QM II
Phys 652

Solutions of HW #2

(1)

Problem #1

$$\Psi(\theta,\varphi) = \frac{1}{\sqrt{5}} Y_1^{-1}(\theta,\varphi) + \sqrt{\frac{3}{5}}\, Y_1^{0}(\theta,\varphi) + \frac{1}{\sqrt{5}} Y_1^{1}(\theta,\varphi)$$

(a) rewrite as a state vector:

$$|\Psi\rangle = \frac{1}{\sqrt{5}}|1,-1\rangle + \sqrt{\frac{3}{5}}|1,0\rangle + \frac{1}{\sqrt{5}}|1,1\rangle$$

Since $L_\pm|l,m\rangle = \hbar\sqrt{l(l+1)-m(m\pm1)}\,|l,m\pm1\rangle \Rightarrow$

$$\langle\Psi|L_+|\Psi\rangle = \left(\frac{1}{\sqrt{5}}\langle 1,-1| + \sqrt{\frac{3}{5}}\langle 1,0| + \frac{1}{\sqrt{5}}\langle 1,1|\right)$$

term $|1,1\rangle$
doesn't survive, since
$L_+|1,1\rangle = 0$

$$\cdot\left(\frac{1}{\sqrt{5}}\hbar\sqrt{1\cdot2-(-1)\cdot0}\,|1,0\rangle + \sqrt{\frac{3}{5}}\hbar\sqrt{1\cdot2-0\cdot1}\,|1,1\rangle\right)$$

$$= \hbar\cdot\sqrt{\frac{3}{5}}\cdot\frac{1}{\sqrt{5}}\cdot\sqrt{2} + \frac{1}{\sqrt{5}}\hbar\cdot\sqrt{\frac{3}{5}}\sqrt{2} = \frac{2}{5}\sqrt{6}\,\hbar$$

(b) If L_z is measured $\Rightarrow$ $m = 0, \pm1$ $\Rightarrow$
$l_z = -\hbar, 0, +\hbar$ are found

Probabilities:

$$P_{\substack{l_z=-\hbar \\ (m=-1)}} = |\langle 1,-1|\psi\rangle|^2 = \frac{1}{5}$$

$$P_{l_z=0} = |\langle 1,0|\psi\rangle|^2 = \frac{3}{5}$$

$$P_{\substack{l_z=\hbar \\ (m=+1)}} = |\langle 1,1|\psi\rangle|^2 = \frac{1}{5}$$

Check: $\frac{1}{5}+\frac{3}{5}+\frac{1}{5}=1$ ✓

(c) After obtaining $l_z=-\hbar$, we are in the state $|1,-1\rangle$.

The uncertainty $\Delta L_x = \sqrt{\langle L_x^2\rangle - \langle L_x\rangle^2}$

$\Delta L_y = \sqrt{\langle L_y^2\rangle - \langle L_y\rangle^2}$

$$L_x = \frac{L_+ + L_-}{2}\ ;\ L_y = \frac{L_+ - L_-}{2i} \Rightarrow \langle L_x\rangle = \langle L_y\rangle = 0$$

$$\langle L_x^2\rangle \underset{\substack{\uparrow \\ \text{see worksheet \#3}}}{=} \langle L_y^2\rangle = \frac{\langle L^2\rangle - \langle L_z^2\rangle}{2} = \frac{\hbar^2}{2}\left[l(l+1)-m^2\right]$$

Since we are in the state with $l=1$, $m=-1 \Rightarrow$

$$\langle L_x^2\rangle = \langle L_y^2\rangle = \frac{\hbar^2}{2}\left[1\cdot 2-1\right] = \frac{\hbar^2}{2} \Rightarrow$$

$$\Delta L_x = \Delta L_y = \frac{\hbar}{\sqrt{2}}$$

Problem #2

$$\Psi(x,y,z) = \frac{1}{4\sqrt{\pi}} \frac{2z^2 - x^2 - y^2}{r^2} + \sqrt{\frac{3}{\pi}} \frac{xz}{r^2}$$

(a) First present $\Psi(x,y,z)$ in terms of spherical harmonics

(i) $2z^2 - x^2 - y^2 = 2r^2\cos^2\theta - r^2\sin^2\theta\cos^2\varphi - r^2\sin^2\theta\sin^2\varphi = 2r^2\cos^2\theta - r^2\underbrace{\sin^2\theta}_{1-\cos^2\theta} = 3r^2\cos^2\theta - r^2 = r^2(3\cos^2\theta - 1)$

From p. 457 of Sakurai ← 2nd edition $\Rightarrow$ $3\cos^2\theta - 1 = Y_2^0 \cdot \sqrt{\frac{16\pi}{5}}$ $\Rightarrow$

$$\frac{1}{4\sqrt{\pi}} \frac{2z^2 - x^2 - y^2}{r^2} = \frac{1}{4\sqrt{\pi}}(3\cos^2\theta - 1) = \frac{1}{4\sqrt{\pi}} \cdot Y_2^0 \cdot \sqrt{\frac{16\pi}{5}} = \frac{1}{\sqrt{5}} Y_2^0$$

