LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

# Solution to written exam in QUANTUM PHYSICS F0047T

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1. The eigenfunctions and eigenvalues of the free-particle Hamiltonian are found by solving the time-independent Schrödinger equation

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

with $V(x)$ zero everywhere. Thus, the eigenvalue equation reads

$$\frac{d^2u(x)}{dx^2} + k^2u(x) = 0,$$

where $k^2 = 2mE/\hbar^2$. The eigenfunctions are given by the plane waves $e^{ikx}$ and $e^{-ikx}$, or linear combinations of these, as *e.g.* $\sin kx$ and $\cos kx$.

(a) The wave function of the particle at $t = 0$ is given by

$$\psi(x,0) = \cos^3(kx) + \sin^5(kx).$$

This is not an eigenfunction in itself but it can be written as using the Euler relations

$$\psi(x,0) = \left(\frac{e^{ikx} + e^{-ikx}}{2}\right)^3 + \psi(x,0) = \left(\frac{e^{ikx} - e^{-ikx}}{2i}\right)^5 = \quad (1)$$

$$\frac{1}{8}\left(e^{i3kx} + 3e^{ikx} + 3e^{-ikx} + e^{-i3kx}\right) + \quad (2)$$

$$\frac{1}{32i}\left(e^{i5kx} - 5e^{i3kx} + 10e^{ikx} - 10e^{-ikx} + 5e^{-i3kx} - e^{-i5kx}\right) = \quad (3)$$

$$\frac{3}{4}\cos(kx) + \frac{1}{4}\cos(3kx) + \frac{1}{16}\sin(5kx) - \frac{5}{16}\sin(3kx) + \frac{10}{16}\sin(kx) \quad (4)$$

Thus, $\psi(x,0)$ can be written as a superposition of plane waves with three different values of $k_1 = k$, $k_2 = 3k$ and $k_3 = 5k$

(b) The energy of a plane wave $e^{ikx}$ is given by $E = \hbar^2k^2/2m$. Thus, the energy of $e^{ik_1x}$ (or $e^{-ik_1x}$) is $E_1 = \hbar^2k^2/2m$ and the energy of $e^{ik_2x}$ (or $e^{-ik_2x}$) is $E_2 = \hbar^2k_2^2/2m = 9\hbar^2k^2/2m$. and the energy of $e^{ik_3x}$ (or $e^{-ik_3x}$) is $E_3 = \hbar^2k_2^2/2m = 25\hbar^2k^2/2m$.

(c) The function $u(x) = e^{ikx}$ is a solution to the the time-independent Schrödinger equation. The corresponding solutions to the time-dependent Schrödinger equation are given by $u(x)T(t)$,with $T(t) = e^{-iEt/\hbar}$. Therefore, $u(x)T(t) = e^{i(kx-Et/\hbar)}$. A sum of solutions of this form is also a solution, since the Schrödinger equation is linear. This means that if $\psi(x,0)$ is given by equation (4), then the time dependent solution is given by

$$\psi(x,t) = \frac{1}{8}\left(e^{i3kx} + e^{-i3kx}\right)e^{-iE_2t/\hbar} + \frac{3}{8}\left(e^{ikx} + e^{-ikx}\right)e^{-iE_1t/\hbar} + \quad (5)$$

$$\frac{1}{32i}\left(e^{i5kx} - e^{-i5kx}\right)e^{-iE_3t/\hbar} - \frac{5}{32i}\left(e^{i3kx} - e^{-i3kx}\right)e^{-iE_2t/\hbar} + \frac{10}{32i}\left(e^{ikx} - e^{-ikx}\right)e^{-iE_1t/\hbar} = \quad (6)$$

$$(7)$$

where

$$E_1 = \frac{\hbar^2k^2}{2m} \quad \text{and} \quad E_2 = \frac{9\hbar^2k^2}{2m} \quad \text{and} \quad E_3 = \frac{25\hbar^2k^2}{2m} \quad (8)$$

2. (a) The parity of a hydrogen eigenfunction $\psi_{nlm_l}(\mathbf{r})$ is given by $(-1)^l$. The given wave function $\Psi(\mathbf{r})$ is a mixture of eigenfunctions of different parity. Hence $\Psi(\mathbf{r})$ cannot have a definite parity.

