Physics 606 Final Solution

1\. (a) $\hat{H} = \frac{1}{2I_x}\hat{L}^2 + \left(\frac{1}{2I_z} - \frac{1}{2I_x}\right)\hat{L}_z^2$

(b) $\langle \hat{L}^2 \rangle = \langle \ell m | \hat{L}^2 | \ell m \rangle = \ell(\ell+1)\hbar^2$

$\langle \hat{L}_z \rangle = \langle \ell m | \hat{L}_z | \ell m \rangle = m\hbar$

$\Rightarrow \langle \hat{H} \rangle = \frac{1}{2I_x}\ell(\ell+1)\hbar^2 + \left(\frac{1}{2I_z} - \frac{1}{2I_x}\right)m^2\hbar^2 \equiv E_{\ell m}$

(c) $\langle \hat{H} \rangle = \left(\sum_{\ell m} \langle \ell m | \psi^*_{\ell m}\right)\hat{H}\left(\sum_{\ell' m'} \psi_{\ell' m'} |\ell' m'\rangle\right)$

$= \sum_{\ell m}\sum_{\ell' m'} \psi^*_{\ell m}\psi_{\ell' m'} E_{\ell' m'} \delta_{\ell\ell'}\delta_{mm'}$

$= \sum_{\ell m} |\psi_{\ell m}|^2 E_{\ell m}$, $E_{\ell m}$ defined above

(d) This is a single energy eigenstate, so at <u>any</u> time t

$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle = e^{-i\hat{H}t}|3,0\rangle = e^{-iE_{3,0}t}|3,0\rangle$, so

$\boxed{\langle\psi(t)|\hat{L}_x|\psi(t)\rangle =} \langle 3,0| e^{+iE_{3,0}t}\frac{1}{2}(\hat{L}_+ + \hat{L}_-)e^{-iE_{3,0}t}|3,0\rangle$

$= \frac{1}{2}\left(\langle 3,0|\hat{L}_+|3,0\rangle + \langle 3,0|\hat{L}_-|3,0\rangle\right)$

$= \boxed{0}$

since $\hat{L}_+|\ell m\rangle \propto |\ell, m+1\rangle$ & $\hat{L}_-|\ell m\rangle \propto |\ell, m-1\rangle$.

(e) Use your own numbers, but

$I_z \sim Mr^2$ with $r \sim$ nuclear radius $\sim 10^{-4}R$

where $R \sim$ internuclear separation $\sim 1\,\text{Å}$,

with $I_x \sim MR^2$.

Then $\frac{I_z}{I_x} \sim \left(\frac{r}{R}\right)^2 \sim 10^{-8}$.

minimum angular momentum excited $\sim \hbar$

$\Rightarrow$ minimum energy for excitation of z-axis rotation

$\sim \frac{\hbar^2}{I_z} \sim 10^8 \frac{\hbar^2}{I_x}$

and temperature to excite z-axis rotation

$\sim 10^8 \times$ temperature to excite x & y rotations

2. $\int_b^a k(x)\,dx = (n+\frac{1}{2})\pi$ with $k(x)=0$ for $x=a$ and b

$$\frac{\hbar^2 k(x)^2}{2m} + \frac{1}{2}Kx^2 = E \Rightarrow k(x) = \pm\left(\frac{2m}{\hbar^2}E - \frac{mK}{\hbar^2}x^2\right)^{1/2}$$

$$= \pm\frac{(2mE)^{1/2}}{\hbar}\left(1-u^2\right)^{1/2}$$

where $u \equiv \left(\frac{\hbar^2}{2mE}\cdot\frac{mK}{\hbar^2}\right)^{1/2} x$

$$= \left(\frac{K}{2E}\right)^{1/2} x \quad , \quad \text{and} \quad dx = \left(\frac{2E}{K}\right)^{1/2} du$$

Then $\int_b^a k(x)\,dx = \frac{(2mE)^{1/2}}{\hbar}\int_{-1}^{1}(1-u^2)^{1/2}\cdot\left(\frac{2E}{K}\right)^{1/2} du$

$$= \frac{2E}{\hbar\omega}\cdot\frac{\pi}{2} \quad \text{since } \omega = \left(\frac{K}{m}\right)^{1/2}$$

so $\frac{2E}{\hbar\omega}\frac{\cancel{\pi}}{\cancel{2}} = (n+\frac{1}{2})\cancel{\pi}$

or $\boxed{E = (n+\frac{1}{2})\hbar\omega}$.

3. (a) $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$

$\boxed{\text{Note: A table of Gaussian integrals was provided.}}$

$$\frac{d\psi}{dx} = Ae^{-\alpha x^2} + Ax\,e^{-\alpha x^2}(-2\alpha x)$$

$$\frac{d^2\psi}{dx^2} = 3Ae^{-\alpha x^2}(-2\alpha x) + Ax\,e^{-\alpha x^2}(-2\alpha x)^2$$

$$1 = \int_{-\infty}^{\infty} \psi^*\psi\, dx = |A|^2 \int_{-\infty}^{\infty} dx\; x^2 e^{-2\alpha x^2} = |A|^2 \cdot \frac{1}{4\cdot 2\alpha}\sqrt{\frac{\pi}{2\alpha}}$$

