PHYS 487 – Homework 3 due **Friday Sep 18** at **midnight**

Problem 1 : The Rigid Rotor

Two particles of mass m are attached to the ends of a massless rigid rod of length a. The system is free to rotate in three dimensions about its center of mass (CM), but the CM point itself is fixed.

(a) What is the energy spectrum of this "rigid rotor"?

▶ Massive hint: First express the Hamiltonian in terms of the total angular momentum of the rotor.

(b) What are the normalized eigenfunctions for this system? What is the degeneracy of the n^{th} energy level?

Problem 2 : Spin ½ Particle in a Constant B-field

A negatively-charged spin-½ particle is at rest in a constant, uniform magnetic field $\vec{B} = B_0\,\hat{z}$ of external origin, where B_0 is a constant. The particle's spin gives it a magnetic moment of magnitude μ, which interacts with the magnetic field through the interaction energy

$$H = \mu\vec{\sigma}\cdot\vec{B} \quad \ldots \quad \text{or in terms of the particle's gyromagnetic ratio } \gamma,\ \ H = -\gamma\vec{s}\cdot\vec{B}\,.$$

(NOTE: The sign change between the two formulae is because of the particle's negative charge, which gives it a negative gyromagnetic ratio γ.) The vector $\vec{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ denotes the usual vector of Pauli matrices for a spin ½ particle.

▶ Reminders from 486: The spin operator $\hat{\vec{s}} = (\hat{s}_x, \hat{s}_y, \hat{s}_z)$ has units of angular momentum. For a spin ½ particle, each of its components has two eigenvalues: $+\hbar/2$ and $-\hbar/2$ (i.e. spin-up and -down along any axis). The $\hbar$ carries units of angular momentum. For convenience, we factor out the $\hbar/2$ when defining the Pauli spin matrices $\sigma_x, \sigma_y, \sigma_z$, which are the 2×2 matrices describing the spin operators for spin-½ particles: $\hat{\vec{s}} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$. These matrices are on the 486 formula sheet. As with anything in the matrix representation, we must know the basis in which these matrices are written in order to use them. The Pauli matrices are written in the basis of the eigenstates of $\hat{s}_z$, meaning $\begin{pmatrix}1\\0\end{pmatrix} \equiv \left|+\frac{1}{2}\right\rangle_{m_s}$ and $\begin{pmatrix}0\\1\end{pmatrix} \equiv \left|-\frac{1}{2}\right\rangle_{m_s}$
If you are unclear on any of this, you must ask!

(a) At $t = 0$, a measurement determines that the spin is pointing in the $+x$ direction. What is the probability that it will be pointing in the $-y$ direction at a later time t ?

(b) Calculate the expectation values of the particle's two spin-components s_y and s_z as functions of time.

▶ You will find that the spin precesses around the magnetic field at the frequency $\omega = \gamma B_0$, which you may recognize as the classical **Larmor frequency** for the precession of a magnetic dipole in a magnetic field. Recall the general statement of Ehrenfest's theorem: expectation values obey classical laws.

Problem 3 : NMR = Nuclear Magnetic Resonance

A spin-½ nucleus is placed in a constant, uniform magnetic field $\vec{B} = B_0\,\hat{z}$ of external origin, where B_0 is a constant. This magnetic field is sometimes called a "**holding field**". Now, an oscillating magnetic field B_1 that is much smaller than B_0 is applied in the xy-plane, i.e. transverse to the holding field. This smaller "**RF field**" is made to oscillate at a radio frequency ω. The resulting total field is

$$\vec{B} = \left(B_1 \cos\omega t,\, B_1 \sin\omega t,\, B_0\right)$$

What will this rotating RF field do? Perhaps it will drag the nuclear spin around with it at frequency ω ? Hmm … let's calculate it! (So great that we can do that ☺) The Hamiltonian of the nucleus is

$$H = -\gamma \vec{s} \cdot \vec{B} \ = \ -\mu \vec{\sigma} \cdot \vec{B}$$

The sign difference with problem 2 is because the nucleus is positively charged, so now γ is positive.

For the following questions, use these two frequency symbols : $\Omega_0 \equiv \dfrac{\mu B_0}{\hbar} = \dfrac{\gamma B_0}{\mathbf{2}}$ and $\Omega_1 \equiv \dfrac{\mu B_1}{\hbar} = \dfrac{\gamma B_1}{\mathbf{2}}$.

(a) At $t = 0$, the nuclear spin is pointing in the $+z$ direction, parallel to the holding field B_0. What is the probability that it points in the –z direction at later times t ? (If it does so at all, that would be cool → that would mean that the nucleus underwent a spin flip!)

▶ **PROCEDURE** : This is actually a new sort of problem for us. With that rotating RF field, we are encountering for the first time a **time-dependent Hamiltonian**. The way we have determined the time-dependence of states up until now is to project them onto the eigenstates of the Hamiltonian, and then apply to each such projection the factor $e^{-iEt/\hbar}$… but that most excellent procedure was derived for time-**IN**dependent Hamiltonians back in the early lectures of 486, by applying separation of variables to the Schrödinger equation

$$i\hbar \frac{d\Psi}{dt} = \hat{H}\Psi \ .$$

With the Hamiltonian now *itself* dependent on time, you must go back to the Schrödinger equation and solve it from scratch. To get you started, note that this problem deals entirely with a spin state; the particle isn't moving so there is no spatial part of our wavefunction – no $\psi(r,\theta,\phi)$ or $\psi(x,y,z)$ to worry about. The state of our stationary spin-½ particle is just a pure two-component spinor, χ. You must find the general solution of

$$i\hbar \frac{d\chi}{dt} = \hat{H}\chi \quad \text{where} \quad \chi(t) = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} \quad \text{and} \quad \hat{H} \ \text{is a } 2\times 2 \text{ matrix.}$$

Once you put the Hamiltonian in 2x2 matrix form, and plug in that generic 2-component spinor $\chi(t)$, you will have two coupled differential equations for the spinor components a(t) and b(t) → you must find the general solution of those. Final note: remember that a and b are complex (of course), and they are not independent as the spinor must be normalized. Good to go? Have at it! A brand new solution of the Schrödinger equation, how exciting! ☺

(b) This method of causing nuclei to flip their spins is called **Nuclear Magnetic Resonance** (**NMR**). It has many applications, notably in medical imaging (MRI = magnetic resonance imaging). Most NMR experiments adjust the magnitude B_0 of the holding field and/or the frequency ω of the RF field so that $|\omega| = 2\Omega_0$.
Why do they do that?

▶ **NOTE**: The absolute-value bars on the resonance condition $|\omega| = 2\Omega_0$ mean that the resonant frequency is
either $\omega = +2\Omega_0$ = counter-clockwise rotation of the RF field
or $\omega = -2\Omega_0$ = clockwise rotation of the RF field.
You figure out which one it is; it will be obvious once you realize what you are trying to maximize … read on ...

▶ **HINT**: The word "resonance" is running around this problem, so it's pretty clear something is maximized when the condition $|\omega| = 2\Omega_0$ is met. In more detail, "**resonance**" means that the magnitude of a system's response to some stimulus is maximized when some resonant condition is met. Here, the response is the nuclear spin flip, and the stimulus is the oscillating RF field that causes it.