25

Rework previous problem for general n

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

$$\rightarrow \quad \langle x \rangle = \frac{a}{2} \quad \forall n$$

$$\langle x^2 \rangle = a^2\left[\frac{1}{3} - \frac{1}{2n^2\pi^2}\right]$$

$$\langle p \rangle = 0 \quad \forall n$$

$$\langle p^2 \rangle = \left(\frac{n\hbar\pi}{a}\right)^2$$

$$\Delta x = a\sqrt{\frac{n^2\pi^2 - 6}{12 n^2\pi^2}}$$

$$\Delta p = n\hbar\pi / a$$

$$\Delta x \Delta p = \hbar\sqrt{\frac{n^2\pi^2-6}{12}}$$

$$= \begin{cases} 0.568\,\hbar & (n=1) \\ 1.67\,\hbar & (\ 2) \\ 2.63\,\hbar & (\ 3) \end{cases}$$

26a Harmonic Oscillator

$$V(x) = \frac{1}{2} m\omega^2 x^2$$

$$\psi_0(x) = A_0 \, e^{-\alpha x^2/2}$$

$$\psi_1(x) = A_1 \, x \, e^{-\alpha x^2/2}$$

$$\left(\alpha = \frac{m\omega}{\hbar}\right)$$

Sch. Eq^n (TISE)

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_n(x)}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi_n(x) = E_n \psi_n(x)$$

Subst $\psi_0(x)$ and $\psi_1(x)$ into TISE

to (i) check that LHS = RHS ✓✓

and (ii) determine E_0 and E_1

$\rightarrow$ $E_0 = \hbar\omega/2$ and $E_1 = \frac{3\hbar\omega}{2}$

\#

Normalize :

$$\int_{-\infty}^{\infty} \psi_0^*(x)\, \psi_0(x)\, dx = 1$$

26b

$$A_0^2 \int_{-\infty}^{\infty} e^{-\alpha x^2} dx = 1$$

$$A_0^2 \sqrt{\frac{\pi}{\alpha}} = 1$$

$$\therefore \quad A_0 = \left(\frac{\alpha}{\pi}\right)^{1/4}$$

$+$

$$\int_{-\infty}^{\infty} \psi_1^*(x)\, \psi_1(x)\, dx = 1$$

$$A_1^2 \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = 1$$

$$A_1^2 \cdot \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}} = 1$$

$$\therefore \quad A_1 = \left(\frac{4\alpha^3}{\pi}\right)^{1/4}$$

27a

$\psi_1(x)$ of Harmonic Oscillator

Kinetic Energy $\quad K = p^2/2m$

$$\langle K \rangle = \frac{\langle p^2 \rangle}{2m}$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \psi_1^*(x)\, \hat{p}^2\, \psi_1(x)\, dx$$

$$= \int_{-\infty}^{\infty} \psi_1^*(x) \left(-\hbar^2 \frac{d^2 \psi_1(x)}{dx^2} \right) dx$$

$$= -\hbar^2 A_1^2 \int_{-\infty}^{\infty} x e^{-\alpha x^2/2} \left[e^{-\alpha x^2/2} (\alpha^2 x^3 - 3\alpha x) \right] dx$$

$$= -\hbar^2 A_1^2 \cdot 2 \left[\alpha^2 \underbrace{\int_0^{\infty} x^4 e^{-\alpha x^2} dx}_{\frac{3}{8}\sqrt{\frac{\pi}{\alpha^5}}} - 3\alpha \underbrace{\int_0^{\infty} x^2 e^{-\alpha x^2} dx}_{\frac{1}{4}\sqrt{\frac{\pi}{\alpha^3}}} \right]$$

$$\therefore \langle p^2 \rangle = \frac{3}{2} \hbar^2 \alpha = \frac{3}{2} m\omega\hbar$$

