

$$\textcircled{6} \text{ equation is: } \hat{H}_x = \frac{\hat{p}_x^2}{2\mu} + \frac{1}{2}\mu\omega_x^2 \hat{x}_x^2; \quad \hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

- This is 1d h.o. Hamiltonian. To solve it we introduce:

$$\hat{a}_x = \sqrt{\frac{\mu\omega_x}{2\hbar}} (\hat{x}_x + \frac{i}{\mu\omega_x} \hat{p}_x);$$

$$\hat{a}_x^\dagger = \sqrt{\frac{\mu\omega_x}{2\hbar}} (\hat{x}_x - \frac{i}{\mu\omega_x} \hat{p}_x);$$

- Then h.o. hamiltonian written in terms of this ladder operators is:

$$\hat{H}_x = \hbar\omega_x (\hat{a}_x^\dagger \hat{a}_x + \frac{1}{2});$$

- Spectrum of this Hamiltonian is given by:

- eigenstates $|n_x\rangle = \frac{(\hat{a}_x^\dagger)^n}{\sqrt{n!}} |0\rangle$ where $|0\rangle$ is the vacuum state defined by: $\hat{a}_x |0\rangle = 0$.

- eigenvalues (energy levels): $E_x^{(n)} = \hbar\omega_x (n_x + \frac{1}{2})$;

In the same way we can introduce 1d h.o. corresponding to y and z directions:

$$H_i = \frac{\hat{p}_i^2}{2\mu} + \frac{1}{2}\mu\omega_i^2 \hat{x}_i^2; \quad \hat{p}_i = -i\hbar \frac{\partial}{\partial x_i};$$

- ladder operators: $\hat{a}_i = \sqrt{\frac{\mu\omega_i}{2\hbar}} (\hat{x}_i + \frac{i}{\mu\omega_i} \hat{p}_i)$

$$\hat{a}_i^\dagger = \sqrt{\frac{\mu\omega_i}{2\hbar}} (\hat{x}_i - \frac{i}{\mu\omega_i} \hat{p}_i)$$

- Hamiltonian in terms of this ladder operators is

$$\hat{H}_i = \hbar\omega_i (\hat{a}_i^\dagger \hat{a}_i + \frac{1}{2});$$

- spectrum:

- eigenstates are given by $|n_i\rangle = \frac{(\hat{a}_i^\dagger)^{n_i}}{\sqrt{n_i!}} |0\rangle$ where

$|0\rangle$ is vacuum state defined by $\hat{a}_i |0\rangle = 0$;

- eigenvalues are $E_i = \hbar\omega_i (n_i + \frac{1}{2})$; here $i=1, 2, 3$; $x_1=x, x_2=y, x_3=z$

Summarizing we get the following:

- ⑦
- Complete Hamiltonian is given by:
$$H = \sum_{i=1}^3 H_i = \hbar \left(\sum_{i=1}^3 \omega_i \hat{a}_i^\dagger \hat{a}_i + \frac{3}{2} \sum_{i=1}^3 \omega_i \right)$$
 - We will denote eigenstates of this Hamiltonian by 3 numbers: $|n_1, n_2, n_3\rangle \equiv \frac{(\hat{a}_1^\dagger)^{n_1}}{\sqrt{n_1!}} \cdot \frac{(\hat{a}_2^\dagger)^{n_2}}{\sqrt{n_2!}} \cdot \frac{(\hat{a}_3^\dagger)^{n_3}}{\sqrt{n_3!}} |0\rangle$ where $|0\rangle$ is vacuum state annihilated by all 3 lowering operators: $\hat{a}_i |0\rangle = 0, i=1,2,3.$
 - Eigenvalues are given by:
$$E_n = \hbar (\omega_1 n_1 + \omega_2 n_2 + \omega_3 n_3 + \frac{3}{2} \sum_{i=1}^3 \omega_i) \quad n \equiv (n_1, n_2, n_3);$$

this eigenvalue is the one corresponding to the eigenstate $|n_1, n_2, n_3\rangle;$

⑧ Discuss the degeneracies of the energy levels if $\omega_1 = \omega_2 = \omega_3 = \omega;$

