1. Eigenstates of potential

$$\psi_{n_x n_y n_z}(x,y,z) = \left(\frac{2}{a}\right)^{3/2} \sin\frac{n_x \pi x}{a} \sin\frac{n_y \pi y}{a} \sin\frac{n_z \pi z}{a}$$

Also have spins s_1 and s_2. Write states $\psi_\uparrow(s)$, $\psi_\downarrow(s)$

a) Ground state

Energy lowest if both elections have $n_x = n_y = n_z = 1$

But then spatial part of wavefunction is symmetric, so spin part needs to be antisymmetric

So

$$\boxed{\Psi(\vec{r}_1, s_1, \vec{r}_2, s_2) = \psi_{111}(\vec{r}_1)\psi_{111}(\vec{r}_2)\frac{1}{\sqrt{2}}\left[\psi_\uparrow(s_1)\psi_\downarrow(s_2) - \psi_\downarrow(s_1)\psi_\uparrow(s_2)\right]}$$

Only one state, so degeneracy $\boxed{d = 1}$

b) Excited state

Now can have one $n_i = 2$
Could be n_x, n_y, or n_z: 3 choices

If spatial part is symmetric, need antisymmetric spin $\equiv |00\rangle$

But if spatial part is antisymmetric, can have symmetric spin:
3 possibilities
$\psi_\uparrow(s_1)\psi_\uparrow(s_2) \equiv |11\rangle$ state
$\frac{1}{\sqrt{2}}\left[\psi_\uparrow(s_1)\psi_\downarrow(s_2) + \psi_\downarrow(s_1)\psi_\uparrow(s_2)\right] = |10\rangle$ state
$\psi_\downarrow(s_1)\psi_\downarrow(s_2) = |1\,{-1}\rangle$ state

Four possibilities for spin, so $3 \times 4 = 12$ states total
$\boxed{d = 12}$

List states:

$$\frac{1}{\sqrt{2}}\left[\psi_{211}(\vec{r}_1)\psi_{111}(\vec{r}_2)+\psi_{111}(\vec{r}_1)\psi_{211}(\vec{r}_2)\right]|00\rangle$$

$$\frac{1}{\sqrt{2}}\left[\psi_{121}(\vec{r}_1)\psi_{111}(\vec{r}_2)+\psi_{111}(\vec{r}_1)\psi_{121}(\vec{r}_2)\right]|00\rangle$$

$$\frac{1}{\sqrt{2}}\left[\psi_{112}(\vec{r}_1)\psi_{111}(\vec{r}_2)+\psi_{111}(\vec{r}_1)\psi_{112}(\vec{r}_2)\right]|00\rangle$$

$$\frac{1}{\sqrt{2}}\left[\psi_{211}(\vec{r}_1)\psi_{111}(\vec{r}_2)-\psi_{111}(\vec{r}_1)\psi_{211}(\vec{r}_2)\right]|11\rangle$$

$$\{ \qquad \text{''} \qquad \}|10\rangle$$

$$\{ \qquad \text{''} \qquad \}|1\,{-1}\rangle$$

$$\frac{1}{\sqrt{2}}\left[\psi_{121}(\vec{r}_1)\psi_{111}(\vec{r}_2)-\psi_{111}(\vec{r}_1)\psi_{121}(\vec{r}_2)\right]|11\rangle$$

$$\{ \qquad \text{''} \qquad \}|10\rangle$$

$$\{ \qquad \text{''} \qquad \}|1\,{-1}\rangle$$

$$\frac{1}{\sqrt{2}}\left[\psi_{112}(\vec{r}_1)\psi_{111}(\vec{r}_2)-\psi_{111}(\vec{r}_1)\psi_{112}(\vec{r}_2)\right]|11\rangle$$

$$\{ \qquad \qquad \}|10\rangle$$

$$\{ \qquad \qquad \}|1\,{-1}\rangle$$

2. a) Distinguishable particles

Label configurations by number of particles in state A $\equiv N_A$

Can have $N_A = 0, 1, 2, 3, 4, 5$ or 6 : seven configurations

For each configuration, have $Q(N_A)$ states

$Q(0) = 1$: all particles in ψ_B

$Q(1) = 6$: six ways to choose which particle in ψ_A

$Q(2) = \frac{6 \cdot 5}{2} = 15$: six choices for first particle, five for second, but order doesn't matter, divide by 2

