LULEÅ UNIVERSITY OF TECHNOLOGY **Division of Physics**

Solution to written exam in QUANTUM PHYSICS F0047T Examination date: 2015-03-17

The solutions are just suggestions. They may contain several alternative routes.

1. (a) As

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos(\theta)$$
 and $Y_{1,\pm 1} = \sqrt{\frac{3}{8\pi}}\sin(\theta)e^{\pm\phi}$

the wave function can be written as

$$\psi = \frac{1}{4\pi} \left(e^{i\phi} \sin(\theta) + \cos(\theta) \right) g(r) = \sqrt{\frac{1}{3}} (-\sqrt{2}Y_{1,1} + Y_{1,0}) g(r).$$

Hence the possible values of L_z are $+\hbar$ and 0.

(b) Since

$$\int |\psi|^2 = \frac{1}{4\pi} \int_0^\infty |g(r)|^2 r^2 dr \int_0^\pi d\theta \int_0^{2\pi} (1 + \cos\phi\sin 2\theta) \sin\theta d\phi = \frac{1}{2} \int_0^\pi \sin\theta \, d\theta = 1,$$

the given wave function is normalised. The probability density is then given by $P = |\psi|^2$. Thus the probability of $L_z = +\hbar$ is $|\sqrt{\frac{2}{3}}|^2 = \frac{2}{3}$ and that of $L_z = 0$ is $|\sqrt{\frac{1}{3}}|^2 = \frac{1}{3}$.

(c) The expectation value of L_z is

$$< L_z >= |\sqrt{\frac{2}{3}}|^2 (+\hbar) + |\sqrt{\frac{1}{3}}|^2 (0) = \frac{2}{3}\hbar$$

- 2. The rotational and vibrational energy levels of a molecule are given by
 - $E_{n,l} = (n + \frac{1}{2})\hbar\omega + \frac{\hbar^2}{2I}l(l+1)$. In an electrical dipole transition the quantum number l changes by one unit $\Delta l = \pm 1$ as the photon carries an angular momentum.

I) If the vibrational state does **not** change $(\Delta n = 0)$, we can observe radiation with the following energies $E_i - E_f = E_{n,l+1} - E_{n,l} = \frac{\hbar^2}{2I}(l+1)(l+2) - \frac{\hbar^2}{2I}l(l+1) = \frac{\hbar^2}{I}(l+1), l = 0, 1, 2, 3,$ which gives the following photon energies: $\frac{\hbar^2}{I}, 2\frac{\hbar^2}{I}, 3\frac{\hbar^2}{I}, 4\frac{\hbar^2}{I}, ...$

II) If however the vibrational state changes by **one** unit $\Delta n = -1$ (note emission), we find two series

one for
$$\Delta n = -1$$
, and $\Delta l = -1$:

 $E_i - E_f = E_{n,l+1} - E_{n-1,l} = \hbar\omega + \frac{\hbar^2}{I}, \hbar\omega + 2\frac{\hbar^2}{I}, \hbar\omega + 3\frac{\hbar^2}{I}, \hbar\omega + 4\frac{\hbar^2}{I}, \dots$ the second series for $\Delta n = -1$, and $\Delta l = +1$:

 $E_i - E_f = E_{n,l} - E_{n-1,l+1} = \hbar\omega - \frac{\hbar^2}{I}, \hbar\omega - 2\frac{\hbar^2}{I}, \hbar\omega - 3\frac{\hbar^2}{I}, \hbar\omega - 4\frac{\hbar^2}{I}, \dots$ Note that the spacing between the transition energies is of equal energy except for one. It seems there is one transition energy missing corresponding to $\hbar\omega$. This transition would however violate $\Delta l = \pm 1$.

The separation between the maxima corresponds to $\Delta E = \frac{\hbar^2}{I} = hc\Delta\lambda^{-1}$ inserting the appropriate data taken from graph $\Delta\lambda^{-1} = \frac{2968.7 - 2824.0}{7} = 20.67 \text{cm}^{-1}$. Now we can calculate $I = \mu R^2 = \frac{m_H m_{Cl}}{m_H + m_{Cl}}$ to arrive at $R = \sqrt{\frac{h}{4\pi^2 c\Delta\lambda^{-1}\mu}} = 1.30 \text{\AA}$.

