P3317 HW from Lecture 7+8 and Recitation 4

Due Friday Tuesday September 25

Problem 1. In class we argued that an ammonia atom in an electric field can be modeled by a two-level system, described by a Schrodinger equation

$$i\hbar\partial_t \left(\begin{array}{c} \psi_L\\ \psi_R\end{array}\right) = \left(\begin{array}{cc} E_0 + \epsilon & -\Delta\\ -\Delta & E_0 - \epsilon\end{array}\right) \left(\begin{array}{c} \psi_L\\ \psi_R\end{array}\right).$$
 (1)

The constant E_0 plays no role in the dynamics: this is supposed to represent the energy when the Nitrogen atom is at one of its two potential minima. The term Δ accounts for tunneling, and ϵ is proportional to the electric field applied along the symmetry axis of the molecule.

Experiments show good agreement with this model, and the most accurate way to determine ϵ and Δ is not from a theoretical calculation, but by fitting the prediction of this model to experiment. One finds $\Delta = 10^{-4}$ eV, and $\epsilon = \mu \mathcal{E}$, where \mathcal{E} is the electric field strength. The proportionality constant is the electric dipole moment, $\mu = 1.6$ debye. A debye is the CGS unit for electric dipole moments: 1 debye= 3.3×10^{-30} Cm. A debye is a typical electric dipole moment for a molecule – it is equal to the charge of the electron times a distance of roughly 0.39 Bohr.

1.1. Derive an expression for the energy eigenvalues as a function of E_0 , Δ , and ϵ . Make a sketch of Energy vs ϵ for fixed E_0 and Δ . Please do not substitute in numbers – I just want to know the shape of the curve. Please do label the axes though. Unlike "graphing" problems, a hand-drawn sketch is fine here (though a computer generated one is also fine).

As an aside, you should see that one state is "high field seeking" – meaning its energy is lowest in regions of large field, while the other is "low field seeking". This property is what is used for creating an inverted population for an ammonia Maser.

1.2. Cavities vary greatly in the fields they contain. Some of the highest intensity microwave cavities are used in particle accelerators. For example, the next generation "Energy Recovering Linac" being built at Cornell has superconducting cavities with electric fields as large as 50 MV/m. For these extremely high-intensity cavities, how does ϵ compare with Δ ? [More concretely, what is the ratio ϵ/Δ ?] Would the perturbation theory we did in class be appropriate for these cavities? The original MASER experiments had much smaller fields.

Note, in the past I have found that some students do not have a very systematic approach to unit conversion. My *strong* recommendation is to keep all units at all stages of your calculation – and do the conversions by multiplying and dividing by ratios which equal 1. For example, if I wanted to convert 60 miles per hour into meters per second, I would look up on google that there are 1609 meters in 1 mile, and write

$$v = \frac{60 \text{ miles}}{\text{hour}} \times \frac{1609 \text{ m}}{\text{mile}} \times \frac{1 \text{ hour}}{60 \text{ minutes}} \times \frac{1 \text{ minute}}{60 \text{ s}} = 27 \text{ m/s.}$$
(2)

In fact, any time I am working with dimensional quantities, I write down the units, and carry them through all of the arithmetic. I can't tell you how many times I have tracked down an error by finding that the units don't work out properly. It makes me cringe when (even as an intermediate step) I see someone write something like v = 3, when v is supposed to be dimensional. Of course I am happy when students first explicitly adimensionalize their equations, then work simply with numbers.

Problem 2.

2.1. Two-level Hamiltonians, are often described in terms of 2×2 matrices

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{4}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{5}$$

Are these Hermitian, Unitary, both?

2.2. What are the eigenvalues of the Hamiltonian

$$H = E_0 \mathbf{1} + B_x \sigma_x + B_y \sigma_y + B_z \sigma_z, \tag{6}$$

where **1** is the identity matrix? No need to find the eigenvectors, I just want the eigenvalues as a function of E_0 and the vector B_x, B_y, B_z . This is a good result to remember (and I often calculate the eigenvalues of 2x2 matrices by writing them in this form).

2.3. The notation $\sigma_x, \sigma_y, \sigma_z$ comes from the fact that in the case of *spin*, the object $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ transforms under rotation as a vector. Feynman Lectures volume 3, chapter 6 works you through the logic that proves it. Furthermore, we can interpret the positive eigenvectors of Eq. (6) as a quantum state in which the spin is pointing in the direction of $\tilde{\mathbf{B}} = (B_x, B_y, B_z)$. You do not need to prove this, but it turns out that you can write this eigenstate as

$$|\hat{n}\rangle = \begin{pmatrix} \cos(\theta/2)e^{i\phi/2}\\ \sin(\theta/2)e^{-i\phi/2} \end{pmatrix},\tag{7}$$

where $\tan \theta = \sqrt{B_x^2 + B_y^2}/B_z$ and $\tan \phi = B_y/B_x$ describe the direction of the vector **B**. For convenience we label the state with the unit vector $\hat{n} = \tilde{\mathbf{B}}/|B|$.