$$\Rightarrow |A|^2 = 8\alpha\sqrt{\frac{2\alpha}{\pi}}$$

so $$\langle \hat{H} \rangle = 8\alpha\sqrt{\frac{2\alpha}{\pi}}\left[-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\; x\,e^{-\alpha x^2}(-6\alpha x + 4\alpha^2 x^3)e^{-\alpha x^2} + \frac{1}{2}m\omega^2\int_{-\infty}^{\infty} dx\; x^4 e^{-2\alpha x^2}\right]$$

$$= 8\alpha\cancel{\sqrt{\frac{2\alpha}{\pi}}}\left[-\frac{\hbar^2}{2m}\left(-6\cancel{\alpha}\cdot\frac{1}{4\cdot 2\cancel{\alpha}}\cancel{\sqrt{\frac{\pi}{2\alpha}}} + 4\cancel{\alpha^2}\cdot\frac{3}{8(2\cancel{\alpha})^2}\cancel{\sqrt{\frac{\pi}{2\alpha}}}\right) + \frac{1}{2}m\omega^2\cdot\frac{3}{8(2\alpha)^2}\cancel{\sqrt{\frac{\pi}{2\alpha}}}\right]$$

$$= -\frac{\hbar^2}{2m}(-6\alpha + 3\alpha) + \frac{1}{2}m\omega^2 \cdot \frac{3}{4\alpha}$$

$$= 3\frac{\hbar^2}{2m}\alpha + \frac{3}{8}m\omega^2\alpha^{-1}$$

$$0 = \frac{d\langle\hat{H}\rangle}{d\alpha} = 3\frac{\hbar^2}{2m} - \frac{3}{8}m\omega^2\alpha^{-2} \Rightarrow \boxed{\alpha = \frac{1}{2}\frac{m\omega}{\hbar}}$$

(b) Then $\boxed{\langle\hat{H}\rangle =}\; 3\frac{\hbar^{\cancel{2}}}{2\cancel{m}}\cdot\frac{1}{2}\frac{\cancel{m}\omega}{\cancel{\hbar}} + \frac{3}{8}\cancel{m}\omega^{\cancel{2}}\cdot 2\frac{\hbar}{\cancel{m}\cancel{\omega}}$

$$= \frac{3}{4}\hbar\omega + \frac{3}{4}\hbar\omega$$

$$= \boxed{\frac{3}{2}\hbar\omega}$$

(c) yes if the excited state is automatically orthogonal to all the lower states by symmetry, as for the $n=1$ state here

4. This is, in fact, a quite simplistic model of e.g. a quantum dot. More sophisticated models require more sophisticated treatments, with off-diagonal elements in degenerate perturbation theory (as in the Stark effect for the H atom) or 2nd-order perturbation theory, or a lot more for actual realism.

But for this model, which is the 3d version of the infinite square well:

(a) $|1\,1\,2\rangle$, $|1\,2\,1\rangle$, $|2\,1\,1\rangle$

(b) For this picture,

$$\psi_{112} = \sqrt{\frac{8}{a^3}}\,\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi y}{a}\right)\sin\left(\frac{2\pi z}{a}\right) \quad \text{etc.}$$

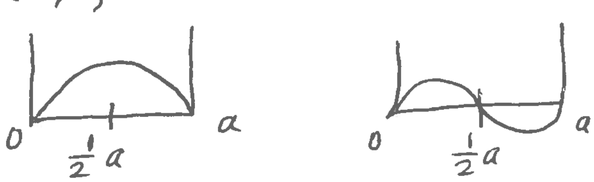
Now, the average value of $\sin^2$ over a half period is $\frac{1}{2}$, or one can evaluate $\int_0^a dx\,\sin^2\left(\frac{\pi x}{a}\right)$ using $\sin^2 u = \frac{1}{2}(1-\cos 2u)$. Similarly, one can evaluate e.g. $\int_0^a dz\; z\,\sin^2\left(\frac{\pi z}{a}\right)$ with this same replacement, plus $\int_0^\pi dv\; v\cos v = \int_0^\pi v\; d(\sin v)$ with integration by parts to get $\int_0^a dz\; z\,\sin^2\left(\frac{\pi z}{a}\right) = \frac{a^2}{4}$.

One can then get

$$\langle 1\,1\,2|z|1\,1\,2\rangle = \langle 1\,2\,1|z|1\,2\,1\rangle = \langle 2\,1\,1|z|2\,1\,1\rangle = \frac{1}{2}a$$

and show that the off-diagonal matrix elements $= 0$.

However, one can also get these results just from symmetry, with the basic idea



so $\langle z\rangle = \frac{1}{2}a$.

Then one has a diagonal matrix for $\langle n_x n_y n_z|V|n_x n_y n_z\rangle$ and the shifts are all $\boxed{\frac{1}{2}e\mathcal{E}a}$.

as for degenerate perturbation theory on pp. 231–234 of Baym.

5. Expand $e^{i\hat{L}\cdot\vec{\omega}\, t/\hbar}$ in a Taylor series and use the given commutation relations on the cover sheet. When the resulting series are written as sin and cos, the result is (after substantial algebra)

$$\hat{x}_{stat}(t) = \hat{x}\cos\omega t - \hat{y}\sin\omega t$$

$$\hat{y}_{stat}(t) = \hat{x}\sin\omega t + \hat{y}\cos\omega t$$

$$\hat{z}_{stat}(t) = \hat{z}$$

This is the same as we would have for ordinary vectors.