3. Hydrogenic atoms have eigenfunctions $\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta,\varphi)$. Using the COLLECTION OF FORMULAE we find

$$\begin{split} \psi_{100}(\boldsymbol{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0} \\ \psi_{200}(\boldsymbol{r}) &= \left(\frac{Z^3}{8\pi a_0^3}\right)^{1/2} \left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0} \\ \psi_{210}(\boldsymbol{r}) &= \left(\frac{Z^3}{32\pi a_0^3}\right)^{1/2} \frac{Zr}{a_0} \cos \theta e^{-Zr/2a_0} \\ \psi_{21\pm 1}(\boldsymbol{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} \frac{Zr}{8a_0} \sin \theta e^{\pm i\varphi} e^{-Zr/2a_0} \end{split}$$

where a_0 is the Bohr radius. The β -decay instantaneously changes $Z = 1 \rightarrow Z = 2$. According to the expansion theorem, it is possible to express the wave function $u_i(\mathbf{r})$ before the decay as a linear combination of eigenfunctions $v_i(\mathbf{r})$ after the decay as

$$u_i(\boldsymbol{r}) = \sum_j a_j v_j(\boldsymbol{r})$$

where

$$a_j = \int v_j^*(\boldsymbol{r}) u_i(\boldsymbol{r}) d^3 r.$$

The probability to find the electron in state j is given by $|a_j|^2$.

(a) Here $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{200}(Z = 2)$. This gives

$$a = \left(\frac{1}{\pi a_0^3}\right)^{1/2} \left(\frac{2^3}{8\pi a_0^3}\right)^{1/2} \int_0^\infty e^{-r/a_0} \left(1 - \frac{2r}{2a_0}\right) e^{-2r/2a_0} 4\pi r^2 dr$$
$$= \frac{4}{a_0^3} \int_0^\infty e^{-2r/a_0} \left(r^2 - \frac{r^3}{a_0}\right) dr = \frac{4}{a_0^3} \left[2\left(\frac{a_0}{2}\right)^3 - \frac{6}{a_0}\left(\frac{a_0}{2}\right)^4\right] = -\frac{1}{2}.$$

Thus, the probability is 1/4 = 0.25.

(b) For $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{210}(Z = 2)$ the θ -integral is

$$\int_0^\pi \cos\theta \sin\theta d\theta = \frac{1}{2} \int_0^\pi \sin 2\theta d\theta = \left[-\frac{\cos 2\theta}{4} \right]_0^\pi = 0.$$

For $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{21\pm 1}(Z = 2)$ the φ -integral is

$$\int_0^{2\pi} e^{\pm i\varphi} d\varphi = 0$$

Thus, the probability to find the electron in a 2p state is zero.

(c) Here $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{100}(Z = 2)$. This gives

$$a = \left(\frac{1}{\pi a_0^3}\right)^{1/2} \left(\frac{2^3}{\pi a_0^3}\right)^{1/2} \int_0^\infty e^{-r/a_0} e^{-2r/a_0} 4\pi r^2 dr = \frac{8\sqrt{2}}{a_0^3} \int_0^\infty e^{-3r/a_0} r^2 dr$$
$$= \frac{8\sqrt{2}}{a_0^3} \frac{a_0^3}{3^3} \int_0^\infty e^{-x} x^2 dx = \frac{8\sqrt{2}}{27} \int_0^\infty e^{-x} x^2 dx = \frac{8\sqrt{2}}{27} \int_0^\infty 2e^{-x} dx = \frac{16\sqrt{2}}{27}$$

Thus, the probability is $512/729 \approx 0.70233$.

(The probability to find the electron in $\psi_{100}(Z=2)$ is 512/729 = 0.702. Therefore, the electron is found with 95% probability in one of the states 1s or 2s.)

(d) No l has to be less than n.

4. First choose a coordinate system. Let the direction of the incoming photon λ be along the x-axis's positive direction and let the outgoing photon λ' nearly go out along the y-axis (15 degrees of) in positive direction.

We can start with the observation that as all momentum before the incident is in the positive x-direction this has to be true also after the collision. So as momentum is conserved and the outgoing photon λ' leaves in the positive y direction, we make the following conclusions about the electron. The electron must have the same y-momentum in opposite direction to keep the total y momentum zero. The momentum the electron obtains in the x-direction has to be the difference between the incident photon and the outgoing photon's momentum in the x-direction.

