LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Quantum Physics F0047T

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1. The eigenfunctions of the infinite square well are (Physics handbook)

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

The correction to the eigenenergies due to perturbation is given by:

$$E_n^1 = < H_1 > \quad \text{where} \quad H_1 \quad \text{is the deviation in the potential from the infinite square well.}$$

$$E_n^1 = \int_0^{a/2} \frac{2\epsilon}{a} \sin^2 \frac{n\pi x}{a} dx = \int_0^{a/2} \frac{2\epsilon}{a2} \left(1 - \cos \frac{2n\pi x}{a}\right) dx = \frac{\epsilon}{a} \left[x - \frac{a}{2n\pi} \sin \frac{2n\pi x}{a}\right]_0^{a/2} = \frac{\epsilon}{2}$$

This is the same for all n. The corrections in energy for the n=1 and n=2 levels are of intrest (**answer to a)**).

$$E_1^1 = E_2^1 = \frac{\epsilon}{2} = 0.235\text{eV}.$$

The two lowest unperturbed eigenergies are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{n^2h^2}{8ma^2} \quad [n = 1] \quad E_1 = \frac{n^2 6.6260710^{-34}}{8 \cdot 9.1093810^{-31} 2.0^2 \cdot 10^{-20}} = 1.5061625 \cdot 10^{-18}\text{J} =$$

$$= 9.4007\text{eV} \quad \text{and} \quad E_2 = 37.60285\text{eV}$$

To calculate the transition energy between two perturbed levels we first calculate the new energys, due to the perturbation, for the two lowest levels:

$$E_1^* = 9.4007125 + 0.235 = 9.6357125\text{eV} \quad \text{and} \quad E_2^* = 37.60285 + 0.235 = 37.83785\text{eV}$$

The transition energy between the perturbed levels will be 37.83785 - 9.6357125 = 28.20214 eV. The same would be for the unperturbed levels as the perturbation changes all levels by the same energy (to first order).

2. (a) $i\hbar\frac{\partial^2}{\partial t^2} \sin \omega t = i\hbar\omega\frac{\partial}{\partial t} \cos \omega t = -i\hbar\omega^2 \sin \omega t$ **YES**

   (b) $-i\hbar\frac{\partial}{\partial z} C(1 + z^2) = -i\hbar C(0 + 2z)$ **NO**

   (c) $-i\hbar\frac{\partial^2}{\partial z^2}(C_1 e^{ikz} + C_2 e^{-ikz}) = -i\hbar ik\frac{\partial}{\partial z}(C_1 e^{ikz} - C_2 e^{-ikz}) = -i\hbar k^2(C_1 e^{ikz} + C_2 e^{-ikz})$ **YES**

   (d) $-\frac{\hbar}{2}\frac{\partial}{\partial z} Ce^{-3z} = -\frac{\hbar}{2} C(-3)e^{-3z} \propto \psi(z)$ **YES**

   (e) $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} =?$ This has to be done in some steps. Start by doing this derivative first: $-\frac{\partial^2}{\partial z^2} ze^{-\frac{1}{2}z^2} = -\frac{\partial}{\partial z}(e^{-\frac{1}{2}z^2} - z^2e^{-\frac{1}{2}z^2}) = -(-ze^{-\frac{1}{2}z^2} - 2ze^{-\frac{1}{2}z^2} + z^3e^{-\frac{1}{2}z^2}) = 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}$.
   Now you go back to the start: $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} = \frac{C}{2}(z^3e^{-\frac{1}{2}z^2} + 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}) = \frac{C}{2}(+3ze^{-\frac{1}{2}z^2}) = \propto \psi(z)$ **YES**

   (f) $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})e^{-\frac{1}{2}z^2} = \frac{C}{2}(z^2e^{-\frac{1}{2}z^2} - \frac{\partial}{\partial z}(-ze^{-\frac{1}{2}z^2})) = \frac{C}{2}(z^2e^{-\frac{1}{2}z^2} - (-e^{-\frac{1}{2}z^2} + z^2e^{-\frac{1}{2}z^2})) = \frac{C}{2}e^{-\frac{1}{2}z^2} \propto \psi(z)$ **YES**

3. 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

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

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. (1), *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 $|b|^2 = |1/\sqrt{2}|^2 = 1/2$.

4. 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 β-decay instantaneously changes $Z = 1 \rightarrow Z = 2$. 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 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 $v_j = \psi_{21\pm1}(Z=2)$ 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

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

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.

5. (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.