For $\omega_1 = \omega_2 = \omega_3 = \omega$ case we get the following spectrum:

- eigenstates $|n_1, n_2, n_3\rangle$ are the same as before.
- corresponding eigenvalues are

$$E_n = \hbar \omega (n_1 + n_2 + n_3 + \frac{3}{2}) = \hbar \omega (n + \frac{3}{2})$$

Now as usually the question is how many states corresponding to the same energy level $E_n = \hbar \omega (n + \frac{3}{2})$, or how many combinations of (n_1, n_2, n_3) such that $n = n_1 + n_2 + n_3$ exist, as w.l.o.g. correspond to different combinations of (n_1, n_2, n_3) :

- Let's first fix n_3 , as $n_1 + n_2 + n_3 = n$, the sum of n_1 and n_2 is fixed too. If we now fix one of them, say n_2 then $n_1 = n - n_2 - n_3$ is completely defined.

Thus we should sum over n_3 from 0, n , and n_2 from 0 to $n - n_3$. This will give us complete number of states:

$$D = \sum_{n_3=0}^n \sum_{n_2=0}^{n-n_3} 1 = \sum_{n_3=0}^n (n - n_3 + 1) = \sum_{n_3=0}^n (n+1) - \sum_{n_3=0}^n n_3 = (n+1)^2 - \frac{1}{2} n(n+1)$$

(8) Thus finally $D = (n+1) \left(\frac{1}{2}n + 1 \right) = \frac{1}{2}(n+1)(n+2)$, so degeneracy of energy level $E_n = \hbar\omega(n + \frac{3}{2})$ equals to $D = \frac{1}{2}(n+1)(n+2)$;

Problem II. Consider the potential $V(x, y, z) = \frac{1}{2}\mu e^2(x^2 + y^2 + z^2)$

(a) Solve the Schrödinger equation using spherical coordinates.

Before solving this problem let's remember how separation of variables works in spherical coordinates.

Theory:

- Let's start with Schrödinger equation for central potential

$$V(\vec{r}) = V(r); \text{ where } r^2 = x^2 + y^2 + z^2;$$

$$-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(x, y, z) + V(r) \psi(r) = E \psi(r);$$

- Laplacian in spherical coordinates is:

$$\Delta \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}$$

So that we get equation:

$$-\frac{\hbar^2}{2\mu} \left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right) \psi(r) + V(r) \psi(r) = E \psi(r);$$

- Now we use spherical separation of variables ansatz:

$$\psi(r) = R_e(r) Y_{lm}(\theta, \varphi);$$

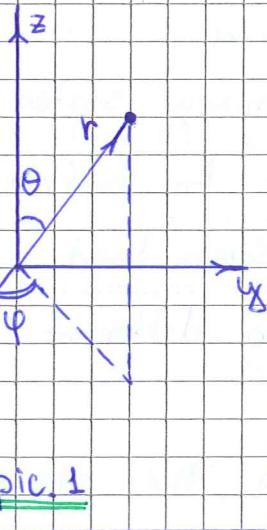
Meaning of indices will become more clear after

This ansatz gives:

$$\left(-\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial R_e}{\partial r}) + V(r) R_e \right) Y_{lm}(\theta, \varphi) +$$

$$+ \frac{R_e}{r^2} \cdot \left(\frac{1}{\sin \theta} \cdot \frac{\partial}{\partial \theta} \sin \theta \frac{\partial Y_{lm}}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y_{lm}}{\partial \varphi^2} \right) = E R_e Y_{lm} \cdot \frac{1}{R_e Y_{lm}};$$

pic. 1



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$$\bullet \frac{1}{R_e} \left(-\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{dR_e}{dr} + V(r) R_e \right) - \frac{\hbar^2}{2\mu r^2} \left(\frac{1}{Y_{em}} \sin\theta \frac{\partial Y_{em}}{\partial \theta} + \frac{1}{Y_{em} \sin^2 \theta} \frac{\partial^2 Y_{em}}{\partial \varphi^2} \right) = 0$$

(r-dependent) (θ, φ)-dependent.

