Creighton University | Professor G. Duda
Physics 531: Quantum Mechanics | Fall 2013

Project #3: Spin and Nuclear Magnetic Resonance

Stage 1 - Preliminary Calculation: Before we handle the more interesting and difficult case of NMR, we need to work out how a particle with spin behaves in a magnetic field. Let's choose the z-axis to be the direction of a constant and uniform magnetic field, $\vec{B} = B_0\hat{k}$, and take the charge of our spin 1/2 particle to be -e, that is, the electron charge. The Hamiltonian for this spin 1/2 particle in a magnetic field is given by:

$$\hat{H} = -\hat{\mu} \cdot \vec{B} = -\frac{ge}{2mc}\hat{S} \cdot \vec{B} = \frac{ge}{2mc}\hat{S}_z B_0 = \omega_0 \hat{S}_z,$$

where we've used Eq. 1.3 from Townsend to relate the magnetic moment of the spin 1/2 particle to its intrinsic spin and have defined $\omega_0 = geB_0/(2mc)$.

a) Suppose that our system starts in the state $|\psi(t=0)\rangle = |+x\rangle$. Find $|\psi(t)\rangle$.

b) Find the probability of our system at a time t later to be in the state $|+x\rangle$.

c) Find the probability of our system at a time t later to be in the state $|-x\rangle$.

d) Find $< \hat{S}_x >$ and show it oscillates in time.

e) Find the probability of our system at some time later t to be in the state $|+y\rangle$, $|-y\rangle$, and calculate $< \hat{S}_y >$.

f) Show that the expectation values for $\hat{S}_x$ and $\hat{S}_y$ obey

$$\frac{d}{dt} < \hat{A} >= \frac{i}{\hbar}\left\langle\psi|[\hat{H}, \hat{A}]|\psi\right\rangle$$

Stage 2 - The Rabi Paper: In his seminal paper (for which he wins the Nobel Prize) Rabi examines the behavior of a spin 1/2 particle in an oscillating magnetic field. We'll take the magnetic field to be (a bit simpler than what Rabi considers):

$$\vec{B} = B_1 \cos(\omega t)\hat{\imath} + B_1 \sin(\omega t)\hat{\jmath} + B_0 \hat{k}$$

In practice one uses a strong dipole magnet to make the constant field in the z-direction and something like a radio wave to created an oscillatory field in the x and y directions. Now, just like in Stage 1, our Hamiltonian is just $\hat{H} = \mu\hat{\vec{\sigma}} \cdot \vec{B}$.

a) First of all, show that in the usual S_z representation, the matrix representation of the Hamiltonian $\hat{H}$ is given by:

$$\mu \begin{pmatrix} B_0 & B_1 e^{-i\omega t} \\ B_1 e^{i\omega t} & -B_0 \end{pmatrix}$$

b) The whole point of the Rabi paper is that he solves the time dependent Schrodinger Equation for a spin in a time dependent magnetic field. We want to duplicate his results. Rabi writes the spin state of the particle at a given time t as

$$|\psi(t)\rangle \rightarrow \begin{pmatrix} C_{1/2} \\ C_{-1/2} \end{pmatrix}$$

where both $C_{1/2}$ and $C_{-1/2}$ are time dependent. In Dirac notation this just looks like

$$|\psi(t)\rangle = C_{1/2}(t)|{+z}\rangle + C_{-1/2}(t)|{-z}\rangle$$

We want to solve for $C_{1/2}(t)$ and $C_{-1/2}(t)$.

As a first step, show that the time dependent Schrodinger Equation can be written as:

$$\begin{pmatrix} \omega_0 & \omega_1 e^{i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix} \begin{pmatrix} C_{1/2} \\ C_{-1/2} \end{pmatrix} = 2i \frac{\partial}{\partial t} \begin{pmatrix} C_{1/2} \\ C_{-1/2} \end{pmatrix}$$

In the above equation we've let $\omega_0 = 2\mu B_0/\hbar$ and $\omega_1 = 2\mu B_1/\hbar$.

c) We want to solve the T.D.S.E. above subject to the initial condition that the state at $t = 0$ is an eigenstate of S_z with the eigenvalue $+\hbar/2$, i.e. $|{+z}\rangle$. What should $C_{1/2}$ and $C_{-1/2}$ be at $t = 0$?

d) Follow the method presented in the paper to solve this coupled set of first-order D.E.s. Show that your solution is given by

$$|\psi(t)\rangle \rightarrow \begin{pmatrix} e^{-i\omega t/2}\left[\frac{-i}{\delta}(\omega_0-\omega)\sin(\delta t/2)+\cos(\delta t/2)\right] \\ e^{i\omega t/2}\left(\frac{-i\omega_1}{\delta}\right)\sin(\delta t/2) \end{pmatrix},$$

where

$$\delta = \left(\omega^2+\omega_0^2+\omega_1^2-2\omega\omega_0\right)^{1/2} = \left((\omega-\omega_0)^2+(\omega_1)^2\right)^{1/2}$$

e) What is the probability that a measurement of S_z at time t will yield the value $-\hbar/2$?

f) In this whole problem and in the whole class, we have been treating the magnetic field classically. However, we can get a glimpse of how the quantum EM field comes in if we recall (from Einstein) that photons carry an energy $E = \hbar\omega$. Show that, at resonance, the energy $\hbar\omega$ of one photon from the oscillating EM field is the difference in energy between the $S_z = \hbar/2$ and $S_z = -\hbar/2$ states due to their orientation with respect to B_0! Hence we can interpret the change in the probability of part e) as due to transitions between spin-up nd spin-down, which are caused by absorbing and emitting photons.