Spring 2017

HW#4 Solution

10-14 in class we found,

$$\left\langle \frac{1}{r} \right\rangle_N = \frac{1}{n^2} \frac{1}{a_0}$$

$$\langle V \rangle = -e^2 \left\langle \frac{1}{r} \right\rangle = -\alpha \hbar c \left(\frac{1}{n^2 a_0} \right) = -\frac{\alpha^2 \mu c}{N^2}$$

$$= +2 E_N$$

then $E_n = +\frac{1}{2} \langle V \rangle$

$$\langle K \rangle = \langle H \rangle - \langle V \rangle = E_N - \langle V \rangle = -E_N = -\frac{1}{2} \langle V \rangle$$

this is the virial theorem, since

$$\vec{r} \cdot \vec{\nabla} V(r) = -e^2 r \frac{d}{dr} \left(\frac{1}{r} \right) = e^2 \frac{1}{r} = -V$$

and from problem 10,12, $\langle K \rangle = \frac{1}{2} \langle \vec{r} \cdot \vec{\nabla} V \rangle = -\frac{1}{2} \langle V \rangle$.

for the 3D harmonic oscillator,

$$\langle V^2 \rangle = \frac{1}{2} \mu \omega^2 \left\langle \left(x^2 + y^2 + z^2 \right) \right\rangle = \frac{3}{2} \mu \omega^2 \langle x^2 \rangle$$

$$= \frac{3}{2} \mu \frac{\omega^2 \hbar}{\mu \omega} \langle y^2 \rangle = \frac{3}{2} \hbar \omega \, \frac{1}{2} (2N+1)$$

since $\hat{y}^2 |N\rangle = \frac{1}{2} \left(a^2 + a^{+2} + 2a^+a + 1 \right) |N\rangle$

then $\langle V^2 \rangle = (2N+1) \frac{3}{4} \hbar \omega$

$$\langle \hat{K} \rangle = \frac{3}{2\mu} \langle P_x^2 \rangle = \frac{3}{2} \hbar\omega \langle \hat{q}^2 \rangle$$

again, $\hat{q}^2 = \left(\frac{i}{\sqrt{2}}\right)^2 (\hat{a}^\dagger - \hat{a})^2 = -\frac{1}{2}\left(a^{\dagger 2} + \hat{a}^2 - 2a^\dagger a - 1\right)$

so $\langle \hat{q}^2 \rangle = \frac{2N+1}{2}$

so $\langle K \rangle = \frac{3}{4} \hbar\omega (2N+1) = \langle \hat{V} \rangle$

from the virial theorem, we expect -

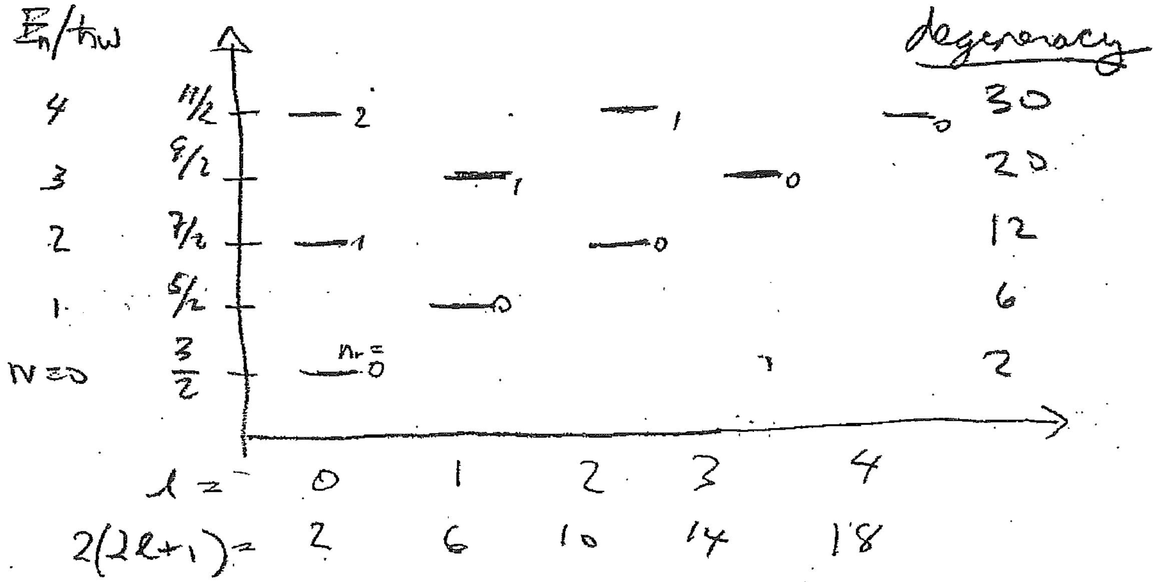
$$\vec{r} \cdot \vec{\nabla} V(r) = \left(x\frac{d}{dx} + y\frac{d}{dy} + z\frac{d}{dz}\right)\left(\frac{1}{2}\mu\omega^2\right)(x^2 + y^2 + z^2)$$

$$= 2V(r)$$

so we expect $\langle \hat{K} \rangle = \langle \hat{V} \rangle$.