(b) The probability is given by the absolute square of the coefficients. The probabilities are (in order) $\frac{4}{15}$, $\frac{9}{15}$, $\frac{1}{15}$, $\frac{1}{15}$. as a check they sum up to 1 as they should do.

(c) The energy of a single state is given by: $E_n = -\frac{13.56}{n^2}$ eV. The expectation value is given by $< E >= \frac{4}{15}(-\frac{13.56}{1^2}) + \frac{9}{15}(-\frac{13.56}{2^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) = -13.56(\frac{4}{15} + \frac{9}{60} + \frac{1}{135} + \frac{1}{135}) = -5.851$ eV

The operator $\mathbf{L}^2$ has eigenvalues $\hbar^2 l(l+1)$. The expectation value is given by $< \mathbf{L^2} >= \frac{4}{15}\cdot 0 + \frac{9}{15}\cdot 0 + \frac{1}{15}(\hbar^2 1(1+1)) + \frac{1}{15}(\hbar^2 2(2+1)) = \frac{8}{15}\hbar^2$

The operator $L_z$ has eigenvalues $\hbar m_l$. The expectation value is given by $< L_z >= \frac{4}{15}\cdot 0 + \frac{9}{15}\cdot 0 + \frac{1}{15}\cdot 0 + \frac{1}{15}(\hbar 2) = \frac{2}{15}\hbar$

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

$$\begin{aligned}
\psi_{100}(\boldsymbol{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0} \\
\psi_{200}(\boldsymbol{r}) &= \left(\frac{Z^3}{8\pi a_0^3}\right)^{1/2} \left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0} \\
\psi_{210}(\boldsymbol{r}) &= \left(\frac{Z^3}{32\pi a_0^3}\right)^{1/2} \frac{Zr}{a_0} \cos\theta e^{-Zr/2a_0} \\
\psi_{21\pm1}(\boldsymbol{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} \frac{Zr}{8a_0} \sin\theta e^{\pm i\varphi} e^{-Zr/2a_0}
\end{aligned}$$

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

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

where

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

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

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

Thus, the probability is $1/4 = 0.25$.

(b) For $u_i = \psi_{100}(Z=1)$ and $v_j = \psi_{210}(Z=2)$ the $\theta$-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 $v_j = \psi_{21\pm1}(Z=2)$ the $\varphi$-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

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

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. (a) i. $\hat{\Pi}C\left(\sin(\frac{\pi x}{L})+\sin(\frac{3\pi x}{L})\right) = C\left(\sin(\frac{-\pi x}{L})+\sin(\frac{-3\pi x}{L})\right) = -C\left(\sin(\frac{\pi x}{L})+\sin(\frac{3\pi x}{L})\right)$, the eigenvalue is -1

ii. $\hat{\Pi}Ce^{-a\sqrt{x^2+y^2+z^2}} = CCe^{-a\sqrt{(-x)^2+(-y)^2+(-z)^2}} = Ce^{-a\sqrt{x^2+y^2+z^2}}$, the eigenvalue is +1

iii. $\hat{\Pi}Cf(r)\left(\cos(\theta)+cos^3(\theta)\right)\ e^{i\phi} = Cf(r)\left(\cos(\pi-\theta)+cos^3(\pi-\theta)\right)\ e^{i(\phi+\pi)} = Cf(r)\left(-\cos(\theta)+-cos^3(\theta)\right)\ (-e^{i\phi}) = Cf(r)\left(\cos(\theta)+cos^3(\theta)\right)\ e^{i\phi}$, the eigenvalue is +1

(b) i. $\hat{\Pi}(2\psi_+(x,y,z)+3\psi_-(x,y,z)) = +2\psi_+(x,y,z)+-3\psi_-(x,y,z) \neq \lambda(2\psi_+(x,y,z)+3\psi_-(x,y,z))$, not an eigenfunction.

