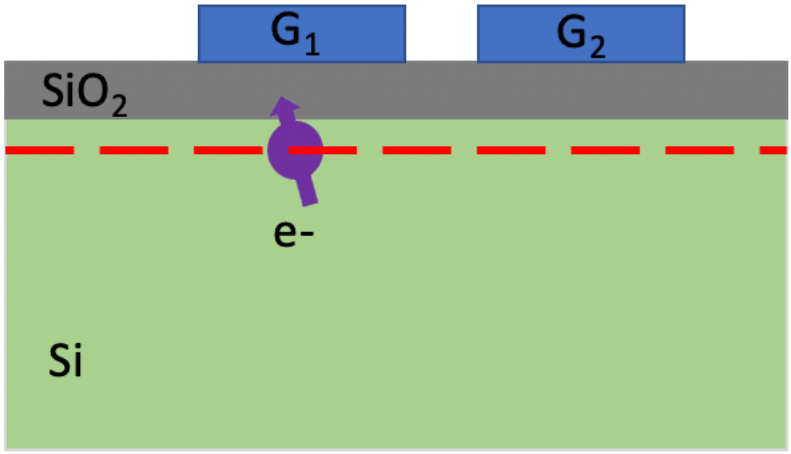

Figure 1 Double Quantum Dot device in silicon with a trapped electron under gate G_1. Either the charge or the spin of the electron can be used to encode quantum information. An insulating dielectric SiO_2 separates the metal gates from Si.

Here, we will investigate a "charge qubit", which uses the localization of the electronic charge to define a two-level quantum system. Whether the electron is localized in the left QD ($|L\rangle$) or right QD ($|R\rangle$) can be measured by a nearby charge sensor (usually through an electrostatic shift in current flowing between two metal contacts). So, the two-level basis for this qubit can be encoded as $|0\rangle = |L\rangle$ and $|1\rangle = |R\rangle$. This means we can use one energy level (the ground state) per QD. By applying voltages to gates G_1 and G_2, the electron can be moved from one dot to another. Device engineers can also control the spacing between the gates during fabrication. This controls the separation between the dots. Let us first implement and solve a simple model of this device using a 1D (time independent) Schrodinger equation with the finite difference technique. The x-direction will be taken along the dotted red line of Figure 1. With energy eigenvalue E and wavefunction $\psi(x)$, the equation to be solved is

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

For each QD, the electrostatic potential from the gates along the separation axis can be approximated as a parabolic potential of the form $V(x) = \alpha(x - x_1)^2$, where x_1 is the centre of the QD, and α is a constant that defines the curvature of the potential. x denotes the separation axis of the dots. For a double quantum dot (DQD), the potential can be approximated as $V(x) = \min[\alpha(x - x_1)^2, \alpha(x - x_2)^2]$, where x_1 and x_2 are the centres of the two QDs. The 'min' function returns the minimum of two numbers. You are provided a Python code for the time independent Schrodinger equation in 1D with a "particle in a box" potential discretised and solved by the finite difference method. The code assumes energies in eV and distances in nanometres (nm). Let us assume the quantum dots are in silicon so that the effective mass of electrons, $m^* = 0.2\, m_0$, where m_0 is the electron rest mass.

Change the code or write your own code to implement the single QD and double QD potential and solve the 1D Schrodinger equation with finite difference method to answer the following questions.

Part B

(i) First, solve the single QD, and obtain the lowest two eigenvalues and wavefunctions. Plot the two probability distributions as a function of x. Plot the difference between the two eigenvalues as a function of α (choose suitable ranges at your discretion). If we want to engineer an energy splitting of about 4 meV (approximately) between these two states, what value of α should we choose? Discuss how you think α can be engineered in a real device. What temperature ranges would you expect these qubits to operate at, and why? [Note: you are essentially solving the 1D quantum harmonic oscillator numerically. So, you may want to compare your results to analytic solution for sanity checking.]

(ii) How did you ensure in (i) that your results do not suffer from various numerical artifacts, such as small simulation domain (artificial confinement), inaccurate meshing, and any other issues you can think of? Provide evidence of the tests that you performed.

(iii) Quantum dots are often called 'artificial atoms'. Can you reason why? Compare the length scale of the wavefunction to the Bohr radii of the ground state of a Hydrogen atom (by choosing a similar measure). If the atoms in a silicon crystal along a 1D chain are spaced by 0.543 nm, over how many atoms does a QD (ground state) wavefunction span for energy splitting of about 4 meV as in B(i)?

Part C

(i) Plot the two lowest energy wavefunctions $\psi(x)$ and their corresponding probability distributions ($|\psi(x)|^2$) as function of x for a double quantum dot (DQD) for a choice of α (that produces about 4 meV level splitting for a single QD) and separation distance R between the dots (choose your values such that you cover two regimes of weak and strong interaction between the dots). What differences do you observe between the lowest two wavefunctions?