Thus we verify the virial theorem for the 3D harmonic oscillator.

10.15 The Harmonic oscillator energy levels are -



degeneracy $\underline{d_N = (N+1)(N+2)}$

magic numbers: 2, 8, 20, 40, 70

10.17 2D harmonic oscillator

(a) $$\hat{H} = \underbrace{\frac{\hat{P}_x^2}{2\mu} + \frac{1}{2}\mu\omega^2\hat{x}^2}_{\hat{H}_x} + \underbrace{\frac{\hat{P}_y^2}{2\mu} + \frac{1}{2}\mu\omega^2\hat{y}^2}_{\hat{H}_y}$$

The wave function factorizes $|\psi\rangle = |n_x\rangle|n_y\rangle$

$$\hat{H}|\psi\rangle = (\hat{H}_x + \hat{H}_y)|n_x\rangle|n_y\rangle = (E_x + E_y)|n_x\rangle|n_y\rangle$$

$$E = (n_x + \tfrac{1}{2} + n_y + \tfrac{1}{2})\hbar\omega = (N+1)\hbar\omega$$

where $N = N_x + N_y = 0, 1, 2, \ldots$

(b) $$L_z = \hat{x}\hat{P}_y - \hat{y}\hat{P}_x$$

$$\hat{a}_x^\dagger \hat{a}_y = \left(\frac{\mu\omega}{2\hbar}\right)\left(\hat{x} + \frac{i}{\mu\omega}\hat{P}_x\right)^\dagger\left(\hat{y} + \frac{i}{\mu\omega}\hat{P}_y\right)$$

$$= \frac{\mu\omega}{2\hbar}\left(\hat{x}\hat{y} + \frac{i}{\mu\omega}(\hat{x}P_y - \hat{y}\hat{P}_x) - \left(\frac{1}{\mu\omega}\right)^2\hat{P}_x\hat{P}_y\right)$$

then since $[\hat{x},\hat{y}]=0$ and $[\hat{P}_x,\hat{P}_y]=0$,

$$\left(\hat{a}_x^\dagger\hat{a}_y - \hat{a}_x\hat{a}_y^\dagger\right) = \left(\frac{\mu\omega}{2\hbar}\right)\frac{2i}{\mu\omega}\left(\hat{x}\hat{P}_y - \hat{y}\hat{P}_x\right)$$

$$\hat{L}_z = \hat{x}\hat{P}_y - \hat{y}\hat{P}_x = \frac{\hbar}{i}\left(\hat{a}_x^\dagger\hat{a}_y - \hat{a}_x\hat{a}_y^\dagger\right)$$

Since $\hat{H}$ is invariant with respect to rotation about the $\hat{z}$ axis, we expect $[\hat{H}, \hat{L}_z] = 0$.

explicitly, $\hat{H} = \hbar\omega(\hat{a}_x^+ \hat{a}_x + \hat{a}_y^+ \hat{a}_y + 1)$

with $[\hat{a}_x, \hat{a}_x^+] = [\hat{a}_y, \hat{a}_y^+] = 1$ and other commutators $[\hat{a}_x, \hat{a}_y] = 0$, etc.,

$$[\hat{H}, \hat{L}_z] = \frac{\hbar^2\omega}{i}\left[\hat{a}_x^+\hat{a}_x + \hat{a}_y^+\hat{a}_y,\ \hat{a}_x^+\hat{a}_y - \hat{a}_x\hat{a}_y^+\right]$$

$$= \frac{\hbar^2\omega}{i}\Big\{[\hat{a}_x^+\hat{a}_x, \hat{a}_x^+]\hat{a}_y - [\hat{a}_x^+\hat{a}_x, \hat{a}_x]\hat{a}_y^+ + [\hat{a}_y^+\hat{a}_y, \hat{a}_y]\hat{a}_x^+ - [\hat{a}_y^+\hat{a}_y, \hat{a}_y^+]\hat{a}_x\Big\}$$

$[\hat{a}_x^+\hat{a}_x, \hat{a}_x^+] = \hat{a}_x^+$ and $[\hat{a}_x^+\hat{a}_x, \hat{a}_x] = -\hat{a}_x$

so $[\hat{H}, \hat{L}_z] = \frac{\hbar^2\omega}{i}\Big\{\hat{a}_x^+\hat{a}_y + \hat{a}_y^+\hat{a}_x - \hat{a}_y\hat{a}_x^+ + \hat{a}_y^+\hat{a}_x\Big\} = 0$