ii. $\hat{\Pi}^2(2\psi_+(x,y,z)+3\psi_-(x,y,z)) = \hat{\Pi}(+2\psi_+(x,y,z)+-3\psi_-(x,y,z)) = 2\psi_+(x,y,z)+3\psi_-(x,y,z)$, an eigenfunction with eigenvalue +1.

iii. $\hat{\Pi}e^{-ikx} = e^{+ikx} \neq e^{-ikx}$ not an eigenfunction and neither is $e^{ikx}$. We can however form linear combinations that have parity. The function $e^{ikx}-e^{-ikx}$ has parity $\hat{\Pi}e^{+ikx}-e^{-ikx} = e^{-ikx}-e^{+ikx} = -1(e^{+ikx}-e^{-ikx})$ with eigenvalue -1. The function $e^{ikx}+e^{-ikx}$ has parity $\hat{\Pi}e^{+ikx}+e^{-ikx} = e^{-ikx}+e^{+ikx} = +1(e^{+ikx}+e^{-ikx})$ with eigenvalue +1.

5. The eigenfunctions of the infinite square well in one dimension are (Here a solution of the S.E. in one dimesion is adequate). The width of the well is $a$.

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \quad \text{and the eigenenergys are } E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad \text{where} \quad n = 1,2,3,...$$

In three dimensions the eigenfunctions and eigenenergys are (Here an argument about separation of variables is needed to justify the structure of the solution)

$\Psi_{n,m,l}(x,y) = \psi_n(x)\cdot\psi_m(y)\cdot\psi_l(z)$ and eigenenergys $E_{n,m} = E_n + E_m + E_l$ where the indecies are $n = 1,2,3,..$ , $m = 1,2,3,..$ and $l = 1,2,3,..$

**a**) The eigenfunctions inside the box are (note the sidelength is $a/2$ for one of the sides)

$$\Psi_{n,m,l}(x,y,z) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\cdot\sqrt{\frac{2}{a}}\sin\frac{m\pi y}{a}\cdot\sqrt{\frac{4}{a}}\sin\frac{l\pi 2z}{a} \quad \text{where} \quad n = 1,2,3,.., m = 1,2,3,.. \text{ and } \quad l = 1,2,3,..$$

The eigenfunctions outside the box are $\Psi_{n,m,l}(x,y,z) = 0$

**b**) The seven lowest eigenenergys are (note the 4 associated to the quantum number $l$ this is due to that the length of the box along the $z$ direction is only half of the other two that are of equal length):

$$E_{n,m,l} = \frac{\pi^2\hbar^2}{2ma^2}(n^2+m^2+4l^2), \quad \text{where the 7 lowest are} \quad (n^2+m^2+4l^2) = 6, 9, 12, 14, 18, \text{ and } 21.$$

**c**) The seven lowest eigenenergys have degeneracys (different ways to choose $n, m, l$ to form the same energy) (either one, two or four) as follows:

$$E_{1,1,1} = \text{ one state } \; (n^2+m^2+4l^2 = 6)$$

$$E_{1,2,1} = E_{2,1,1} = \text{ two states } \; (n^2+m^2+4l^2 = 9)$$
$$E_{2,2,1} = \text{ one state } \; (n^2+m^2+4l^2 = 12)$$
$$E_{1,3,1} = E_{3,1,1} = \text{ two states } \; (n^2+m^2+4l^2 = 14)$$
$$E_{2,3,1} = E_{3,2,1} = \text{ two states } \; (n^2+m^2+4l^2 = 17)$$
$$E_{1,1,2} = \text{ one state } \; (n^2+m^2+4l^2 = 18)$$

Energy number 7 is special as the degeneracy is 4 but all four are not connected through a symmetry operation, ie some of these states are accidentally degenerated. These four can be grouped in the following way.

$$E_{1,2,2} = E_{2,1,2} = \text{ two states } \; (n^2+m^2+4l^2 = 21)$$

$$E_{1,4,1} = E_{4,1,1} = \text{ two states } \; (n^2+m^2+4l^2 = 21)$$