Homework [4] SOLUTIONS

$$\hat{H} = \frac{\hat{p}^2}{2m} \qquad \hat{H}\psi(x) = E\psi(x) = \int \frac{-h^2}{2m} \frac{d^2\psi}{dx^2} - E\psi = 0 = \int \frac{d^2\psi}{dx^2} + k^2\psi = 0$$
(with $k^2 = \frac{2mE}{h^2}$)
So $\psi(x) = Ae^{-ikx} + Be^{-ikx}$

Now
$$\psi(x) = \psi(x+L)$$
. In particular $\psi(0) = \psi(L) = Ae^{ikL} + Be^{-ikL}$
Also for $x = \frac{\pi}{2k}$, $\psi(\frac{\pi}{2k}) = (\frac{\pi}{2k} + L) = iAe^{ikL} - iBe^{-ikL} = iA-iB$

Add the two above equations to get 2Aeikl = 2A

So A=0 or
$$e^{ikL} = 1$$

$$kL = 2nTT \left(n = 0, \pm 1, \pm 2, \pm 3,\right)$$

IF A=0, Be-ikh = B, so once again KL = 2nTT (nEZ) since both A and B cannot both be O.

So
$$\psi_n(x) = A e^{\frac{2\pi i n x}{L}}$$
 (neZ)

Normalize:
$$1 = \int_0^L dx |\psi_n(x)|^2 = \int_0^L dx |A|^2 e^{\frac{2\pi i \pi x}{L}} = |A|^2 L$$
So $|\psi_n(x)| = \frac{1}{\sqrt{L}} e^{\frac{2\pi i \pi x}{L}} (n \in \mathbb{Z})$

And
$$E_n = \frac{\hbar^2 k^2}{2m} = \left(\frac{2n\pi t}{L}\right)^2 \frac{\hbar^2}{2m} = \left[\frac{2}{m} \left(\frac{n\pi k}{L}\right)^2\right]$$

Note: Except for n=0, all states all doubly degenerate (±n states have the same energy)

$$\langle n|H'|n\rangle = V \cdot \frac{1}{L} \int_{0}^{L} dx e^{-\frac{\lambda^{2}}{2}} e$$

$$\frac{-\sqrt{\ln a}}{L} \pm \sqrt{\frac{2}{2}} \cdot \sqrt{\frac{a\sqrt{\pi}}{L}} = \frac{-\frac{4\pi^2n^2a^2}{L^2}}{\sqrt{\frac{a\sqrt{\pi}}{L}}}$$

$$= \frac{-4\pi^2n^2a^2}{L^2}$$

$$= \frac{4\pi^2n^2a^2}{L^2}$$

(c) We can work out the good states By from the above matrix, but we can also figure out the good basis by using the Parity operator,
$$P:x \to -x$$

$$|n_{s}\rangle = \frac{1}{12}(|n\rangle + |-n\rangle)$$
 $P|n_{s}\rangle = |n_{s}\rangle$
 $|n_{h}\rangle = \frac{1}{12}(|n\rangle - |-n\rangle)$ $P|n_{h}\rangle = -|n_{h}\rangle$

$$\frac{1}{\sqrt{n_s(x)}} = \frac{2\pi i n x}{\sqrt{2L}} \left(e^{\frac{2\pi i n x}{L}} + e^{\frac{2\pi i n x}{L}} \right) \cdot \frac{1}{\sqrt{2L}}$$

$$\frac{1}{\sqrt{n_s(x)}} = \frac{1}{\sqrt{n_s^2 L}} \left(e^{\frac{2\pi i n x}{L}} - e^{\frac{2\pi i n x}{L}} \right)$$

We can check from the matrix W that these states are actually a good basis

$$\frac{\pi a}{L} \left(\frac{1}{e} + \frac{\pi a}{L^2} \right) \left(\frac{1}{L} \right) = \frac{\pi a}{L} \left(\frac{1}{L} + e^{\frac{\pi a}{L^2}} \right) \left(\frac{1}{L} \right)$$

$$\frac{\sqrt{\pi} \alpha}{L} \left(\frac{e^{-\frac{4\pi^2n^2\alpha^2}{L^2}}}{e^{-\frac{4\pi^2n^2\alpha^2}{L^2}}} \right) \left(\frac{1}{-1} \right) = \frac{\sqrt{\pi} \alpha}{L} \left(1 - e^{-\frac{4\pi^2n^2\alpha^2}{L^2}} \right) \left(\frac{1}{-1} \right) = \frac{\sqrt{\pi} \alpha}{L} \left(1 - e^{-\frac{4\pi^2n^2\alpha^2}{L^2}} \right) \left(\frac{1}{-1} \right) = \frac{\sqrt{\pi} \alpha}{L} \left(1 - e^{-\frac{4\pi^2n^2\alpha^2}{L^2}} \right) \left(\frac{1}{-1} \right) = \frac{\sqrt{\pi} \alpha}{L} \left(1 - e^{-\frac{4\pi^2n^2\alpha^2}{L^2}} \right) \left(\frac{1}{-1} \right) = \frac{\sqrt{\pi} \alpha}{L} \left(\frac{1$$