(c) $E_1 = 2\hbar\omega$ is doubly degenerate

$|n_x, n_y\rangle = |1,0\rangle$, $|n_x, n_y\rangle = |0,1\rangle$

$\hat{L}_z|1,0\rangle = \frac{\hbar}{i}(\hat{a}_x^+\hat{a}_y - \hat{a}_x\hat{a}_y^+)|1,0\rangle = i\hbar|0,1\rangle$

$\hat{L}_z|0,1\rangle = -i\hbar|1,0\rangle$

so $[L_z] = i\hbar\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

$$i\hbar \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \varepsilon \hbar \begin{pmatrix} a \\ b \end{pmatrix}$$

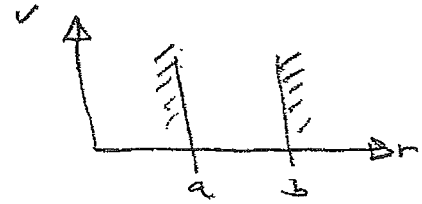
$$\begin{pmatrix} \varepsilon & i \\ -i & \varepsilon \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0$$

$$\varepsilon^2 = 1$$

eigenvalues $\pm\hbar$: $|\pm\rangle = \frac{1}{\sqrt{2}}\left(|1,0\rangle \pm i\, |0,1\rangle \right)$

10.18

$$V(r) = \begin{cases} 0 & a<r<b \\ \infty & \text{elsewhere} \end{cases}$$



in the interval $a<r<b$, the particle is free. We therefore have the free particle solution subject to the boundary condition $\Psi(a)=\Psi(b)=0$.

$$\Psi = \frac{U}{r} Y_{\ell m}$$

for $\ell=0$, $\quad U'' = -k^2 U \quad , \quad k^2 = \frac{2\mu E}{\hbar^2}$

$$U(r) = A \sin\left(k(r-a)\right) \quad \text{where } k(b-a) = n\pi$$

$$E_n = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{(b-a)^2} \qquad n=1,2,\ldots$$

$$\Psi_{1,0} = \frac{A}{r}\sin\left(\frac{\pi(r-a)}{b-a}\right)$$

$$\Psi_{2,0} = \frac{A}{r}\sin\left(\frac{2\pi(r-a)}{b-a}\right)$$

for $\ell \neq 0$ we would have to impose the boundary conditions on the general solutions, $j_\ell(\rho)$, $n_\ell(\rho)$.

10.19 $\hat{H} = \frac{\hat{P}_1^2}{2m_1} + \frac{\hat{P}_2^2}{2m_2} + V_a(r) + \left(\frac{1}{4} - \frac{\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2}{\hbar^2}\right) V_b(r)$

distinguishable

Since $\hat{H}$ is rotationally invariant, $|\psi\rangle = |\psi_{cm}\rangle |\psi_{rel}\rangle$
where $|\psi_{rel}\rangle = |space\rangle |spin\rangle$

$V_a(r)$ confines particle to $r < a$

$V_b(r)$ confines particle to $r < b$

write $\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left(\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2\right)$ and $\frac{1}{2} \otimes \frac{1}{2} = \underset{\text{triplet}}{1} \oplus \underset{\text{singlet}}{0}$

$s = 1, 0$

$$\left\langle \frac{1}{4} - \frac{\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2}{\hbar^2} \right\rangle = \frac{1}{4} - \frac{1}{2}\left[s(s+1) - 2\left(\tfrac{1}{2}\right)\left(\tfrac{1}{2}+1\right)\right]$$

$$= 1 - \frac{1}{2}s(s+1) = \begin{cases} 1 & s=0 \\ 0 & s=1 \end{cases}$$

Ground state energy for ∞ spherical well gives

$$E_{1\,\substack{l=0\\ s=0}} = \frac{\hbar^2}{2\mu}\left(\frac{\pi}{b}\right)^2$$

$$E_{\substack{l=0\\ s=1}} = \frac{\hbar^2}{2\mu}\left(\frac{\pi}{a}\right)^2 < E_{\substack{l=0\\ l=1}}$$

First excited state - $E_{1\,\substack{l=1\\ s=1}} = \frac{\hbar^2}{2\mu}\left(\frac{4.49}{a}\right)^2$

condition for $E_{1\,\substack{l=0\\ s=0}} < E_{1\,\substack{l=1\\ s=1}}$ to be first excited is

$$\frac{\pi}{b} < \frac{4.49}{a}$$

$$\frac{b}{a} < \frac{\pi}{4.49} \cong 0.7$$