$$\therefore \langle K \rangle = \frac{3}{4} \hbar\omega$$

27b

$$V = \frac{1}{2} m\omega^2 x^2$$

$$\langle V \rangle = \frac{1}{2} m\omega^2 \langle x^2 \rangle$$

$$\langle x^2 \rangle = A_1^2 \int_{-\infty}^{\infty} x e^{-\alpha x^2/2} \cdot x^2 \cdot x e^{-\alpha x^2/2} dx$$

$$= 2A_1^2 \int_0^{\infty} x^4 e^{-\alpha x^2} dx$$

$$= 2A_1^2 \cdot \frac{3}{8}\sqrt{\frac{\pi}{\alpha^5}}$$

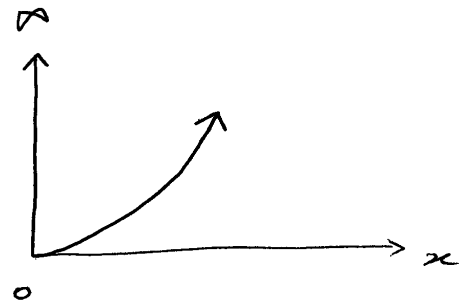
$$= \frac{3}{2\alpha} = \frac{3\hbar}{2m\omega}$$

So $\langle V \rangle = \frac{3}{4}\hbar\omega \quad = \langle K \rangle$

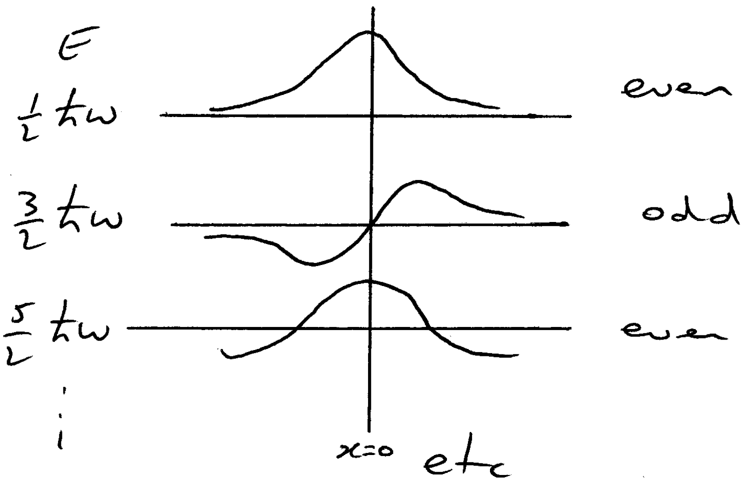
$$\langle V \rangle + \langle K \rangle = \frac{3}{2}\hbar\omega$$

$= E_1$ from previous problem ✓

A semi-harmonic oscillator



The $\psi_n(x)$ for the full harmonic oscillator are



In the semi-H.O. $V \to \infty$ at $x=0$

$$\therefore \quad \psi_n(x) = 0 \quad \text{at } x = 0$$

$\therefore$ only the 'odd' $\psi_n(x)$ apply

$$\therefore E_{semi} = \frac{3}{2}\hbar\omega, \ \frac{7}{2}\hbar\omega, \ \frac{11}{2}\hbar\omega \ldots$$

29 $\quad \psi(r) = e^{-r/a_0}$

Radial form of TISE

$$-\frac{\hbar^2}{2m}\cdot\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi(r)}{dr}\right) - \frac{e^2}{4\pi\varepsilon_0 r}\psi(r) = E\,\psi(r)$$

$$\Rightarrow -\frac{\hbar^2}{2m}e^{-r/a_0}\left[\frac{1}{a_0^2} - \frac{2}{a_0 r}\right] - \frac{e^2}{4\pi\varepsilon_0 r}e^{-r/a_0} = E\,e^{-r/a_0}$$

$$\Rightarrow E = -\frac{\hbar^2}{2m}\left[\frac{1}{a_0^2} - \frac{2}{a_0 r}\right] - \frac{e^2}{4\pi\varepsilon_0 r}$$