2 (Graffiaks 6.8)

Ground State:

$$E_{0}^{(1)} = \langle \Psi_{111} | H' | \Psi_{111} \rangle = \int dx dy dz \left(\int_{a}^{a} \right) \sin^{2} \left(\frac{\pi x}{a} \right) \sin^{2} \left(\frac{\pi x}{a} \right) \sin^{2} \left(\frac{\pi z}{a} \right) \cdot \frac{3}{4} V_{0} S(x - \frac{\pi}{4}) S(x - \frac{3}{4}) S($$

1st Excited State

We'll guess that the good states are simply, (4112), (4211) call them: (a) (b) 10>

Note that,

lote that,
$$\left(Y_{n_1 n_2 n_3} \mid H' \mid Y_{n_1 n_2 n_3}\right) = \int d\kappa d\gamma dz \left(\sqrt{\frac{2}{\alpha}}\right) \sin \left(\frac{n_1 \pi x}{\alpha}\right) \sin \left(\frac{n_2 \pi y}{\alpha}\right) \sin \left(\frac{n_2 \pi y}{\alpha}\right) \sin \left(\frac{n_3 \pi x}{\alpha}\right) \sin \left(\frac{n_3 \pi x}{\alpha}\right) \sin \left(\frac{n_2 \pi y}{\alpha}\right) \sin$$

Note + had if n=2 or m=2 => <4,n,n,3/H'/4,m,m,3/=0

Need to calculate the other values

$$\langle 112|H'|112\rangle = \sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)$$

$$\langle 112|H'|211\rangle = \sin(\frac{\pi}{4})\sin(\frac{\pi}{2$$

$$\langle 211 | H' | 211 \rangle = \sin(\frac{\pi}{2}) \sin(\frac{\pi}{2}) \sin(\frac{\pi}{2}) \sin(\frac{3\pi}{4}) \sin(\frac{3\pi}{4}) \cdot 8V_{o}$$

5*

$$2\langle T \rangle = \langle \overrightarrow{P}, \overrightarrow{\nabla} V \rangle$$
 Virial theorem

$$\langle \vec{r}, \vec{\nabla} v \rangle = \langle r \frac{e^2}{4\pi\epsilon_0} \rangle = \frac{e^2}{4\pi\epsilon_0} \langle \frac{1}{r} \rangle$$

So
$$\frac{e^2}{4\pi\epsilon_0} \frac{1}{an^2} = \frac{e^2}{4\pi\epsilon_0} \left\langle \frac{1}{r} \right\rangle = \frac{1}{an^2}$$

$$\Rightarrow a = \frac{4\pi \epsilon_0 h^2}{me^2} \left(Bohr radius \right)$$

OR Use Feynman-Hellmann as I did in section!
$$\frac{\partial E_n}{\partial \lambda} = \langle \Psi_n | \frac{\partial \hat{H}}{\partial \lambda} | \Psi_n \rangle$$

Choose for instance >= Eo.

And
$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 \Gamma}$$
. So $\langle \Psi_n | \frac{\partial \hat{H}}{\partial \epsilon_0} | \Psi_n \rangle = \langle \frac{e^2}{4\pi\epsilon_0^2 \Gamma} \rangle = \frac{e^2}{4\pi\epsilon_0^2 \Gamma} \langle \frac{1}{\Gamma} \rangle$

So
$$\langle \frac{1}{r} \rangle = \frac{4\pi \varepsilon_0^2}{e^2} \frac{me^4}{\hbar^2 (4\pi)^2 \varepsilon_0^3} \frac{1}{n^2} = \frac{me^2}{4\pi \varepsilon_0 \hbar^2} \frac{1}{n^2} = \frac{1}{an^2}$$
 as promised!

Feynman-Hellmann theorem 4. (Griffing 6.16)

a) We'll do everything using index notation since its much easier.

I.S = LiS; We'll use "Einstein Summation" notation. This means that whenever you see on index twice (e.g. j). that means that its summed over,

i.e. $L_jS_j = \sum_{j=1}^{2} L_jS_j$

[L.S, L] = [L; S, Lkêk]

= ê,S; Ejka tla

= ê,Sj [Lj, Lk] since [Sj, Lk] = 0 [êx, 4]=0 [ex, Sj.]=0

Here ne've vied [Lx, Ly] = th Lz, etc.