$Q(3) = \frac{6 \cdot 5 \cdot 4}{2 \cdot 3} = 20$

$Q(4) = \frac{6 \cdot 5 \cdot 4 \cdot 3}{2 \cdot 3 \cdot 4} = 15$

$Q(5) = \frac{6 \cdot 5 \cdot 4 \cdot 3 \cdot 2}{2 \cdot 3 \cdot 4 \cdot 5} = 6$

$Q(6) = 1$

Generally, $\boxed{Q(N) = \frac{6!}{N!\,(6-N)!} = \binom{6}{N}}$

Probability to have all particles in same state

$$= \frac{Q(0) + Q(6)}{\Sigma Q} = \frac{2}{64} = \boxed{\frac{1}{32}}$$

2.(b) Bosons

Same seven configurations as before.

But now there is just one state for
each configuration = totally symmetric state

So $\boxed{Q(N_A) = 1}$ for all N_A

Probability that all particles in same state
is $\frac{Q(0)+Q(6)}{\Sigma Q} = \boxed{\frac{2}{7}}$

3. Unperturbed states $\psi_n^0(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$

$E_n^0 = \frac{\hbar^2 n^2 \pi^2}{m a^2}$

a) Fermions

Ground state: Can't put two fermions in same state, so $\psi^0(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)\right]$

$\rightarrow$ no degeneracy

So $E^{(1)} = \langle \psi^0 | H' | \psi^0 \rangle = U a \int \psi^*(x_1, x_2)\, \delta(x_1 - x_2)\, \psi(x_1, x_2)\, dx_1 dx_2$

But $\psi(x_1, x_2) = 0$ if $x_1 = x_2$

So $\boxed{E^{(1)} = 0}$

The same will be true for any state, since $\psi(x_1, x_2) = 0$ always if $x_1 = x_2$

So $E^{(1)} = 0$ for all states: $\boxed{E_n = E_n^0}$

b) Bosons

Ground state: $\psi^0(x_1, x_2) = \psi_1(x_1)\psi_1(x_2)$

$\rightarrow$ no degeneracy

$E^{(1)} = U a \frac{4}{a^2} \int_0^a \int_0^a \sin^2 \frac{\pi x_1}{a} \sin^2 \frac{\pi x_2}{a}\, \delta(x_1 - x_2)\, dx_1 dx_2$

$= 4U \frac{1}{a} \int_0^a \sin^4 \frac{\pi x}{a}\, dx$

$u = \frac{\pi x}{a}$

$= \frac{4}{\pi} U \int_0^\pi \sin^4 u\, du$

From Dwight, $\int_0^{\pi} \sin^4 u \, du = \frac{3\pi}{8}$

So $E^{(1)} = \frac{4}{\pi} U \cdot \frac{3\pi}{8} = \boxed{\frac{3}{2} U}$

Excited state

Have one particle in ψ_1, one in ψ_2

$$\psi(x_1, x_2) = \frac{\sqrt{2}}{a}\left[\sin\frac{\pi x_1}{a} \sin\frac{2\pi x_2}{a} + \sin\frac{2\pi x_1}{a} \sin\frac{\pi x_2}{a}\right]$$

Only one state, so no degeneracy

$$E^{(1)} = Ua \iint \psi^*(x_1, x_2)\, \delta(x_1 - x_2)\, \psi(x_1, x_2)\, dx_1 dx_2$$

$$= Ua \int_0^a \psi(x, x)^2 \, dx$$

But $\psi(x, x) = \frac{2\sqrt{2}}{a} \sin\frac{\pi x}{a} \sin\frac{2\pi x}{a}$

So $E^{(1)} = Ua \frac{8}{a^2} \int_0^a \sin^2\frac{\pi x}{a} \sin^2\frac{2\pi x}{a} \, dx$ $\quad v = \frac{\pi x}{a}$