There are two parts - r-dependent and angle-dependent.

In order for equation to be satisfied both of terms should be constant.

- angular equation

$$\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial Y_{em}}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y_{em}}{\partial \varphi^2} = C Y_{em};$$

• how we separate variable θ and φ using ansatz:

$$Y_{em}(\theta, \varphi) = P_e^m(\theta) F_m(\varphi);$$

With this ansatz angle-dependent equation takes form:

$$\underbrace{\frac{1}{P_e^m \sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial P_e^m}{\partial \theta}}_{\theta\text{-dependent}} + \underbrace{\frac{1}{F_m} \frac{d^2 F_m}{d\varphi^2}}_{\varphi\text{-dependent}} = C$$

• putting φ-dependent part to constant we get:

$$\frac{1}{F_m} \frac{d^2 F_m}{d\varphi^2} = -m^2 \quad \text{sign here is taken in order}$$

for final solution to be normalizable (for theory and conventions see FMM course). So we get:

$$F_m(\varphi) = C e^{im\varphi}, \text{ here } C \text{ is integration constant.}$$

• Equation for θ-dep. part is then:

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{dP_e^m}{d\theta} \right) + \left(-C - \frac{m^2}{\sin^2 \theta} \right) P_e^m(\theta) = 0;$$

This is Legendre equation which as solutions

have associated Legendre polynom and $C = -l(l+1)$, $l=0, 1, 2, \dots$

• Final solution for angular equations is

$$Y_{em}(\theta, \varphi) = B P_e^m(\cos\theta) e^{im\varphi}; \quad B \text{ is norm. constant} \quad \int d\Omega |Y_{em}|^2 = 1;$$

Where $P_e^m(\cos\theta)$ is associated Legendre polynom and

$$C = -l(l+1); \quad l=0, 1, 2, \dots$$

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- radial equation:

$$-\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{dR_e}{dr} + \frac{\hbar^2 l(l+1) R_e}{2\mu r^2} + V(r) R_e = E R_e$$

Note: usually sum $V_{eff}(r) = \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)$ is

called effective potential, part of which comes from angular motion of particle.

- To solve radial equation we usually introduce

$$U_e(r) = R_e \cdot r \text{ function}$$

Note that in order $R_e(r)$ to be finite at the origin ($r=0$) $U_e(0)=0$;

Normalization condition for R_e is

$$\int_0^\infty dr \cdot r^2 |R_e(r)|^2 = 1 \text{ so that for } U_e(r) \text{ function}$$

it gives: $\int_0^\infty dr \cdot r |U_e(r)|^2 = 1$;

- Let's find radial equation for $U_e(r)$:

$$\frac{1}{r^2} \frac{d}{dr} r^2 \frac{dR_e}{dr} = \frac{1}{r^2} \frac{d}{dr} \left(-r^2 \frac{1}{r^2} U_e + \frac{r^2}{r} U'_e \right) = -\frac{U''_e}{r^2} + \frac{U'_e}{r^2} + \frac{1}{r} U''_e$$

and radial equation turns into:

$$-\frac{\hbar^2}{2\mu} U''_e + V_{eff} U_e = E U_e;$$

Now we can go to our particular potential $V(r) = \frac{1}{2} \mu \omega^2 r^2$;

- Equation for U_e reads

$$-\frac{\hbar^2}{2\mu} U''_e + \left(\frac{\hbar^2 l(l+1)}{2\mu r^2} + \frac{1}{2} \mu \omega^2 r^2 \right) U_e = E U_e$$

- Now let's change U_e variable to $Z = \frac{U_e}{\alpha}$, where $\alpha = \sqrt{\frac{\hbar^2}{\mu \omega}}$; and $E = \frac{E}{\hbar \omega}$; and equations turns into:

$$\left(-\frac{d^2}{dz^2} + \frac{l(l+1)}{z^2} + z^2 - 2\epsilon \right) U_e = 0;$$

- in $Z \rightarrow \infty$ we get: $\left(\frac{d^2}{dz^2} - z^2 \right) U_e = 0$, suitable solution to this is $U_e = e^{-z^2/2}$;