This is expressed in index notation as

[Li, Li] = 60kthL

where $E_{ijk} = \begin{cases} 1 & \text{if } ijk = 123,231,312 \\ -1 & \text{if } ijk = 132,321,213 \end{cases}$

Note also that if

Ros AxB=C

Book & Gr

AxB = Exik A; B; Ek

= to Sile êx Ejre = Ezik

= + LoSjêx Erjk

b) [2.5,5] = [L;S;, S,êk]

= Ljêr[Sj,Sk]

- Liêr tejhe &

= LLi Seek Ejke

= LL; Seek Ezjk

=(\(\frac{1}{5}\)\)

(c)
$$= [\vec{L} \cdot \vec{S}, \vec{J}] = [\vec{L} \cdot \vec{S}, \vec{L} + \vec{S}]$$

 $= [\vec{L} \cdot \vec{S}, \vec{L}] + [\vec{L} \cdot \vec{S}, \vec{S}]$
 $= + \vec{L} \times \vec{S} + + + \vec{S} \times \vec{L}$
 $= + \vec{L} \times \vec{S} - + + \vec{L} \times \vec{S} = 0$

(f)
$$[\vec{c} \cdot \vec{s}, \vec{J}^2] = [\vec{c} \cdot \vec{s}, (\vec{c} + \vec{s}) \cdot (\vec{c} + \vec{s})]$$

$$= [\vec{c} \cdot \vec{s}, \vec{c}^2 + \vec{s}^2 + 2\vec{s} \cdot \vec{c}]$$

$$= [\vec{c} \cdot \vec{s}, \vec{L}^2] + [\vec{c} \cdot \vec{s}, \vec{s}^2] + 2[\vec{c} \cdot \vec{s}, \vec{s} \cdot \vec{c}] = 0$$

$$= (0)$$

Weed to calculate the matrix,

To do so. "It helps to write H'= K'xy in terms of raising and lowering operators,

H'= K'.
$$\sqrt{\frac{t}{2\pi\omega}} \left(\frac{a^{t}+a}{a^{t}} - \sqrt{\frac{t}{2\pi\omega}} \left(\frac{b^{t}+b}{a^{t}} \right) \right)$$

raising and raising and lowering for y direction

$$= \frac{K't}{2\pi\omega} \left(\frac{a^{t}+a}{a^{t}} \right) \left(\frac{b^{t}+b}{a^{t}} \right) = \frac{K't}{2\pi\omega} \left(\frac{a^{t}}{a^{t}} + \frac{a^{t}}{a^{t}} + a^{t}} + \frac{a^{t}}{a^{t}} + a^{t}} \right)$$

$$H'|20\rangle = \frac{k't}{2m\omega} \left(atb^{\dagger}|20\rangle + atb|20\rangle + ab^{\dagger}|20\rangle + ab|20\rangle \right)$$

$$= \frac{k't}{2m\omega} \left(\sqrt{3} |31\rangle + \sqrt{2} |11\rangle + (0) \right)$$

$$H'|02\rangle = \frac{K'h}{2m\omega} \left(atb^{\dagger}|02\rangle + atb|02\rangle + ab^{\dagger}|02\rangle + ab^{\dagger}|02\rangle + ab^{\dagger}|02\rangle$$

$$= \frac{K'h}{2m\omega} \left(\sqrt{3}|13\rangle + \sqrt{2}|11\rangle + 0 + 0$$

$$\frac{(20)H'(02)=0}{(11)H'(02)=\sqrt{2}} = \sqrt{2} \cdot \frac{K'h}{2mw}$$

$$H'|H'| = \frac{K't_1}{2mw} \left(a^{\dagger}b^{\dagger}|H'| + a^{\dagger}b|H'| +$$

:
$$\langle 11|H'|11\rangle = 0$$

 $\langle 20|H'|11\rangle = \frac{\sqrt{2} \, K' h}{2 \, m \omega}$
 $\langle 02|H'|11\rangle = \frac{\sqrt{2} \, K' h}{2 \, m \omega}$

$$\int_{\mathbb{R}^{3}} d\alpha (W-\lambda \mathbb{I}) = \int_{\mathbb{R}^{3}} (-\lambda^{\frac{1}{3}} - \lambda^{\frac{1}{3}} + 2\lambda)$$

$$= \lambda (2-\lambda^{\frac{1}{3}}) = \frac{1}{2} (\lambda - \sqrt{2}) (\lambda + \sqrt{2}) \cdot -\lambda = 0$$

: The eigenvalues are
$$\begin{cases} \lambda=0 \\ \lambda=\sqrt{2} \end{cases}$$

$$E_{1}^{(i)} = 0$$

$$E_{2}^{(i)} = \sqrt{2} \cdot \frac{\sqrt{2} \cdot k' h}{2 m \omega} = \frac{k' h}{m \omega}$$

$$E_{3}^{(i)} = -\frac{\sqrt{2} \cdot k' h}{2 m \omega} = -\frac{k' h}{m \omega}$$