$$= \frac{8}{\pi} U \int_0^{\pi} \sin^2 v \sin^2 2v \, dv$$

$$= \frac{32}{\pi} U \int_0^{\pi} \sin^4 v \cos^2 v \, dv$$

$$= \frac{32}{\pi} U \int_0^{\pi} \sin^4 v - \sin^6 v \, dv$$

$$= \frac{32}{\pi} U \left(\frac{3\pi}{8} - \frac{5\pi}{16}\right) \quad \text{(Dwight)}$$

$$= \frac{32}{\pi} U \left(\frac{\pi}{16}\right) = \boxed{2U}$$

3.c) Distinguishable particles

<u>Ground state</u>: Both particles in ground state

$$\psi^0(x_1,x_2) = \psi_1(x_1)\psi_1(x_2)$$

Same as bosons, so $\boxed{E^{(1)} = \frac{3}{2}U}$

<u>Excited state</u>: One particle in $n=2$ state

Two states: $\psi_A^0 = \psi_1(x_1)\psi_2(x_2)$

$\psi_B^0 = \psi_2(x_1)\psi_1(x_1)$

These are degenerate: need to use degenerate PT

Try to find a basis where H' is diagonal:

Note H' commutes with exchange operator P

So use $\psi_\pm^0 = \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) \pm \psi_2(x_1)\psi_1(x_2)\right]$

Check $\langle\psi_+|H'|\psi_-\rangle$

$= Ua\int dx_1 dx_2\, \psi_+^*(x_1,x_2)\,\delta(x_1-x_2)\,\psi_-(x_1,x_2)$

$= 0$, since $\psi_-(x,x) = 0$

So we have $E_\pm^{(1)} = \langle\psi_\pm|H'|\psi_\pm\rangle$

But we already evaluated these for (a) and (b)!

$$\boxed{E_+^{(1)} = 2U \qquad E_-^{(1)} = 0}$$

4. Unperturbed states $\psi(\vec{r}) = R_{n\ell}(\vec{r})\, Y_\ell^m(\theta,\phi)$

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$$

$$R_{20} = \frac{1}{\sqrt{2}\, a^{3/2}}\left(1-\frac{r}{2a}\right)e^{-\frac{r}{2a}}$$

$$R_{21} = \frac{1}{\sqrt{24}}\frac{1}{a^{3/2}}\,\frac{r}{a}\,e^{-r/2a}$$

(From Chapter 4)

We have 4 degenerate states.
No obvious basis where H' will be diagonal, so
just work out complete W matrix.

Label states

$A = \quad \ell = 0 \quad m = 0$
$B = \quad \ell = 1 \quad m = -1$
$C = \quad \ell = 1 \quad m = 0$
$D = \quad \ell = 1 \quad m = +1$

$$W_{AA} = \underbrace{\int r^2 dr\, |R_{20}|^2}_{=1} \int \sin\theta\, d\theta\, d\phi\, |Y_0^0|^2 \beta\cos\theta\cos\phi$$

$$= \frac{1}{4\pi}\int_0^\pi \cos\theta\sin\theta\, d\theta \int_0^{2\pi}\cos\phi\, d\phi = 0$$

Similarly, $W_{ii} = \int \sin\theta\, d\theta\, d\phi\, |Y_\ell^m|^2 \cos\theta\cos\phi$

$$= \int_0^\pi f(\theta)\, d\theta \int_0^{2\pi}\cos\phi\, d\phi = 0 \quad \text{for all states,}$$

since $|Y_\ell^m|^2$ has no ϕ dependence.

$$\boxed{W_{AA} = W_{BB} = W_{CC} = W_{DD} = 0}$$

$$W_{BA} = \underbrace{\int R_{21} R_{20}\, r^2 dr}_{\text{Call this } Q \text{ for now. Only evaluate if we need to}} \int \sin\theta\, d\theta\, d\phi \left(Y_1^{-1}\right)^+ Y_0^0 \cos\theta \cos\phi$$

$$= \frac{Q}{4\pi}\sqrt{\frac{3}{2}} \int_0^\pi \cos\theta \sin^2\theta\, d\theta \int_0^{2\pi} e^{i\phi} \cos\phi\, d\phi$$

$$= \frac{Q}{4\pi}\sqrt{\frac{3}{2}} \underbrace{\frac{\sin^3\theta}{3}\Big|_0^\pi}_{=0} \int_0^{2\pi} e^{i\phi} \cos\phi\, d\phi$$

