LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS F0047T

Examination date: 2010-01-15

1. (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.

2. 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

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

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

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

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

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

(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

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

3. (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 $< L_z >= \frac{4}{15}\cdot 0 + \frac{9}{15}\cdot 0 + \frac{1}{15}\cdot 0 + \frac{1}{15}(\hbar 2) = \frac{2}{15}\hbar$

4. 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:

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

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

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

$$E_1^1 = E_2^1 = \frac{\epsilon}{2} = 0.055\text{eV}.$$

The two lowest eigenergies are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{n^2h^2}{8ma^2} \quad [n=1] \quad E_1 = 6.02465\cdot 10^{-20}\text{J} = 0.376028\text{eV} \quad \text{and} \quad E_2 = 1.504114\text{eV}$$

The new energys for the two lowest levels are:

$$E_1^* = 0.376028 + 0.055 = 0.431028\text{eV} \quad \text{and} \quad E_2^* = 1.504114 + 0.055 = 1.559114\text{eV}$$

The case of $\epsilon = 1.08$ eV. This energy is much higher than the groundstate energy of the unperturbed model. You cannot use perturbation here. The model is more like a square well of width $a/2$. The answer of such a perturbation calculation would not give a trustworthy result.

5. The rotational energy of a molecule is given by

$$E_l = \frac{\hbar^2}{2I} l(l+1)$$

The emitted photon energy for a transition $l+1$ to l is given by

$$E_{photon} = \frac{\hbar^2}{2I}\left((l+1)(l+2) - l(l+1)\right) = \frac{\hbar^2}{2I}\left(l^2 + 3l - 2 - l^2 - l\right) = \frac{\hbar^2(l+1)}{I}$$

This is the energy for one line and there will be a set of lines all for different l. The separation between two adjecent lines in energy will be

$$E_{photon,l+2} - E_{photon,l+1} = \frac{\hbar^2(l+2)}{I} - \frac{\hbar^2(l+1)}{I} = \frac{\hbar^2}{I}$$

The energy of a photon is $E_{photon} = \frac{hc}{\lambda}$ and hence

$$\frac{\hbar^2}{I} = hc\left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2}\right) = 1.2398 \cdot 10^{-6}\left(\Delta\frac{1}{\lambda}\right)\text{eV m} = 1.2398 \cdot 10^{-6} \cdot 20.68cm^{-1} = 2.564 \cdot 10^{-3}\text{eV}$$

$$I = \frac{(1.055 \cdot 10^{-34})^2}{2.564 \cdot 10^{-3} \cdot 1.602 \cdot 10^{-19}} = 2.71 \cdot 10^{-47}\text{kg m}^2$$

The moment of inertia is $I = mr^2$ where $m = m_H m_{Cl}/(m_H + m_{Cl}) = 35/36 m_H$ and r is the average separation. $r = \sqrt{\frac{I}{m}} = \sqrt{\frac{36 \cdot\ 2.71 \cdot 10^{-47}}{35 \cdot\ 1.673 \cdot 10^{-27}}} = 1.29 \cdot 10^{-10}\text{m}$

$E_l = \frac{2.56 \cdot 10^{-3}}{2} l(l+1)\text{eV}$
$E_0 = 0\text{eV}$,
$E_1 = 2.56 \cdot 10^{-3}\text{eV} = 4.10 \cdot 10^{-22}\text{J}$,
$E_2 = 7.68 \cdot 10^{-3}\text{eV} = 1.23 \cdot 10^{-21}\text{J}$,
$E_3 = 15.4 \cdot 10^{-3}\text{eV} = 2.47 \cdot 10^{-21}\text{J}$,
$E_3 = 25.6 \cdot 10^{-3}\text{eV} = 4.10 \cdot 10^{-21}\text{J}$.