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• in the limit $\underline{z \rightarrow 0}$ equation goes to

$$\left(-\frac{d^2}{dz^2} + \frac{l(l+1)}{z^2} \right) u_e = 0 ;$$

Natural ansatz for this equation is $u=z^\alpha$ then eq goes to algebraic one

$$-\alpha(\alpha-1) + l(l+1) = 0 \text{ so that } \alpha = l+1$$

$$\alpha^2 - \alpha + l(l+1) = 0 \quad \alpha = -l$$

$\alpha = -l$ is not proper solution as z^{-l} is divergent at the origin $z=0$. While it should be $u_e(z) \xrightarrow[z \rightarrow 0]{} 0$

So we get $u_e(z) \xrightarrow[z \rightarrow 0]{} z^{l+1}$;

• So reasonable ansatz is $\underline{u_e(z) = e^{-\frac{z^2}{2}} \cdot z^{l+1} f(z)}$;

where $f(z)$ is some polynomial such that $f(z) \xrightarrow[z \rightarrow 0]{} \text{const}$;

Then:

$$u_e' = f' \cdot z^{l+1} e^{-\frac{z^2}{2}} + f \cdot (l+1) z^l e^{-\frac{z^2}{2}} - f \cdot z^{l+2} e^{-\frac{z^2}{2}};$$

$$u_e'' = (f'' z^{l+1} + 2f'(l+1) z^l - f \cdot z^{l+2}) e^{-\frac{z^2}{2}};$$

$$u_e''' = (f''' z^{l+1} + 2f''(l+1) z^l - 2f' \cdot z^{l+2} + l(l+1) f \cdot z^{l-1} - (l+1)f \cdot z^{l+2} - (l+2)f \cdot z^{l+1} + f \cdot z^{l+3}) e^{-\frac{z^2}{2}};$$

Then equation turns into:

$$-u_e''' + \frac{1}{z^2} l(l+1) u_e + z^2 \cdot u_e - 2z \cdot u_e = 0$$

$$\Downarrow$$

$$z^l \cdot e^{-\frac{z^2}{2}} (f''' z + 2(l+1)f' - 2f' z^2 + \frac{1}{z} l(l+1) f - f z (2l+3) + f z^3 - \frac{1}{2} l(l+1) f - z^3 f + 2 \cdot z \cdot \varepsilon \cdot f) = 0 . \text{ So that we get}$$

equation for z -polynom:

$$\underline{f''' z + 2(l+1)f' - 2f' z^2 + f z (-2l-3+2\varepsilon) = 0}$$

Now if we introduce $x = z^2$, we get:

$$\frac{d^2 f}{dz^2} = 2\sqrt{x} \frac{d}{dx} 2\sqrt{x} \frac{df}{dx} = 2 \frac{df}{dx} + 4x \frac{d^2 f}{dx^2}, \quad \frac{df}{dz} = 2\sqrt{x} \frac{df}{dx}; \text{ so that}$$

we get equation:

$$\underline{4x \frac{d^2 f}{dx^2} + 2 \frac{df}{dx} + 2 \frac{df}{dx} (2(l+1) - 2x) - f (-l-3+2\varepsilon) = 0}, \text{ or}$$

$$\boxed{\underline{x \frac{d^2 f}{dx^2} + \frac{df}{dx} (l+\frac{3}{2}-x) + \frac{f}{4} (2\varepsilon+3-2l) = 0}};$$

(12) Solution to this equation is Laguerre polynomials

(generalized) :

$f(x) = L_n^{(l)}(x)$ where $n = \frac{1}{4}(2\varepsilon - 3 - 2l)$ $\in \mathbb{Z}$ and

$l = l + \frac{1}{2}$ so that:

$$R_n(r) = \frac{1}{r} U_n(r) = \frac{1}{r} e^{-\frac{1}{2}\frac{r^2}{a^2}} \left(\frac{r}{a}\right)^{l+\frac{1}{2}} L_{n-l}^{(l+\frac{1}{2})}\left(\frac{r^2}{a^2}\right); \text{ and final}$$

