LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS MTF067

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1. (a) The eigenfunctions and eigenvalues of the particle are found by solving the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V(x)u(x)=Eu(x),$$

for $0 \le x \le a$ where $V(x)=0$. This gives

$$\frac{d^2u(x)}{dx^2}+k^2u(x)=0, \text{ with } k=\sqrt{\frac{2mE}{\hbar^2}}.$$

The general solution is $A\sin(kx)+B\cos(kx)$ for $0\le x\le a$. The boundary conditions give

$$\begin{aligned} u(0) &= 0 \Longrightarrow B=0 \\ u(a) &= 0 \Longrightarrow \sin(ka)=0 \Longrightarrow ka=n\pi \text{ where } n=1,2,3,... \end{aligned}$$

Normalization gives

$$1=\int |u|^2\, dx=\int_0^a |A|^2\sin\left(\frac{n\pi x}{a}\right)\, dx=|A|^2\frac{a}{2}\Longrightarrow A=\sqrt{\frac{2}{a}}.$$

Thus

$$u_n=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right).$$

The energy eigenvalues are given by

$$E=\frac{\hbar^2k^2}{2m}\Longrightarrow E_n=\frac{n^2\pi^2\hbar^2}{2ma^2}.$$

(b) The states $n=1$ and $n=2$ have $E\le\frac{3\hbar^2\pi^2}{ma^2}$. It is possible to do the expansion

$$\alpha(x)=\sum_{i=1}^{\infty}c_iu_i \text{ where } c_i=\int u_i^*(x)\alpha(x)\, dx.$$

The probability to measure E_1 or E_2 is $|c_1|^2+|c_2|^2$, where

$$\begin{aligned} c_1 &= \int_0^a\sqrt{\frac{2}{a}}\sin\left(\frac{1\pi x}{a}\right)Nx(a-x)\, dx=...=N\frac{a^2\sqrt{a}\,4\sqrt{2}}{\pi^3}, \text{ and} \\ c_2 &= \int_0^a\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)Nx(a-x)\, dx=...=0. \end{aligned}$$

Normalization of $\alpha(x)$ gives

$$1=\int_0^a|\alpha(x)|\, dx=|N|^2\int_0^a x^2(a-x)^2\, dx=...=|N|^2\frac{a^5}{30}\Longrightarrow |N|^2=\frac{30}{a^5}.$$

The probability is

$$|c_1|^2+|c_2|^2=\left|N\frac{a^2\sqrt{a}\,4\sqrt{2}}{\pi^3}\right|^2+0=\frac{960}{\pi^6}.$$

2. (a) Use the spherical coordinates

$$\begin{cases} x &= r\sin\theta\cos\varphi \\ x &= r\sin\theta\sin\varphi \\ x &= r\cos\theta \end{cases}$$

to expand the wave function $\psi(x,y,z)$ as a sum of functions $R(r)Y_{lm}(\theta,\phi)$. This gives

$$\begin{aligned} \psi &= Nr^2\sin\theta\cos\varphi\sin\theta\sin\varphi e^{-\alpha r} = Nr^2\sin^2\theta\sin\varphi\cos\varphi e^{-\alpha r} \\ &= \tfrac{1}{2}Nr^2\sin^2\theta\sin 2\varphi e^{-\alpha r} = \tfrac{1}{2}N\sin^2\theta\tfrac{1}{2i}\left(e^{2i\varphi}-e^{-2i\varphi}\right)r^2e^{-\alpha r} \\ &= \tfrac{1}{2}N\tfrac{1}{2i}\sqrt{\tfrac{32\pi}{15}}\left(Y_{22}-Y_{2-2}\right)r^2e^{-\alpha r} = N'\left(Y_{22}-Y_{2-2}\right)r^2e^{-\alpha r}, \end{aligned}$$

where Y_{lm} are taken from the COLLECTION OF FORMULAS. From the expansion we see that the only possible values of l and m are $l=2$ and $m=\pm 2$. Therefore, a measurement of L^2 will give the value $L^2 = 2(2+1)\hbar^2 = 6\hbar^2$ with probability $P(L^2 = 6\hbar^2) = 1$. A measurement of L_z will give the values $L_z = \pm 2\hbar$ with probabilities $P(L_z = +2\hbar) = P(L_z = -2\hbar) = 1/2$.

(b) The expectation value can be calculated as $\langle A\rangle = \sum_i P_i A_i$, where P_i is the probability to measure the value A_i. Therefore we have
$\langle L^2\rangle = 1\cdot 6\hbar^2 = 6\hbar^2$ and
$\langle L_z\rangle = 1/2\cdot 2\hbar + 1/2\cdot(-2\hbar) = 0$.

(c) The Schrödinger equation in spherical coordinates is given by

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r\cdot + \frac{\boldsymbol{L}^2}{2mr^2} + V(r)\right)N'\left(Y_{22}-Y_{2-2}\right)r^2e^{-\alpha r} = EN'\left(Y_{22}-Y_{2-2}\right)r^2e^{-\alpha r}$$

If we use the fact that $L^2\psi = 6\hbar^2$ and that

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r\left(r^2e^{-\alpha r}\right) = -\frac{\hbar^2}{2m}\left(\frac{6}{r^2}-\frac{6\alpha}{r}+\alpha^2\right)r^2e^{-\alpha r},$$

we can write the Schrödinger equation as

$$\left\{-\frac{\hbar^2}{2m}\left(\frac{6}{r^2}-\frac{6\alpha}{r}+\alpha^2\right)+\frac{6\hbar^2}{2mr^2}+V(r)-E\right\}\psi = 0,$$

or

$$-\frac{\hbar^2}{2m}\left(\frac{6}{r^2}-\frac{6\alpha}{r}+\alpha^2\right)+\frac{6\hbar^2}{2mr^2}+V(r)-E = 0. \tag{1}$$