– no r-dependence

$$\therefore \quad \frac{\hbar^2}{m a_0 r} = \frac{e^2}{4\pi\varepsilon_0 r}$$

$$\rightarrow \quad a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$$

$$E = -\frac{\hbar^2}{2ma_0^2} = -\frac{me^4}{2\hbar^2(4\pi\varepsilon_0)^2} = -13.6\ \text{eV}$$

30a

$$\psi(r) = A e^{-r/a_0}$$

Normalize:

$$A^2 \int_0^\infty e^{-2r/a_0} \cdot 4\pi r^2 \, dr = 1$$

$$4\pi A^2 \underbrace{\int_0^\infty r^2 e^{-2r/a_0} \, dr}_{\frac{2!}{(2/a_0)^3}} = 1$$

$$\Rightarrow \quad A = \frac{1}{\sqrt{\pi a_0^3}}$$

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

$$\therefore \quad \langle V \rangle = -\frac{e^2}{4\pi\varepsilon_0} \left\langle \frac{1}{r} \right\rangle$$

$$\left\langle \frac{1}{r} \right\rangle = A^2 \int_0^\infty \frac{1}{r} e^{-2r/a_0} \cdot 4\pi r^2 \, dr$$

$$= \frac{4\pi}{\pi a_0^3} \underbrace{\int_0^\infty r e^{-2r/a_0} \, dr}_{1/(2/a_0)^2} = \frac{1}{a_0}$$

30b

$$\therefore \langle V \rangle = \frac{-e^2}{4\pi\varepsilon_0 a_0}$$

$$= -27.2 \text{ eV}$$

$$= -2 \times E$$

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$$\psi(r) = C \cdot \frac{r}{a_0} e^{-r/2a_0}$$

Probability : $P(r) = 4\pi r^2 \psi^*(r)\psi(r)$

$$= \frac{4\pi C^2}{a_0^2} r^4 e^{-r/a_0}$$

"Most likely" means maximum probability

$$\therefore \frac{dP(r)}{dr} = 0$$

$$\therefore \frac{d}{dr}\left[r^4 e^{-r/a_0}\right] = 0$$

$$4r^3 = \frac{r^4}{a_0}$$

$$\therefore r = 4a_0$$

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Lyman series : $n_{final} = 1$

transitions $n_{initial} = 2 \rightarrow 1$

$3 \rightarrow 1$

$$\Delta E = hf = \frac{hc}{\lambda} = 13.6\left(1 - \frac{1}{n_i^2}\right) \text{ eV}$$

$n_i = 2$ $\Delta E = 10.2$ eV

$\lambda = 1.219 \times 10^{-7}$ m

$n_i = 3$ $\Delta E = 12.09$ eV

$\lambda = 1.028 \times 10^{-7}$ m

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$$E_n = -\frac{13.6}{n^2} \text{ eV}$$

transition $(n+1) \rightarrow n$

$$\Delta E = 13.6\left[\frac{1}{n^2} - \frac{1}{(n+1)^2}\right] \text{ eV}$$

$$= 13.6\left[\frac{2n+1}{n^2(n+1)^2}\right]$$

33b

For large n

$$\frac{2n+1}{n^2(n+1)^2} \sim \frac{2n}{n^4} = \frac{2}{n^3}$$

$$\therefore \Delta E = 13.6 \times \frac{2}{n^3} = \frac{27.2}{n^3} \text{ eV}$$

$$= \frac{27.2e}{n^3} \text{ J}$$

$$= hf$$

$$\therefore f = \frac{27.2e}{hn^3} \text{ Hz}$$

34a

$$x = r \sin\theta \cos\phi$$

$$y = r \sin\theta \sin\phi$$

$$z = r \cos\theta$$

Chain Rule

$$\frac{\partial}{\partial \phi} = \frac{\partial}{\partial x} \cdot \frac{\partial x}{\partial \phi} + \frac{\partial}{\partial y} \cdot \frac{\partial y}{\partial \phi} + \frac{\partial}{\partial z} \cdot \frac{\partial z}{\partial \phi}$$