What is the +z-eigenstate, $|\hat{z}\rangle$? [You can use Eq. (7), or go back to Eq. (6) – either is fine.]

2.4. What is the +x-eigenstate, |x̂⟩? [You can use Eq. (7), or go back to Eq. (6) – either is fine.]
2.5. What is the +y-eigenstate, |ŷ⟩? [You can use Eq. (7), or go back to Eq. (6) – either is fine.]

2.6. In class we introduced the notation $\langle \psi | \phi \rangle$ for the dot-product between two vectors in an abstract Hilbert space. In particular, if

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \tag{8}$$

$$|\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \tag{9}$$

then we define

$$\langle \psi | \phi \rangle = \psi_1^* \phi_1 + \psi_2^* \phi_2. \tag{10}$$

Calculate the overlap $\langle \hat{x} | \hat{z} \rangle$.

2.7. Find the overlap $\Lambda = \langle \cos(\theta_1)\hat{z} + \sin(\theta_1)\hat{x} | \cos(\theta_2)\hat{z} + \sin(\theta_2)\hat{x} \rangle$. Show that Λ is only a function of $\delta\theta = \theta_1 - \theta_2$.

This is a special case of a more general relation that $|\langle \hat{n} | \hat{n}' \rangle|$ is only a function of the angle between the two unit vectors \hat{n} and \hat{n}' .

Problem 3. In the next problem we will use the following integral

$$I = \int dx \frac{\sin^2 x}{x^2} = \pi. \tag{11}$$

Here you will verify that result using a trick called "integrating under the integral." [Apparently Feynman was fond of tricks like this.]

3.1. By integrating over t_1 and t_2 , show

$$I = \frac{1}{4} \int_{-\infty}^{\infty} dx \int_{-1}^{1} dt_1 \int_{-1}^{1} dt_2 \, e^{ix(t_1 + t_2)} \tag{12}$$

3.2. Perform the x integral in EQ. (12), using the identity

$$\int_{-\infty}^{\infty} dx \, e^{ixs} = 2\pi\delta(s). \tag{13}$$

3.3. Now the t_1 and t_2 integrals should now be straightforward. Perform them.

Problem 4. Although we did not spend much time exploring it, in class we showed that the probability of an ammonia atom absorbing radiation of detuning δ in time t is

$$P = 4\epsilon^2 t^2 \frac{\sin^2(\delta t/2)}{(\delta t/2)^2},$$
(14)

where ϵ is proportional to the electric field (so ϵ^2 is proportional to the intensity of the light, I_0 .) Imagine we have many ammonia atoms, and light of many frequencies. The total energy absorbed from the light in that time is then

$$E \propto I_0 t^2 \int d\delta \frac{\sin^2(\delta t/2)}{(\delta t/2)^2}.$$
(15)

Use the identity

$$\int dx \frac{\sin^2 x}{x^2} = \pi \tag{16}$$

to show that the absorbed **power** is a constant, independent of time.

Problem 5. Here we will use dimensional analysis to estimate the ionization energy of hydrogen. The various quantities which come to mind as being involved are: The ionization energy E_0 , the proton mass m_p , electron mass m_e , Coulomb's constant $k = e^2/(4\pi\epsilon_0)$, planck's constant h (or equivalently $\hbar = h/2\pi$. The physics is non-relativistic, so we don't expect to need c.

5.1. How many independent dimensionless quantities can you construct from these parameters? Write them down.

5.2. What is the most general expression for E_0 which only involves these scales, and is dimensionally consistent.

5.3. If we assume that m_p drops out, what do you find for the ionization energy? [Note, that as with any other dimensional argument, all you get is an order of magnitude.] Give a number in eV.

Problem 6. The Schrodinger equation for a simple harmonic oscillator reads

$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x) + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x).$$
 (17)

Rescale the variables so that $y = x/x_0$ and $E = \mathcal{E}/E_0$ to reduce this to the dimensionless equation

$$-\frac{1}{2}\partial_y^2\psi + \frac{1}{2}y^2\psi = \mathcal{E}\psi.$$
(18)

What is x_0 and E_0 ?

Problem 7. A typical model for the potential between two atoms is

$$V = \frac{\alpha}{x^{12}} - \frac{\beta}{x^6},\tag{19}$$

where α and β are constants which depend on the atom. This is often known as a "6-12" potential.

7.1. Sketch this potential.

7.2. What are the units of α and β ?

7.3. There is a unique length-scale r_0 you can make out of α and β . What is r_0 ?

7.4. Since there is only one length-scale here, the location of the minimum of V, must roughly be given by r_0 . Use calculus to find the location of the minimum r^* , and calculate r^*/r_0 .

Problem 8. Feedback

8.1. How long did this homework take?

8.2. Which of the following words come to mind when you think about this homework (feel free to add your own words if you have something better): frustrating, fun, tedious, insightful, hard, easy, useful, useless, fair, unfair