1. This is a variation on Sakurai’s problem 4.10, which is confused because you can’t prove what he asks you to prove in part (c) (it involves a phase convention). Do this instead:

(a) Let $U(R)$ be a rotation operator on the state space of any system (however complex). Show that $[\Theta, U(R)] = 0$ for all $R$.

(b) Denote the basis states in a single irreducible subspace under rotations of any system by $|jm\rangle$. By considering $\Theta U(R)|jm\rangle$, show that

$$[D^j_{m',m}(R)]^\dagger = (-1)^{m-m'} D^j_{-m',-m}(R).$$  

(c) Show that if $T_q^k$ is an irreducible tensor operator, then so is

$$S_q^k = (-1)^q (T_q^k)^\dagger.$$

Operator $S^k$ is regarded as the Hermitian conjugate of $T^k$.

2. Compute the shifts in the energy levels of a single-electron (hydrogen-like) atom of nuclear charge $Z$ due to the finite size of the nucleus. Treat the nucleus as a uniform sphere of charge of radius $r_0 A^{1/3}$, where $r_0 = 1.0 \times 10^{-13}$ cm and $A$ is the number of nucleons. Express your answer as some number of eV times some function of $Z$, $A$, and the quantum numbers of the atomic state. Only treat those atomic states for which the effect is the largest. This is called the volume effect. You may use

$$R_{n0}(0) = 2 \left( \frac{Z}{na_0} \right)^{3/2},$$

valid in hydrogen-like atoms, where $a_0 = \hbar^2/me^2$ is the Bohr radius.

The volume effect induces a splitting between the $2s$ and $2p$ levels of hydrogen. Compare this to the Lamb shift (another splitting of the same two levels). The Lamb shift
suppresses the $2p$ level relative to the $2s$ level by approximately 1.05 GHz in frequency units.


4. In this problem, set $\hbar = 1$ for simplicity. The Hamiltonian for a rigid body is

$$H = \frac{1}{2} \left( \frac{L_1^2}{I_1} + \frac{L_2^2}{I_2} + \frac{L_3^2}{I_3} \right),$$

where $(I_1, I_2, I_3)$ are the principal moments of inertia and where $(L_1, L_2, L_3) = (L_x, L_y, L_z)$ are angular momentum operators satisfying the commutation relations,

$$[L_i, L_j] = i \epsilon_{ijk} L_k.$$

You may assume that the angular momentum takes on only integer values. The Hamiltonian (4) describes the rotational spectrum of molecules. Physically, the quantities $L_i$ are the negatives of the components of the angular momentum with respect to the body frame.

In the case of a spherical top, such as methane, we have $I_1 = I_2 = I_3 = I$. The Hamiltonian is

$$H = \frac{L^2}{2I},$$

and the energy levels are

$$E_{\ell} = \frac{\ell(\ell + 1)}{2I},$$

which is $(2\ell + 1)$-fold degenerate since $E_{\ell}$ is independent of $m$.

In the case of a symmetric top such as ammonia, we have $I_1 = I_2 = I_\perp \neq I_3$. The Hamiltonian is

$$H = \frac{1}{2} \left( \frac{L_1^2}{2I_\perp} + \frac{L_2^2}{2I_\perp} + \frac{L_3^2}{2I_3} \right),$$

and the energy levels are

$$E_{\ell m} = A + B m^2,$$

where

$$A = \frac{\ell(\ell + 1)}{2I_\perp}, \quad B = \frac{1}{2} \left( \frac{1}{I_3} - \frac{1}{I_\perp} \right),$$

and where $m$ is the usual quantum number of $L_z$.

Now consider the case of a slightly asymmetric top. (Water is an example of an asymmetric top molecule.) Let

$$\frac{1}{I_1} = \frac{1 + \epsilon}{I_\perp}, \quad \frac{1}{I_2} = \frac{1 - \epsilon}{I_\perp},$$

$$\frac{1}{I_3} = \frac{1}{I_\perp},$$

(11)
where $\epsilon$ is small. These equations are equivalent to defining

$$I_\perp = \frac{2I_1I_2}{I_1 + I_2}, \quad \epsilon = \frac{I_2 - I_1}{I_1 + I_2}. \quad (12)$$

Write the Hamiltonian as $H = H_0 + \epsilon H_1$, where $H_0$ is the symmetric top Hamiltonian in Eq. (8).

You may find the following relations useful:

$$\langle m|L_+^2|m'\rangle = \langle m'|L_+^2|m\rangle^*, \quad (13a)$$
$$\langle m|L_+^2|m'\rangle = (-1)^{m+m'}\langle -m'|L_+^2|\epsilon\rangle, \quad (13b)$$

but if you use Eq. (13b) you must prove it.

(a) Consider the state $m = 0$. Find the first order of perturbation theory at which the energy shift does not vanish, and compute the energy shift at that order. In addition to the abbreviations (10), use

$$C = \frac{1}{4I_\perp}, \quad (14)$$

and express your answer in terms of the constants $A$, $B$ and $C$.

(b) Find the first order of perturbation theory at which the energy shifts for the $m = \pm 1$ levels do not vanish, and compute them at that order.

(c) Find the first order of perturbation theory at which the energy shifts for the $m = \pm 2$ levels do not vanish, and compute them at that order. Express your answer in terms of

$$X = \frac{\ell(\ell - 1)(\ell + 1)(\ell + 2)}{4B}, \quad Y = \frac{(\ell - 3)(\ell - 2)(\ell + 3)(\ell + 4)}{12B}. \quad (15)$$

See also Sakurai’s problem 12, p. 348. Notice the appearance of a sum over “intermediate states.”

(d) What order of perturbation theory do you have to go to in order to find the first nonvanishing correction to the energy in the case of $m = \pm 3$? $m = \pm 4$?