Since the spherically symmetric potential $V(r)\to 0$ as $r\to\infty$ we have

$$E = -\frac{\hbar^2\alpha^2}{2m}.$$

When this result is inserted into equation (1) we get

$$V(r) = -\frac{3\alpha\hbar^2}{mr}.$$

3. Use a test function $f(r,\theta,\phi)$ to calculate the commutator.

$$\begin{aligned}
[L_z, \sin\phi]\, f(r,\theta,\phi) &= \left[-i\hbar\frac{\partial}{\partial\phi}, \sin\phi\right] f(r,\theta,\phi) \\
&= -i\hbar\frac{\partial}{\partial\phi}\sin\phi f(r,\theta,\phi) - \sin\phi\left(-i\hbar\frac{\partial}{\partial\phi}\right) f(r,\theta,\phi) \\
&= -i\hbar\cos\phi f - i\hbar\sin\phi\frac{\partial f}{\partial\phi} + i\hbar\sin\phi\frac{\partial f}{\partial\phi} \\
&= -i\hbar\cos\phi f(r,\theta,\phi).
\end{aligned}$$

Thus, $[L_z, \sin\phi] = -i\hbar\cos\phi$.

4. (a) For a hydrogen atom we have the quantum numbers n, l, m, and s. Here we neglect the spin quantum number s. From FYSIKALIA we find that the energy is given by

$$E_n = -\frac{\mu e^4}{8\varepsilon_0^2 h^2}\cdot\frac{Z^2}{n^2} = -13.6\cdot\frac{Z^2}{n^2}\text{ eV}.$$

For a given n we have $l = 0, 1, 2, ..., n-1$ and for a given l we have $m = -l, -l+1, ..., l-1, l$. Thus, for a given n there is a n-fold l-degeneracy and each state with a given l exhibits a $(2l+1)$-fold m-degeneracy. Therefore, the energy level E_n is

$$\sum_{l=0}^{n-1}(2l+1) = n^2\text{-fold degenerate.}$$

(b) The first order energy correction $E_n^{(1)}$ for the perturbation H_1 is

$$E_n^{(1)} = \langle\phi_n|H_1|\phi_n\rangle\,,$$

if the Hamiltonian is $H = H_0 + H_1$ and ϕ_n are eigenstates to H_0. Here we have $H_1 = \epsilon/r^3$ and $\phi = \psi_{nlm} = R_{nl}(r)Y_{lm}(\theta,\varphi)$. Thus,

$$E_n^{(1)} = \epsilon\left\langle\psi_{nlm}|r^{-3}|\psi_{nlm}\right\rangle = \frac{\epsilon}{n^3 l(l+1/2)(l+1))}\left(\frac{Z}{a_0}\right)^3.$$

The expectation value $\langle r^{-3}\rangle$ is taken from the COLLECTION OF FORMULAE.

(c) The the spin-orbit interaction will cause a small amount of energy splitting between the l-degenerate states.

5. (a) The solution to the time-independent Schrödinger equation is

$$\begin{cases} u(x) = e^{ikx} + Re^{-ikx} & ,k = \frac{\sqrt{2mE}}{\hbar} \quad ,x<0, \\ u(x) = Te^{iqx} & ,q = \frac{\sqrt{2m(E-V_0)}}{\hbar} \quad ,x>0 \end{cases}$$

The continuity conditions at $x = 0$ give

$$\begin{cases} T = 1 + R \\ iqT = ik(1-R) \end{cases} \Rightarrow T = \frac{2k}{k+q}\text{ , and } R = \frac{k-q}{k+q}$$

Thus,

$$\begin{cases} u(x) = e^{ikx} + \frac{k-q}{k+q}e^{-ikx} & ,x<0, \\ u(x) = \frac{2k}{k+q}e^{iqx} & ,x>0 \end{cases}$$

(b) The transmitted part is given by the transmitted probability flux divided by the incoming probability flux, i.e.

$$\frac{\hbar q}{m}|T|^2 \Big/ \frac{\hbar k}{m} = \frac{q}{k}|T|^2 = \frac{4qk}{(k+q)^2} = \frac{4qk}{(k+q)^2}.$$

Therefore, the number of transmitted particles per time unit is

$$\frac{4qk}{(k+q)^2} N_0.$$

6. A measurement of the spin component in the direction $\hat{n} = \cos\varphi\hat{x} + \sin\varphi\hat{y}$ gives the value $\hbar/2$. The spin operator $S_{\hat{n}}$ is

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

The eigenvalue equation is

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

We find the eigenvalues from

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

(a) The spin state corresponding to $\lambda = +\hbar/2$ must satisfy the eigenvalue equation Eq. (2), *i.e.*

$$\chi_{\hat{n}+} = \begin{pmatrix} a \\ b \end{pmatrix} = b\begin{pmatrix} e^{-i\varphi} \\ 1 \end{pmatrix} \Rightarrow \chi_{\hat{n}+} = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\varphi} \\ 1 \end{pmatrix},$$

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 $\exp(i\alpha)$.

(b) A general spin state can be written as $\chi = a\chi_+ + b\chi_-$, where χ_+ is spin up and χ_- is spin down in z-direction. 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 $|b|^2 = |1/\sqrt{2}|^2 = 1/2$.