So $\boxed{W_{BA} = 0}$

Will have $W_{DA} = 0$ for same reason

$$W_{CA} = Q \frac{\sqrt{3}}{4\pi} \int_0^\pi \cos^2\theta \sin\theta\, d\theta \underbrace{\int_0^{2\pi} \cos\phi\, d\phi}_{=0}$$

So $\boxed{W_{CA} = 0}$ as well.

$$W_{CB} = \beta \underbrace{\int (R_{21})^2 r^2 dr}_{=1} \int \left(Y_1^0\right)^+ Y_1^{-1} \cos\theta \cos\phi \sin\theta\, d\theta\, d\phi$$

$$= \beta \frac{3}{4\pi} \frac{1}{\sqrt{2}} \int_0^\pi \cos^2\theta \sin^2\theta\, d\theta \int_0^{2\pi} e^{-i\phi} \cos\phi\, d\phi$$

$$= \beta \frac{3}{4\pi} \frac{1}{\sqrt{2}} \frac{1}{4} \int_0^\pi \sin^2 2\theta\, d\theta \cdot \frac{1}{2} \int_0^{2\pi} \left(e^{-2i\phi} + 1\right) d\phi$$

$$= \beta \frac{3}{32\pi} \frac{1}{\sqrt{2}} \left(\frac{\pi}{2}\right)\left(2\pi\right)$$

$$= \boxed{\beta \frac{3\pi}{32} \frac{1}{\sqrt{2}}}$$

4. - Continued

$$W_{BD} = \beta \int (R_{21})^2 r^2 dr \int (Y_1^{-1})^+ Y_1^1 \cos\theta \cos\phi \sin\theta d\theta d\phi$$

$$= -\beta \frac{3}{8\pi} \int_0^\pi \cos\theta \sin^3\theta \, d\theta \int_0^{2\pi} e^{2i\phi} \cos\phi \, d\phi$$

$$= -\beta \frac{3}{8\pi} \left. \frac{\sin^4\theta}{4} \right|_0^\pi \frac{1}{2} \left(\int_0^{2\pi} e^{3i\phi} + e^{i\phi} d\phi \right)$$

$$= 0$$

Finally,

$$W_{CD} = \beta \int (R_{21})^2 r^2 dr \int (Y_1^0)^+ Y_1^1 \cos\theta \cos\phi \sin\theta d\theta d\phi$$

$$= -\beta \frac{3}{4\pi} \frac{1}{\sqrt{2}} \int_0^\pi \cos^2\theta \sin^2\theta \, d\theta \int_0^{2\pi} e^{i\phi} \cos\phi \, d\phi$$

$$= -W_{CB}$$

So have

$$W = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha & 0 \\ 0 & \alpha & 0 & -\alpha \\ 0 & 0 & -\alpha & 0 \end{bmatrix} \qquad \alpha = \frac{3\pi}{32} \frac{1}{\sqrt{2}} \beta$$

See that state A is not mixed with other states, and also that it has no energy shift

For B, C, and D states, solve

$$\begin{vmatrix} -\lambda & \alpha & 0 \\ \alpha & -\lambda & -\alpha \\ 0 & -\alpha & -\lambda \end{vmatrix} = 0$$

$$-\lambda^3 + 2\lambda\alpha^2 = 0 \quad \Rightarrow \quad \begin{array}{l} \lambda = 0 \\ \lambda = \pm \alpha\sqrt{2} = \pm \frac{3\pi}{32} \beta \end{array}$$

So energy shifts are:

$$\boxed{E^{(1)} = 0,\ 0,\ -\frac{3\pi}{32}\beta,\ +\frac{3\pi}{32}\beta}$$