(a) for Compton scattering we have the following relation $\lambda' - \lambda = \frac{h}{m_e c} (1 - \cos \theta)$. $\lambda = \frac{hc}{E_{photon}} = \frac{6.626 \cdot 10^{-34} \cdot 2.998 \cdot 10^8}{100 \cdot 10^{-119}} = 1.240 \cdot 10^{-11} \text{m} = 0.1240 \text{ Å}$. The wave length of the outgoing photon will be $\lambda' = \lambda + \frac{h(1 - \cos 75)}{m_e c} = \lambda + \frac{6.626 \cdot 10^{-34} (1 - \cos 75)}{9.109 \cdot 10^{-31} \cdot 2.998 \cdot 10^8} = 1.240 \cdot 10^{-11} + 1.798 \cdot 10^{-12} = 1.4198 \cdot 10^{-11} \text{m}$ = 0.14198 Å. The energy is $E' = \frac{hc}{\lambda'} = \frac{6.626 \cdot 10^{-34} \cdot 2.998 \cdot 10^8}{1.4198 \cdot 10^{-11}} = 1.3991 \cdot 10^{-14} \text{J} = 87.336 \text{keV} = 87.3 \text{keV}$. Another route to the energy may be: $E' = h\nu' = \frac{E}{1 + \alpha(1 - \cos \theta)}$ where $\alpha = \frac{E}{m_0 c_0^2}$. The

dimensionless
$$\alpha = \frac{100 \cdot 10^3 \cdot 1.602 \cdot 10^{-19}}{9.109 \cdot 10^{-31} \cdot (2.998 \cdot 10^8)^2} = 0.19567$$
 and $E' = \frac{100 \cdot 10^3}{1 + 0.19567(1 - \cos 75)} = 87.3$ keV.

- (b) The energy of the electron will be: 100 87.3 = 12.7 keV.
- (c) Use conservation of momentum. To calculate the recoil of the electron we have to calculate the momentum of the photon h/λ .

$$p_x^0 = p_x^1 + p_x^{electron}$$
$$p_y^0 = p_y^1 + p_y^{electron}$$

Before the incident $p_x^0 = \frac{6.626 \cdot 10^{-34}}{1.240 \cdot 10^{-11}} = 5.3435 \cdot 10^{-23}$ kg m/s and $p_y^0 = 0$. After the event the outgoing photon has: $p_y^1 = \frac{6.626 \cdot 10^{-34}}{1.4198 \cdot 10^{-11}} \sin(75) = 4.5078 \cdot 10^{-23}$ kg m/s and $p_x^1 = \frac{6.626 \cdot 10^{-34}}{1.4198 \cdot 10^{-11}} \cos(75) = 1.2079 \cdot 10^{-23}$ kg m/s. This yields for the electron $p_x^{electron} = p_x^0 - p_x^1 = (5.3435 - 1.2079) \cdot 10^{-23} = 4.1356 \cdot 10^{-23}$ kg m/s and $p_y^{electron} = -p_y^1 = -4.5078 \cdot 10^{-23}$ kg m/s. The angle of the recoil α is given by $\tan \alpha = \frac{p_y^{electron}}{p_x^{electron}} = \frac{-4.5078}{4.1356} = -1.0900$ which gives $\alpha = -47.5^o$ (note sign).

 $p_x^{electron} = 4.1356$

Another way to calculate the angle ϕ of the recoiling electron is: Start with $\cos \theta = \frac{2}{(1+\alpha)^2 \tan^2 \phi + 1}$ solving for ϕ yields $\tan \phi = \sqrt{\frac{1}{(1+\alpha)^2} \cdot \frac{1+\cos \theta}{1-\cos \theta}}$ and with $\theta = 75$ we arrive at $\tan \phi = 1.089954$ and hence $\phi = 47.46$.

We can corroborate the result in b) in the following way: The length of the electrons momentum vector is $p^{electron} = \sqrt{4.1356^2 + 4.5078^2} \cdot 10^{-23} = 6.1174 \cdot 10^{-23}$ kg m/s. The kinetic energy of the electron can also be calculated from $E_{kin} = p^2/2m = (6.1174 \cdot 10^{-23})^2/(2 \cdot 9.109 \cdot 10^{-31}) = 2.0542 \cdot 10^{-15}$ J = 12.8keV, the same result as in b) (well nearly).

