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1 Chapter 6 The Hydrogen Atom

6.1
(a) True
(b) False

6.2
(a)needs $V(r)$ to be irrelated to θ, ϕ
(b)the conversion of the equation is step by step:
$-\frac{\hbar^2}{2m}{}^2\Psi + V(r)\Psi = E\Psi$
convert to a spherical coordinate:
$-\frac{\hbar^2}{2m}(\frac{\partial^2\Psi}{\partial r^2} + \frac{2}{r}\frac{\partial\Psi}{\partial r}) + \frac{1}{2mr^2}\hat{L}^2\Psi + V(r)\Psi = E\Psi$
then given $\hat{L}^2$ has eigenvalue $l(l+1)\hbar^2$
Ψ should satisfy both R related function and $\hat{L}^2$'s eigenfunction Y_l^m
so suppose:
$\Psi = R(r)Y_l^m$
the above equation is:
$-\frac{\hbar^2}{2m}(R" + \frac{2}{r}R') + \frac{l(l+1)}{2mr^2}R + V(r)R = ER$
given in this problem $l = 0$ and $V = 0$ when $r < b$
$-\frac{\hbar^2}{2m}(R" + \frac{2}{r}R') = ER$
substitute $R = g(r)/r$
$g" + \frac{2mE}{\hbar^2}g = 0$
$g(r) = rR = Acos(\frac{\sqrt{2mE}}{\hbar}r) + Bsin(\frac{\sqrt{2mE}}{\hbar}r)$
One is from this substitution, $g(0) = 0R = 0$
So $A = 0$
Another is from the boundary condition:
$r = b, g = 0$
Namely:
$\frac{\sqrt{2mE}}{\hbar}b = n\pi$
$E = \frac{n^2h^2}{8mb^2}$
$R(r) = g(r)/r = \frac{B}{r}sin(\frac{\sqrt{2mE}}{\hbar}r)$

6.3

(a) if idential force in all direction
$V = \frac{1}{2}k(x^2 + y^2 + z^2) = \frac{1}{2}kr^2$
irrelevant to θ and ϕ
So the wave function is:
$\Psi = R(r)Y_l^m(\theta, \phi)$
(c) using the same function as in **6.2**
$-\frac{\hbar^2}{2m}(R'' + \frac{2}{r}R') + \frac{l(l+1)}{2mr^2}R + V(r)R = ER$
when $V(r) = \frac{1}{2}kr^2$
(d) verifiying from a harmonic oscillator point of view:
$\Psi = (\alpha/\pi)^{3/4}e^{-\alpha r^2/2}$
there is no θ or ϕ
So in Hamilton operator, it means $\Psi = R(r)Y_l^m(\theta, \phi)$
where $Y_l^m(\theta, \phi) = constant$, namely $l = 0$

6.5

(a) False
(b) True

6.6

two particles are not related to each other
$E = \frac{h^2}{8l^2}(\frac{n_1^2}{m_1} + \frac{n_2^2}{m_2})$
Given the six lowest state:
$(1, 1), (1, 2), (2, 1), (2, 2), (2, 3), (3, 2)$

6.7

(a)True
$\frac{m_1 m_2}{m_1 + m_2} < m_1 < m_2$
(b) True
$V(r)$ is part of the internal wave function potential energy

6.8

(a) True
Since $J = 4$, it has $2 * 4 + 1 = 9$ different m value
(b) False
Distance $E_{div} = 2(J + 1)B$
(c) True
Spacing between teo E_{div} is $2B$
(d) True

the fact is bond length is almost the same, but E_{rot} is different since μ is different
(e) True
It is the same atom

6.9

(a)Given the energy difference between $J = 0$ and $J = 1$:
$E_{div} = \frac{J(J+1)\hbar^2}{2\mu d^2} - 0 = \frac{2\hbar^2}{2\mu d^2}$
where $\mu = \frac{m_1 m_2}{m_1+m_2} = \frac{12*16}{(12+16)*6.02*10^{23}}$
So:
$d = 1.13\mathring{A}$
(b) the first absorption is from $J = 0$ and $J = 1$
the next two is from $J = 1$ to $J = 2$ and $J = 2$ to $J = 3$
where the first is $2(J + 1)B = 2B$
the next two is $2(J + 1)B = 4B$ and $2(J + 1)B = 6B$
so the frequency is twice and three times of the original lowest absorption:
$\nu_2 = 2 * 115271 MHz$
$\nu_3 = 3 * 115271 MHz$
(c) the bond length is almost the same
the difference is in reduced mass μ
$hv_{new} = \frac{1*2\hbar^2}{2\mu_{new} d^2}$

6.10

Given the emission energy:
$E_{div} = hv = 2(J + 1)B = 2 * 3B = h * 126.4GHz$
So $E_{div} = hv_2 = 2(J + 1)B = 2 * (5 + 1)B = 12B = h * v_2$
So:
$v_2 = 2 * v = 252.8GHz$

6.11

$E_{div} = \frac{8*(8+1)\hbar^2}{2\mu d^2} - \frac{7(7+1)\hbar^2}{2\mu d^2} = h\nu$
where $\nu = 104189.7MHz$
So: $d = 2.36\mathring{A}$

6.12

the difference between two emission is $2B = h\nu = h * (921.84 - 806.65)GHz$
the initial emission is $115.19GHz$

6.13

adding the correction to the rigid rotator:

$\Delta E = 2(J+1)Bh - hD[(J+1)^2(J+2)^2 - J^2(J+1)^2]$
$= 2(J+1)Bh - 4hD(J+1)^3$
So emission $\nu_{0-1} = 2B - 4D$
emission $\nu_{4-5} = 10B - 500D$
$D = 0.183MHz$