(ii) Plot the energy difference between the lowest two states of the DQD as a function of the centre-to-centre dot separation, $x_2 - x_1$, for the range of separations you investigated in (i). Which Hamiltonian parameter of the 2×2 matrix from Part A is modified by engineering the dot separation? Physically, in this system, what does this parameter represent, and would this also be present in a classical system? Explain your thoughts on whether a large or small dot-to-dot separation is desirable or whether there is an optimal separation.

(iii) Voltages applied to the two gates G_1 and G_2 are used to create an electric field in the x direction. This controls the localization of the electron between the two dots, and is called a "detuning" bias. We will model this by adding an extra potential energy term for a uniform electric (F) field $V(x) = F\,x$ to the DQD Hamiltonian. Plot the lowest two wavefunction probabilities ($|\psi(x)|^2$) (as a function of x) when there is small detuning bias. What happens when the sign of F is changed? Plot for suitable choices of F (in the order of mV) from positive to negative values, the lowest two eigenvalues, and their differences. Can you relate this to your analytic solution from Part A? Which parameter of the 2×2 Hamiltonian is controlled by this detuning bias? From your simulations, can you identify a range of F, over which the qubit can be operated?

Part D

(i) In practice, charge qubits are controlled by a time varying detuning potential that periodically moves the electron between the left and right dots. This creates an oscillation between the two qubit levels called a "Rabi oscillation". Model this with a numerical solution of the time dependent Schrodinger equation (TDSE) on a DQD subjected to a time varying potential $V(x,t) = F\ x\ \cos(\omega t)$, where F is an electric field value that you have to choose. Assume the system is in the ground state at the start. You may want to check the wavefunctions at several time intervals to make sure your code is working properly. Assume the system is resonantly driven with $\omega = \omega_R = \frac{E_1 - E_0}{\hbar}$ (i.e. the energy difference between the two lowest levels without any detuning bias). Let the two lowest energy states at $t = 0$ be the '0' and the '1' state of the qubit. Simulate time evolution at the qubit resonant frequency, for time between $t = 0$ and t_{max} (chosen to cover at least a full period of oscillation) with suitable timestep Δt. During simulation calculate and store projections of the wavefunction on $|0\rangle$ and $|1\rangle$ states as changing in time i.e. for each time step calculate $p_0(t) = |\langle 0|\Psi(t)\rangle|^2$ and $p_1(t) = |\langle 1|\Psi(t)\rangle|^2$ and store them in some list/array. Plot $p_0\ and\ p_1$ vs. time together in one figure for a fixed value of F. Discuss your findings when you explore the impact of various parameters. Discuss what steps you took to ensure convergence. [For part D, you are not restricted to the simulation parameters from parts B and C but can modify/adjust to make the time evolution work better. However, you must discuss your choice of parameters and reasoning.]

(ii) The resonant transition between the states occurs only at or close to the resonant frequency. When we move away from ω_r the transition becomes less and less probable. Repeat the simulation of (i) from part D for a chosen value of F, but now for the frequency $\omega = 0.95\omega_r$ and see how the oscillations differ in comparison to $\omega = \omega_r$ case. Discuss your findings.

Submission information and expectations

You are required to use Jupyter notebook for this assignment and write in a report format, with an intro/background, results/discussion, and conclusion sections. In the results/discussion sections, you must address the questions posed in this assignment, and show code segments and your findings in a step-by-step manner. Expected report length is roughly 15-20 pages with all plots and codes.

The computational essay will be marked holistically, i.e., based on the submission as a whole (just like the final lab report). We are looking for your ability to use computational tools and techniques to investigate and analyse important Physics problems. We are not looking for exact answers, but trends, reasonable ranges for quantities, and your ability to communicate scientific knowledge through writing. Hence, brevity and to the point discussions are valuable. We will be assessing based on these four categories with roughly equal weighting.

1. Completeness of the tasks (with evidence such as code, equations, etc.)
2. Quality and correctness of the figures and the results.
3. Quality of the write up (organization, format, soundness of arguments, references).
4. Analysis of results, understanding, insights.

To achieve marks in the HD range, we expect to see some creative extension beyond the task described above. To satisfactorily display such creativity, we would expect about 1–2 pages to be devoted to this extension activity, and it is sufficient to explore only one idea.

You can either use your own Python code or build on the template code I provided in the course website. You are free to use any packages in Python, but the method should utilize finite difference in matrix form. You must not use any other codes or packages outside Python. If further clarification is needed on this, I recommend contacting me by email rajib.rahman@unsw.edu.au.

You need to convert the output into a pdf and submit it through Moodle. The due date is Sunday **April 29, 2025, at 11:55 pm.**