(ii) $\frac{xz}{r^2} = \frac{r^2 \sin\theta\cos\theta\cos\varphi}{r^2} = \frac{\sin\theta\cos\theta}{2}(e^{i\varphi} + e^{-i\varphi})$

From p. 451 of Sakurai ⇒

$$Y_2^{\pm 1} = \mp \sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta\, e^{\pm i\varphi} \Rightarrow$$

$$Y_2^{1} - Y_2^{-1} = -\sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta\left(e^{i\varphi} + e^{-i\varphi}\right) \Rightarrow$$

$$\Rightarrow \frac{xz}{r^2}\cdot\sqrt{\frac{3}{\pi}} = \sqrt{\frac{3}{\pi}}\cdot\frac{1}{2}\sqrt{\frac{8\pi}{15}}\left(Y_2^{-1} - Y_2^{1}\right) =$$

$$= \underbrace{\sqrt{\frac{2}{5}}\left(Y_2^{-1} - Y_2^{1}\right)}$$

So, our $\underbrace{\Psi = \frac{1}{\sqrt{5}} Y_2^0 + \sqrt{\frac{2}{5}}\left(Y_2^{-1} - Y_2^{1}\right)}$

Now, $\vec{L}^2\Psi = \frac{1}{\sqrt{5}} \underbrace{\vec{L}^2 Y_2^0}_{= \hbar^2\cdot 2\cdot 3\, Y_2^0} + \sqrt{\frac{2}{5}}\left(\underbrace{\vec{L}^2 Y_2^{-1}}_{= \hbar^2\cdot 2\cdot 3\, Y_2^{-1}} - \underbrace{\vec{L}^2 Y_2^{1}}_{= \hbar^2\cdot 2\cdot 3\, Y_2^{1}}\right) =$

$$= 6\hbar^2\left(\frac{1}{\sqrt{5}} Y_2^0 + \sqrt{\frac{2}{5}}\left(Y_2^{-1} - Y_2^{1}\right)\right) = \underline{6\hbar^2\Psi} \Rightarrow$$

Ψ is an eigenstate of $\vec{L}^2$

$$L_z\Psi = \frac{1}{\sqrt{5}} \underbrace{L_z Y_2^0}_{= 0} + \sqrt{\frac{2}{5}}\left(\underbrace{L_z Y_2^{-1}}_{= -\hbar Y_2^{-1}} - \underbrace{L_z Y_2^{1}}_{= \hbar Y_2^{1}}\right) =$$

$$= -\hbar\sqrt{\frac{2}{5}}\left(Y_2^{-1} + Y_2^{1}\right)$$ ← obviously, Ψ is not an eigenstate of L_z

The total angular momentum is

$$\sqrt{\langle\Psi|\vec{L}^2|\Psi\rangle} = \sqrt{6\hbar^2\langle\Psi|\Psi\rangle} = \underline{\sqrt{6}\,\hbar}$$

(b) $L_+\Psi = ?$

$$L_+\Psi = \frac{1}{\sqrt{5}} L_+ Y_2^0 + \sqrt{\frac{2}{5}}\left(L_+ Y_2^{-1} - L_+ Y_2^1\right) =$$

Use $L_+ Y_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m+1)}\, Y_\ell^{m+1}$

$$= \frac{1}{\sqrt{5}}\cdot\hbar\sqrt{6}\, Y_2^1 + \sqrt{\frac{2}{5}}\,\hbar\left(\sqrt{6}\, Y_2^0 - 2 Y_2^2\right)$$

$\Downarrow$

$\langle\Psi|L_+|\Psi\rangle = ?$ $\Rightarrow L_+|\Psi\rangle = \hbar\sqrt{\frac{6}{5}}\,|2,1\rangle +$ (ℓ m)

$$+\sqrt{\frac{2}{5}}\,\hbar\left(\sqrt{6}\,|2,0\rangle - 2|2,2\rangle\right)$$

$$\langle\Psi| = \frac{1}{\sqrt{5}}\langle 2,0| + \sqrt{\frac{2}{5}}\left(\langle 2,-1| - \langle 2,1|\right)$$

$$\langle\Psi|L_+|\Psi\rangle = \frac{1}{\sqrt{5}}\sqrt{\frac{2}{5}}\,\hbar\sqrt{6}\,\langle 2,0|2,0\rangle - \hbar\sqrt{\frac{6}{5}}\cdot$$

$$\cdot\sqrt{\frac{2}{5}}\,\langle 2,1|2,1\rangle = \underline{0}$$

(c) From part (a), $L_z\overbrace{\Psi}^{=\frac{1}{\sqrt{5}}Y_2^0 + \sqrt{\frac{2}{5}}Y_2^{-1} - \sqrt{\frac{2}{5}}Y_2^1} = -\hbar\sqrt{\frac{2}{5}}\left(Y_2^{-1} + Y_2^1\right)$,

i.e. possible values for L_z are $\pm\hbar$ and 0.