6.14

Given $I = m_1\rho_1^2 + m_2\rho_2^2$
and $m_1\rho_1 = m_2\rho_2$ and $\mu = \frac{m_1 m_2}{m_1+m_2}$
$I = \mu(\rho_1 + \rho_2)^2 = \mu d^2$

6.15

the Coulon force is $F = \frac{e^2}{4\pi\epsilon_0 r^2}$
the gravity force is $G = \frac{Gm_p m_e}{r^2}$
which is negligible

6.17

(a) the energy of H atom:
$\Delta E = -13.598eV * (\frac{1}{6^2} - \frac{1}{3^2}) = h\nu = h\frac{c}{\lambda}$
So $\lambda = 1094.12nm$
(b) for He^+ it has the same energy equation $E = -13.598eV * \frac{Z^2}{n^2}$
where $Z^2 = 4$
So $\nu_{He} = 4\nu_H$
$\lambda = \frac{\lambda_H}{4} = 273.5nm$

6.18

Given the emission wavelengths:
$\lambda = \frac{c}{\nu} = \frac{ch}{\Delta E} = \frac{ch}{\frac{-13.6eV}{n_1^2} - \frac{-13.6eV}{n_2^2}}$
So try different values of n_1 and n_2
They have values $n = 2, 3, 7, 8$

6.23

Given ground state $\Psi_{100} = \frac{1}{\sqrt{\pi}}\frac{Z}{a}^{3/2}e^{-Zr/a}$
So $<r>= \int |\Psi|^2 r d\tau$
In spherical coordinate:
$<r>= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |\Psi|^2 r r^2 sin\theta dr d\theta d\phi = \frac{3a}{2Z}$

6.24

for $2p_0$:
$\Psi_{210} = \frac{1}{\sqrt{\pi}}\frac{Z}{2a}^{5/2} re^{-Zr/2a} cos\theta$
So $< r >= \int |\Psi|^2 r d\tau$
in spherical coordinate:
$< r >= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |\Psi|^2 r r^2 sin\theta dr d\theta d\phi = \frac{5a}{Z}$

6.25
for $2p1$:
$\Psi_{211} = \frac{1}{8\sqrt{\pi}}\frac{Z}{a}^{5/2} re^{-Zr/2a} sin\theta e^{i\phi}$
$< r >= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |\Psi|^2 r r^2 sin\theta dr d\theta d\phi = \frac{30a^2}{Z^2}$

6.26
Given the original:
$< r >= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |\Psi|^2 r r^2 sin\theta dr d\theta d\phi = \int_0^{2\pi} r^3 |R_{nl}|^2 dr \int_0^{\pi}\int_0^{\infty} |Y_l^m|^2 sin\theta d\theta d\phi =$
$\int_0^{2\pi} r^3 |R_{nl}|^2 dr$

6.27
$R_{2s} = b_0(1 - Zr/2a)e^{-Zr/2a}$
using normalization:
$\int_0^{\infty} R_{2s}^2 r^2 dr = 1$
$b_0 = \frac{Z}{a}^{3/2}\frac{1}{\sqrt{2}}$
$R_{2p} = re^{-Zr/2a} b_0$
using the same normalization method:
$R_{2p} = \frac{1}{\sqrt{24}}\frac{Z}{a}^{5/2} re^{-Zr/2a}$

6.28
for s states, for example: $\Psi_{100} = \frac{1}{\sqrt{\pi}}\frac{Z}{a}^{3/2} e^{-Zr/a}$

6.35
$E =< H >= \int \Psi^* H \Psi d\tau = \int \Psi^*(T + V)\Psi d\tau =< T > + < V >$

6.36
$V = -\frac{e^2}{4\pi\epsilon r}$
$E = -\frac{e^2}{8\pi\epsilon r}$
So $T = E - V = \frac{e^2}{8\pi\epsilon r}$
So $T/V = 1/2$

6.38

p_z is p_0 depicted by L_z
p_x is depicted by L_x
p_y is depicted by L_y

6.39

Given $Af = af$ and $Ag = bg$
if $A(c_1 f + c_2 g = c_1 af + c_2 bg = a(c_1 f + c_2 \frac{b}{a} g)$
So we need $a = b$

6.40

(a)for $2p_z$, it is the eigenfunction of $\hat{H}, \hat{L}^2, \hat{L}_z$
(b)for $2p_x$,it is the eigenfunction of $\hat{H}, \hat{L}^2$
(c)for $2p_1$,it is the eigenfunction of $\hat{H}, \hat{L}^2, \hat{L}_z$

6.42

p_x, p_y, p_z orthogonal to each other
$\int_0^{2\pi} cos\phi sin\phi = 0$
$\int_0^{2\pi} cos\phi = 0$
$\int_0^{2\pi} sin\phi = 0$

6.52

(a) dx, from 0 to l
(b) dx, from $-\infty$ to ∞
(c) dxdydz, from $-\infty$ to ∞
(d) $r^2 sin\theta dr d\theta d\phi$, from 0 to ∞, from 0 to π, from 0 to 2π

6.54

(a) harmonic oscillator, since $E = (n + \frac{1}{2})h\nu$
(b) rigid rotator, $\Delta E = 2(J+1)Bh$
(c) H atom, $E = -13.6eV * \frac{Z^2}{n^2}$

6.55

(a) infinite number of bound state energy: particle in a box where $V = \infty$ outside
(b) finite number of bound state energy: particle in a well where $V = a$ outside
(c) particle in a box, $E = \frac{n^2 h^2}{8ml^2}$

6.56

(a) false
(b) true
(c) false, electron is $-e$
(d) true
(e) false, it is not on a circle orbit only
(f) false, s state is not 0 at center
(g) false
(h) true
(i) false