5. A measurement of the spin component in the direction $\hat{n} = \hat{x}\sin(\varphi) + \hat{y}\cos(\varphi)$ gives the value $-\hbar/2$ (or $+\hbar/2$ depending of version of problem).

The spin operator $S_{\hat{n}} = \hat{n} \cdot (S_x, S_y, S_z)$ is

$$S_{\hat{n}} = \frac{\hbar}{2} \begin{pmatrix} 0 & \sin\varphi - i\cos\varphi \\ \sin\varphi + i\cos\varphi & 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 & -ie^{i\varphi} \\ ie^{-i\varphi} & 0 \end{pmatrix} = \frac{-i\hbar}{2} \begin{pmatrix} 0 & e^{i\varphi} \\ -e^{-i\varphi} & 0 \end{pmatrix}$$

The eigenvalue equation is

$$S_{\hat{n}}\chi = \lambda\chi \Leftrightarrow \frac{i\hbar}{2} \begin{pmatrix} 0 & -e^{i\varphi} \\ e^{-i\varphi} & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$
(1)

We find the eigenvalues from

$$\begin{vmatrix} -\lambda & \frac{-i\hbar}{2}e^{i\varphi} \\ \frac{i\hbar}{2}e^{-i\varphi} & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda^2 - (\frac{\hbar}{2})^2 = 0 \Rightarrow \lambda = \pm \frac{\hbar}{2}$$

(a) The spin state corresponding to $\lambda = -\hbar/2$ must satisfy the eigenvalue equation Eq. (1). This yields two equations that are linearly dependent. Take any of these, say $iae^{-i\varphi} = -b$ and choose a = 1 and hence:

$$\chi_{\hat{n}-} = C \begin{pmatrix} 1 \\ -ie^{-i\varphi} \end{pmatrix} \Rightarrow \chi_{\hat{n}-} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -ie^{-i\varphi} \end{pmatrix}, \text{ or differently } \frac{1}{\sqrt{2}} \begin{pmatrix} ie^{i\varphi} \\ 1 \end{pmatrix},$$

where the normalization condition $|a|^2 + |b|^2 = 1$ was used in the last step. Other correct solutions can be found by a multiplication with an arbitrary phase factor $e^{i\alpha}$.

N.B. this is for the other eigenvalue $\lambda = +\hbar/2$, an answer to the + version of the question. The spin state corresponding to $\lambda = \hbar/2$ must satisfy the eigenvalue equation Eq. (1). This yields two equations that are linearly dependent. Take any of these, say $iae^{-i\varphi} = b$ and choose a = 1 and hence:

$$\chi_{\hat{n}+} = C\left(\begin{array}{c}1\\ie^{-i\varphi}\end{array}\right) \Rightarrow \chi_{\hat{n}+} = \frac{1}{\sqrt{2}}\left(\begin{array}{c}1\\ie^{-i\varphi}\end{array}\right), \text{ or differently } \frac{1}{\sqrt{2}}\left(\begin{array}{c}-ie^{-i\varphi}\\1\end{array}\right),$$

where the normalization condition $|a|^2 + |b|^2 = 1$ was used in the last step. Other correct solutions can be found by a multiplication with an arbitrary phase factor $e^{i\alpha}$.

- (b) A general spin state (for the z-direction) can be written as $\chi^z = a\chi_+^z + b\chi_-^z$, where $\chi_+^z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is the spin up and $\chi_-^z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is the spin down spinor in the z-direction. The outcomes of a measurement will be: For $\chi_{\hat{n}-}$ we find that the probability to measure spin up, *i.e.* $S_z = \hbar/2$ is $|a|^2 = |-e^{-i\varphi}/\sqrt{2}|^2 = 1/2$, and that the probability to measure spin down, *i.e.* $S_z = -\hbar/2$ is $|b|^2 = |1/\sqrt{2}|^2 = 1/2$.
- (c) We would get 50% up and 50% down in the \hat{n} direction. The reason is that the states (in b) we start from are eigenstates of S_z and this operator is not present in $S_{\hat{n}}$. Had S_z been part of $S_{\hat{n}}$ there would be a bias.