Probabilities: $\mathcal{P}(L_z = 0) = \frac{1}{5}$; $\mathcal{P}(L_z = \pm\hbar) = \frac{2}{5}$; $\frac{2}{5} + \frac{2}{5} + \frac{1}{5} = 1$ ✓

Problem #3.

Analysis of the paper entitled "Fullerene quantum gyroscope" by M. Krause et al. (*Phys. Rev. Lett.* **93**, 137403 (2004)).

1) **What is the claim of the paper?**

The authors claim the first experimental observation of quantized rotational states of the C_2 molecule encapsulated in solid fullerene.

2) **Did the authors do experiment, calculations or both?**

The authors performed both the experiment and calculations (DFT and MD).

3) **What kind of experiment did the authors do?**

The experimental method was Raman scattering in a backscattering geometry at two laser wavelengths of excitation (647 nm and 514 nm, respectively) as a function of temperature.

4) **What are the measured quantities?**

Spectral content of the scattered light was measured, and dependence of the intensity of the scattered light on the frequency shift with respect to the laser excitation frequency was analyzed at various temperatures.

5) **How is the experimentally measured line separation (see Fig.2) related to the difference in energy levels (e.g. E_l-E_{l-1}) ?**

The line separation ($\Delta\nu$) is $\Delta\nu = \nu_{l+2} - \nu_l = \frac{E_{l+2} - E_l}{h} - \frac{E_l - E_{l-2}}{h}$

(note that we take a difference between the energy levels l and $l \pm 2$ due to selection rules in the case of Raman scattering experiment)

Also note that the line separation is the difference in frequencies, not in energies!

5) In the first column of page 2, the authors state that if the motion of the rotator is confined to a plane, then the energies are E(m)=Bm². Why?

If the motion is confined to a plane (say, x-y plane), then the angular momentum has only z component, i.e. $\vec{L}^2 = L_z^2$. Then the Hamiltonian is $H = \frac{L_z^2}{2\mu r_e^2}$.

Since $H\psi = E\psi$ and $L_z\psi = hm\psi$, then $\frac{L_z^2}{2\mu r_e^2}\psi = \frac{\hbar^2}{2\mu r_e^2}m^2\psi$, from which $E=Bm^2$, where $B = \frac{\hbar^2}{2\mu r_e^2}$.

6) What are the selection rules for Raman scattering? What line separation is expected and why?

The selection rules are $\Delta J=\pm 2$, $\Delta m=\pm 2$.

Strictly speaking, the line separation is

$$\Delta\nu = \nu_{j+2} - \nu_j = \frac{E_{j+2}-E_j}{h} - \frac{E_j - E_{j-2}}{h} = \frac{B}{h}\left((j+2)(j+3) - 2j(j+1) + (j-2)(j-1)\right) = 8\frac{B}{h}$$

Similarly,

$$\Delta\nu = \nu_{m+2} - \nu_m = \frac{E_{m+2}-E_m}{h} - \frac{E_m - E_{m-2}}{h} = \frac{B}{h}\left((m+2)^2 - 2m^2 + (m-2)^2\right) = 8\frac{B}{h}$$

However, note that the rotational constant B, defined in class as $B = \frac{\hbar^2}{2\mu r_e^2}$, has the units of energy (Joules), while the authors define it in the units of cm^{-1}. As a result, their line separation is expressed in terms of the wave numbers (cm^{-1}) and not in the frequencies (s^{-1}), and so their line separation $\Delta\nu$ (in cm^{-1}) is just 8B, not 8B/h.

Also note that the rotational spectrum lines in this paper correspond to transitions 0->2, 2->4, 4->6, … (see Table 1), so only even rotational states are allowed (and odd ones such as 1->3, 3->5,… are disallowed) due to symmetry considerations (page 2, column 2, first paragraph).

7) **How is the rotational constant B derived from the experimental data? What is the obtained value for B?**

The average line separation deduced from the data is $\Delta\nu = 8B = 13.8\ cm^{-1}$, from which $B = 13.8/8 = 1.73\ cm^{-1}$.

8) **What are the obtained values for the moment of inertia and a distance between the atoms (i.e. r_e)?**

$I = 1.617 x 10^{-46}\ kg\ m^2$; $r_e = 0.127\ nm$

9) **Under what conditions the model of an unperturbed rotator is applicable to this "real" system?**

The closer the system to a free rotator (i.e. very low rotational barrier), the better the agreement with the unperturbed model (i.e. $V=0$).

10) **What do the authors introduce in the Schroedinger equation to better describe the experimental results?**

The authors introduce the potential term $V(\gamma)$ in the Schroedinger equation.

12) **Which model provides a better agreement with the experiment (see Table I)?**

At all frequencies, the plane rotor models (both unperturbed and perturbed) provide a better agreement with the data than the free rotor model.
However, the perturbed plane rotor model has an advantage over the unperturbed plane rotor model at low frequencies.