1. Make a C-NOT gate using protons and NMR. (20 points)

The discussion of quantum logic operations that we had in class only briefly discussed how you might actually make any of the quantum logic gates. For example, we very briefly discussed how to make an X-gate, the single qubit gate that flips the qubit. This is the quantum NOT function. You can make it for example by having your qubit be a spin $\frac{1}{2}$ in a magnetic field. The two energy levels can be your two logical states. Electromagnetic waves with energy equal to the energy difference of the two-level system can drive transitions between the two levels. If you start in the ground state and turn on the EM wave for a brief time, you can move the state up into the higher energy state. Similarly, if you start in the high state, turn on the same EM field for the same time, you transfer the system to the low energy state. In nuclear magnetic resonance (NMR) this pulse of EM radiation is called a ‘Pi pulse’. I believe that you can say why …

In this problem, let’s sketch out at least some picture of how you might make a two-qubit controlled NOT or ‘C-NOT’ gate by using protons in some type of molecule.

In class and in Homework 1, we discussed the case of a spin $\frac{1}{2}$ in a magnetic field, with an applied field in the z-direction and of magnitude, $B_0$. Protons in such a magnetic field produce a two-level energy system, with a splitting between the two levels of $\gamma B_0 \hbar$. These levels came from a Hamiltonian that look like:

$$\hat{H} = -\gamma B_0 S_z$$

a) **Remind yourself:** The two-level system can be excited (or de-excited for that matter) by an applied electromagnetic wave. How does the angular frequency of electromagnetic field depend upon the applied magnetic field and the properties of the proton? Look up the required physical properties of the proton and explain at what frequency (in Hertz or Megahertz) you expect a proton to absorb electromagnetic energy if it sits in an applied magnetic field of 1 Tesla.

b) If you put a proton in a molecule, and chemists will do this type of thing all the time, then the magnetic field actually seen by the proton will depend upon what the nearby electrons are doing. Effectively, the various protons will ‘see’ slightly different magnetic fields and therefore absorb EM waves at slightly different frequencies. The relative shifts in frequency can be one part in $10^4$ of the resonance frequency and are easy to measure. Chemists refer to these as ‘chemical shifts’ and they use the shifts to infer the chemical environment around the protons.

Think about two particular protons in some molecule. Now we have two spin $\frac{1}{2}$ particles. I will refer to them as A and B. Let’s assume that they see slightly different magnetic fields, so that the Hamiltonian is approximately give by:
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\[ \hat{H} = -\gamma B_A S_{A,z} - \gamma B_B S_{B,z} \]

Pick a basis of two-particle product states, which are products of the single-proton eigen states of the \( S_z \) operators for the two different particles. Let’s label them as ‘spin-up’ or ‘spin-down’ for each of the particles. Show that these product states are the eigenvectors of the Hamiltonian and make a table of the eigen states and eigen energies.

c) To make a C-NOT gate, you want to have a machine that takes two qubits, call them \( |A\rangle \) and \( |B\rangle \) (these will be the two protons discussed above), and the machine should ‘flip B if A is set’. Look at the quantum logic cheat sheet to remind yourself of how the C-NOT logic is supposed to behave if things are fuzzy. Somehow, you want the state of the control qubit, A, to help flip qubit B. That means you want the two qubits to interact. In NMR systems, the protons often interact through a mechanism referred to as ‘Scalar coupling’ or ‘J-coupling’. Again, a proton talks to the electrons, the electrons talk to each other, and eventually talk to the other proton. Mathematically, the interaction behaves as though it cares mostly about the z-components of the spin. The Hamiltonian gets a new interaction term and looks like:

\[ \hat{H} = -\gamma B_1 S_{1,z} - \gamma B_2 S_{2,z} + JS_{1,z}S_{2,z} \]

where the ‘\( J \)’ is an energy that depends upon the molecule.

Show that this new Hamiltonian still has the same eigen states as in part b), but that the energy levels are different by making a table of the state vectors and the associated energy levels. Look at your result and explain how you could use the state of spin A, along with a Pi-pulse at the correct EM frequency to “flip B if A”.

You have just implemented a C-NOT gate with single qubits.

2. Perturbations to the infinite square-well. (15 pts.)

Griffiths Example 6.1 is all about seeing how first order perturbation theory works with the infinite square well as our \( H_0 \) and with various small extra potential energy bumps. Have a look at the discussion and then:

a) Griffiths first shows you how the energies are predicted to shift if you just raise the bottom of the box by some small amount, \( V_0 \). Of course, you know what’s going to happen, don’t you? Go back to the discussion of the infinite square well in Griffiths section 2.2. Set up a problem where the potential is \( V_0 \) in the box rather than zero in the box. Explain how the new energy levels and the new wave functions are related to the old results, Griffiths Equations 2.27 and 2.28.

b) Griffiths shows you that the first-order non-degenerate perturbation theory result for the expected energy shift (assumes the extra term in the Hamiltonian, namely \( V_0 \), is small) gives you the exactly correct result. Griffiths says, “Evidently for a
constant perturbation all the higher corrections vanish.” Use Equation 6.15 for the second-order energy shift to show that he is correct for the second order result.

c) Show that perturbation theory also gets the wave functions exactly correct. Explain qualitatively, why it is that the constant potential is expected to behave this way, getting everything correct after only the first-order in perturbation theory, for ANY well problem, as Griffiths claims in footnote 3 on page 252.

3. Griffiths Problem 6.5. (15 points)