Physics 221A
Fall 2007
Homework 9
Due Friday, November 2, 2007

Reading Assignment: Sakurai, pp. 197–198; rest of Notes 11, Notes 12, and pp. 1–8 or so of Notes 13. Sakurai discusses magnetic resonance on pp. 320–325, but from a rather different standpoint than we have. You may want to read what he says anyway. He remarks that four Nobel prizes have been awarded for work involving magnetic resonance. The technique of spin echo, which was invented by Erwin Hahn in our department, lies behind modern MRI imaging techniques. We always hoped that Erwin, too, would win a Nobel for his work, but it seems unlikely now. Nevertheless, his work has had tremendous practical impact.

1. A molecule is approximately a rigid body. Consider a molecule such as H_2O, NH_3, or CH_4, which is not a diatomic. First let us talk classical mechanics. Then the kinetic energy of a rigid body is

$$H = \frac{L_x^2}{2I_x} + \frac{L_y^2}{2I_y} + \frac{L_z^2}{2I_z}, \tag{1}$$

where $\mathbf{L} = (L_x, L_y, L_z)$ is the angular momentum vector with respect to the body frame, and (I_x, I_y, I_z) are the principal moments of inertia. The body frame is assumed to be the principal axis frame in Eq. (1). The angular velocity $\boldsymbol{\omega}$ of the rigid body is related to the angular momentum $\mathbf{L}$ by

$$\mathbf{L} = \mathsf{I}\boldsymbol{\omega}, \tag{2}$$

where I is the moment of inertia tensor. When (2) is written in the principal axis frame, it becomes

$$\omega_i = \frac{L_i}{I_i}, \qquad i = x, y, z. \tag{3}$$

Finally, the equations of motion for the angular velocity or angular momentum in the body frame are the *Euler equations*,

$$\dot{\mathbf{L}} + \boldsymbol{\omega}\times\mathbf{L} = 0. \tag{4}$$

By using (3) to eliminate either $\boldsymbol{\omega}$ or $\mathbf{L}$, (4) can be regarded as an equation for either $\mathbf{L}$ or $\boldsymbol{\omega}$. The Euler equations are trivial for a spherical top ($I_x = I_y = I_z$), they are easily solvable in terms of trigonometric functions for a symmetric top ($I_x = I_y = I_\perp \neq I_z$), and they are solvable in terms of elliptic functions for an asymmetric top (I_x, I_y, I_z all unequal). The symmetric top is studied in all undergraduate courses in classical mechanics.

(a) In quantum mechanics, it turns out that the Hamiltonian operator for a rigid body has exactly the form (1). The angular momentum $\mathbf{L}$ satisfies the commutation relations,

$$[L_i, L_j] = -i\hbar\, \epsilon_{ijk}\, L_k, \tag{5}$$

with a minus sign relative to the familar commutation relations because the components of $\mathbf{L}$ are (in this problem) measured relative to the body frame. (We will not justifiy this. If the components of $\mathbf{L}$ were measured with respect to the space or inertial frame, then there would be the usual plus sign in (5).) Compute the Heisenberg equations of motion for $\mathbf{L}$, and compare them with the classical Euler equations. You may take (2) or (3) over into quantum mechanics, in order to define an operator $\boldsymbol{\omega}$ to make the Heisenberg equations look more like the classical Euler equations. (Just get the equataion for L_x, then cycle indices to get the others.) Make your answer look like (4) as much as possible.

(b) It is traditional in the theory of molecules to let the quantum number of L_z (referred to the body frame) be k. Write the rotational energy levels of a symmetric top ($I_x = I_y = I_\perp \neq I_z$) in terms of a suitable set of quantum numbers. Indicate any degeneracies. How is the oblate case ($I_z > I_\perp$) qualitatively different from the prolate case ($I_\perp > I_z$)? Hint: In order to deal with standard commutation relations, you may wish to write $\tilde{\mathbf{L}} = -\mathbf{L}$, so that $[\tilde{L}_i, \tilde{L}_j] = i\hbar\, \epsilon_{ijk}\, \tilde{L}_k$.

2. A spin-1 particle has the component of its spin in the direction

$$\hat{\mathbf{n}} = \frac{1}{\sqrt{3}}(1, 1, 1), \tag{6}$$

measured, and the result is $\hbar$. Find the probabilities for the various outcomes in a subsequent measurement of S_z. Do not diagonalize any matrices; use rotation operators.

3. Consider a particle of spin 1 and magnetic moment $\boldsymbol{\mu} = -\gamma\mathbf{S}$ in the magnetic field,

$$\mathbf{B} = B_0\hat{\mathbf{z}} + B_{10}(\hat{\mathbf{x}}\cos\omega_1 t + \hat{\mathbf{y}}\sin\omega_1 t), \tag{7}$$

employed in magnetic resonance experiments (assume $\gamma > 0$). If at $t = 0$, the particle is in state $m = 0$, find the transition probabilities $P(0 \to \pm 1)$ as a function of time.

4. If we combine Eq. (12.31) with (12.38), we obtain

$$\frac{\partial U}{\partial t} = -\frac{i}{\hbar}\boldsymbol{\omega}(t)\cdot\mathbf{S}\,U, \tag{8}$$

where we write U instead of T for the time evolution operator, which we know is a rotation. Let U be parameterized by its Euler angles, $U = U(\alpha, \beta, \gamma)$. Find equations of motion for the Euler angles, assuming $\boldsymbol{\omega}(t)$ is given. Your answer will be identical to the equations of motion of the Euler angles in classical rigid body theory (for given $\boldsymbol{\omega}(t)$).

5. Consider a biological sample at 300K in a magnetic field of 6T (for example, you in an MRI device). After a certain relaxation time, the nuclear spins will reach thermal equilibrium with their environment (a heat bath). Calculate the fractional magnetization of protons under such circumstances (the magnetization compared to the maximum we would have at 0K). Finally, for a sample of water under the conditions indicated, compute the magnetization due to protons in Gauss.