$$\frac{\partial x}{\partial \phi} = -r \sin\theta \sin\phi = -y$$

$$\frac{\partial y}{\partial \phi} = r \sin\theta \cos\phi = +x$$

$$\frac{\partial z}{\partial \phi} = 0$$

$$\Rightarrow \quad \frac{\partial}{\partial \phi} = -y \frac{\partial}{\partial x} + x \frac{\partial}{\partial y}$$

$$\hat{\underset{\sim}{L}}_z = (\hat{\underset{\sim}{r}} \times \hat{\underset{\sim}{p}})_z \qquad (\underset{\sim}{l} = \underset{\sim}{r} \times \underset{\sim}{p})$$

$$\hat{L}_z = \hat{x} \hat{p}_y - \hat{y} \hat{p}_x$$

34b $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ and $\hat{p}_y = -i\hbar \frac{\partial}{\partial y}$

$$\therefore \hat{L}_z = -i\hbar \left[x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right]$$

$$= -i\hbar \frac{\partial}{\partial \phi}$$

$$\hat{L}_z \psi_{nlm} = -i\hbar \frac{\partial \psi_{nlm}}{\partial \phi}$$

$$= -i\hbar \frac{\partial}{\partial \phi} \left[R(r)\, \Theta(\theta)\, e^{im\phi} \right]$$

$$= -i\hbar R(r)\, \Theta(\theta) \times im e^{im\phi}$$

$$= m\hbar R(r)\, \Theta(\theta)\, e^{im\phi}$$

$$= m\hbar \psi_{nlm}$$

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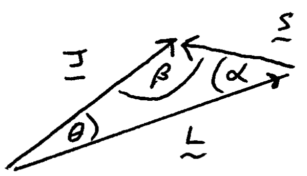
$$^2F_{5/2} = {}^{2S+1}L_J$$

$\therefore S = \frac{1}{2}$, $J = 5/2$

and 'F' means $L = 3$ (S P D F G ....)

$$\left.\begin{aligned} |\underset{\sim}{J}| &= \sqrt{J(J+1)} = \frac{\sqrt{35}}{2} \\ |\underset{\sim}{L}| &= \sqrt{L(L+1)} = \sqrt{12} \\ |\underset{\sim}{S}| &= \sqrt{S(S+1)} = \frac{\sqrt{3}}{2} \end{aligned}\right\} \text{in units of } \hbar$$



Cosine Rule

$$\left(\frac{\sqrt{3}}{2}\right)^2 = \left(\sqrt{12}\right)^2 + \left(\frac{\sqrt{35}}{2}\right)^2 - \frac{2\cdot\sqrt{12}\cdot\sqrt{35}}{2}\cos\theta$$

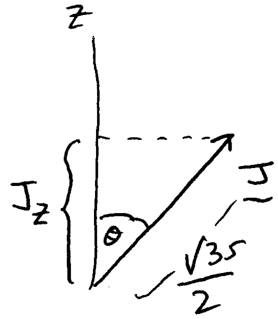
$$\Rightarrow \theta = 12.56^\circ$$

similarly, $\alpha = 48.19^\circ$

$$\beta = 180^\circ - (\alpha + \theta) = 119.25^\circ$$

36 $J = 5/2$

in units of $\hbar$



$$\theta = \cos^{-1}\left(\frac{J_z}{(\sqrt{35}/2)}\right)$$

$2J+1 = 6 \quad \therefore \quad 6$ possible orientations of $\underset{\sim}{J}$

J_z	$\theta(°)$
$+5/2$	32.31
$+3/2$	59.53
$+1/2$	80.27
$-1/2$	99.73
$-3/2$	120.47
$-5/2$	147.69