Answer for the w.f. is:

$$\Psi_{nlm}(\vec{r}) = C R_n(r) Y_{lm}(\theta, \varphi)$$

↑ norm. radial w.f. → spherical
 constant with Laguerre harmonics.
 polynomial

and $n = \frac{1}{4}(2\varepsilon + 3 - 2l)$ gives condition for quantization of energy levels: $E_{nlm} = \hbar\omega(2n + l + \frac{3}{2})$

- There is another way to observe this spectrum for energy:

Let's put $f(x)$ in the form of $f(x) = \sum_{n=0}^{\infty} c_n x^n$;

$$\text{then } f'(x) = \sum_{n=0}^{\infty} c_n \cdot n x^{n-1} = \sum_{n=0}^{\infty} c_{n+1} (n+1) x^n; f'' = \sum_{n=0}^{\infty} c_{n+1} \cdot n (n+1) x^{n-1};$$

Then equation reads:

$$c_{n+1} \cdot n \cdot (n+1) x^n + c_{n+1} (n+1) \left(l + \frac{3}{2}\right) \cdot x^n - c_n \cdot n \cdot x^n + \frac{1}{4} c_n \cdot x^n (2\varepsilon - 2l - 3) = 0$$

$$c_{n+1} (n+1) \left(n + l + \frac{3}{2}\right) = c_n \left(-\frac{1}{4}(2\varepsilon - 2l - 3) + n\right).$$

This is recurrent equation for coefficients of $f(x)$ polynomial. In order for series to be finite we should get $c_{n+1} = 0$ so that:

$$2\varepsilon - 2l - 3 = 4n \Rightarrow E = \hbar\omega(2k + l + \frac{3}{2});$$

which coincides with expression observed above

- (B) Show how your results for the degeneracies are consistent with result from part 2b.

Let's denote $E_n = \hbar\omega(n + \frac{3}{2})$ where $n = 2k + l$;

We calculate degeneracy in the following way:

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- Let's first assume that n is even, then as

$$n=2k+l, l \text{ should be even too and}$$

$$0 < l < n$$

- for each l we have $-l \leq m \leq l$ (for each l and m we have different w.f.)

$$N = \sum_{l \text{ even}}^n (2l+1) = \sum_{k=0}^{\frac{n}{2}} (4k+1) = 4 \cdot \frac{1}{2} \cdot \frac{n}{2} \left(\frac{n}{2} + 1 \right) + \left(\frac{n}{2} + 1 \right) = \frac{(n+1)(n+2)}{2}$$

- for odd n we have similar computation, but now we should sum over odd l :

$$N = \sum_{l \text{ odd}}^n (2l+1) = \sum_{k=0}^{\frac{n-1}{2}} (4k+3) = 4 \cdot \frac{1}{2} \cdot \frac{n-1}{2} \left(\frac{n-1}{2} + 1 \right) + 3 \left(\frac{n-1}{2} + 1 \right) = \frac{(n+1)(n+2)}{2}$$

So we see that in both $n = \text{odd}$ and even number we get degeneracy to be equal to

$$\boxed{N = \frac{(n+1)(n+2)}{2}}, \text{ which is consistent with the}$$

result of problem 2b, q.e.d.

Problem III Consider the 3d potential:

$$V(r) = \begin{cases} -V_0, & r \leq a; \\ 0, & r > a; \end{cases}$$

Find a relation that V_0 and a must satisfy in order for there to be at least one bound state.

- We start with 3d

Schrödinger equation:

$$E\psi = -\frac{\hbar^2}{2\mu} \Delta\psi + V(r)\psi$$

- To use separation of

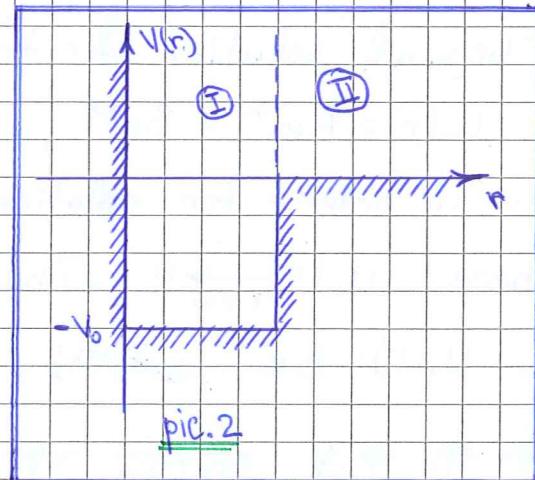
variables method we try

ansatz:

$$\psi(r, \theta, \varphi) = R_e(r) Y_{lm}(\theta, \varphi);$$

$Y_{lm}(\theta, \varphi)$ are spherical harmonics.

- Now we write $R_e = r \cdot u_e(r)$ and equation for



(14) $u_e(r)$ turns out to be:

$$-\frac{\hbar^2}{2\mu} \frac{d^2 u_e}{dr^2} + \left(V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} \right) u_e = E u_e;$$

• Boundary and normalization conditions read:

$$u_e(0) = 0; \int_0^\infty dr |u_e|^2 = 1;$$

• Let's further consider only $l=0$ states, because

① It simplifies problem very much

② Additional potential pushes levels out from the well, so to find the shallow well such that only 1 level exists we are forced to consider $l=0$ states.

• Now we can proceed solving the problem finally:

I inside the well $r < a$: Schrödinger equation takes form:

$$\frac{d^2 u_o}{dr^2} = -\frac{2\mu}{\hbar^2} (E + V_o) u_o \text{ so that}$$

$$u_o(r) = A \cdot \cos kr + B \cdot \sin kr, \text{ where } k = \sqrt{\frac{2\mu(E + V_o)}{\hbar^2}};$$

Using boundary condition $u_o(0) = A = 0$. So that:

$$u_o(r) = B \sin kr, k = \sqrt{\frac{2\mu(E + V_o)}{\hbar^2}}; r < a;$$

II outside the well $r > a$ Schrödinger equation is:

$$\frac{d^2 u_o}{dr^2} = -\frac{2\mu E}{\hbar^2} u_o = \alpha^2 u_o; \text{ where } \alpha = \sqrt{\frac{-2\mu E}{\hbar^2}}; E \in \mathbb{R} \text{ as}$$

For bound states $E < 0$:

• General solution for this equation is:

$$u_o(r) = A e^{-\alpha r} + B e^{\alpha r},$$

• In order for solution to be normalizable we

need $u_o(r) \xrightarrow[r \rightarrow \infty]{} 0$. Thus $B = 0$ and we get:

$$u_o(r) = B e^{-\alpha r}, r > a; \alpha = \sqrt{\frac{-2\mu E}{\hbar^2}};$$

III To find energy of the bound state we apply continuity conditions:

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$$U_I(a) = U_{II}(a) \Rightarrow A \sin ka = B e^{-\alpha a};$$

$$U'_I(a) = U'_{II}(a) \Rightarrow kA \cdot \cos ka = -\alpha B e^{-\alpha a};$$

Dividing one equation with another we get:

$$\underline{k \cot(ka)} = -\alpha; \rightarrow \text{this equation defines boundary}$$

state. Note that this is exactly equation for odd levels in symmetric square well of width $2a$.

We can't solve equation exactly but we can obtain qualitative picture graphically.

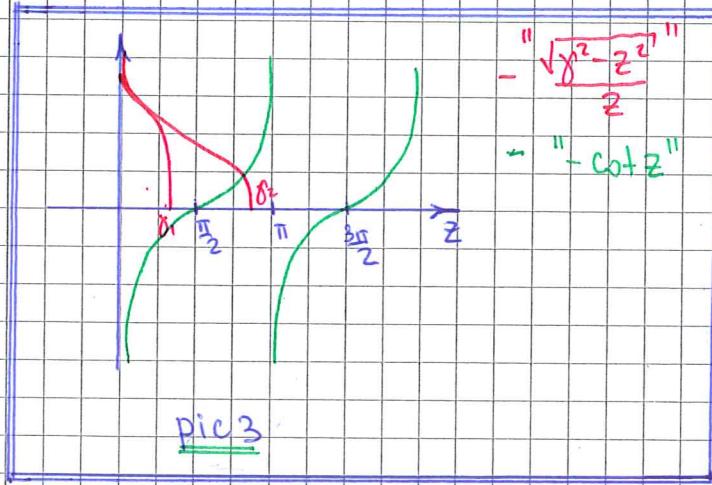
If we denote:

$$ka = z, \alpha a = \frac{a}{\hbar} \sqrt{2\mu(-E - V_0 + V_0)} = \sqrt{\gamma^2 - z^2}, \text{ where } \gamma = \frac{a}{\hbar} \sqrt{2\mu V_0};$$

we get equation:

$$\cot z = -\frac{\sqrt{\gamma^2 - z^2}}{z}$$

We have drawn 2 sides of the equation on the picture below:



As we see solution corresponding to the intersection of 2 graphs exists only if

$$\gamma \geq \frac{\pi}{2}$$

$$a^2 V_0 \geq \frac{\pi^2 \hbar^2}{8 \mu}$$

which is

the solution we were asked to find.

① Seminar 11 (angular momentum)

Theory • In classical mechanics we have concept of the angular momentum: $\vec{L} = \vec{r} \times \vec{p}$. To generalize this to quantum mechanics we just put operators instead of functions into this formula. In particular, we replace \vec{p} with nabla operator:

$$\vec{p} \rightarrow -i\hbar \vec{\nabla} = -i\hbar \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix}; \text{ so that}$$

$$\hat{L} = -i\hbar \vec{r} \times \vec{\nabla};$$

- In components we have

$$\hat{L}_x = \hat{y} \cdot \hat{p}_z - \hat{z} \cdot \hat{p}_y; \quad \hat{L}_y = \hat{z} \cdot \hat{p}_x - \hat{x} \cdot \hat{p}_z; \quad \hat{L}_z = \hat{x} \cdot \hat{p}_y - \hat{y} \cdot \hat{p}_x;$$

another combinations that will be useful to us are

$$\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y$$

- Sometimes it will be useful to solve problems in spherical coordinates:

$$\begin{cases} x = r \cdot \sin\theta \cdot \cos\phi; \\ y = r \cdot \sin\theta \cdot \sin\phi; \\ z = r \cdot \cos\theta; \end{cases}$$

In this coordinate system angular momentum operators take form:

$$\hat{L}_x = +i\hbar (\sin\phi \frac{\partial}{\partial \theta} - \cot\theta \cdot \cos\phi \cdot \frac{\partial}{\partial \phi});$$

$$\hat{L}_y = -i\hbar (\cos\phi \frac{\partial}{\partial \theta} + \cot\theta \cdot \sin\phi \frac{\partial}{\partial \phi});$$

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

$$\hat{L}^2 = -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right);$$

$$\hat{L}_{\pm} = \hbar e^{\pm i\phi} \left(\pm \frac{\partial}{\partial \theta} + i \cot\theta \frac{\partial}{\partial \phi} \right);$$

② Important things about this formulas are:

- All angular momentum operators act only on angular variables, and don't act on radial variable r .
- \hat{L}^2 looks like angular part of 3d laplace operator.

$$\Delta = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) + \frac{1}{r^2} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \cdot \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right);$$

- Useful commutators are:

$[L_x, L_y] = i\hbar L_z;$	$[L_y, L_z] = i\hbar L_x;$	$[L_x, L_z] = i\hbar L_y;$
$[L_i, L^2] = 0 \quad i=x, y, z;$	$[L_z, L_{\pm}] = \pm \hbar L_{\pm};$	

- Remember that commuting operators can have common eigenstates (or, speaking physically, can be measured simultaneously). For us this means that we can have system of simultaneous eigenstates of L^2 and, following usual conventions, L_z

In particular:

$\hat{L}^2 l, m\rangle = \hbar^2 l(l+1) l, m\rangle;$	$-l \leq m \leq l;$
$L_z l, m\rangle = m l, m\rangle;$	

- If we go to coordinate representation

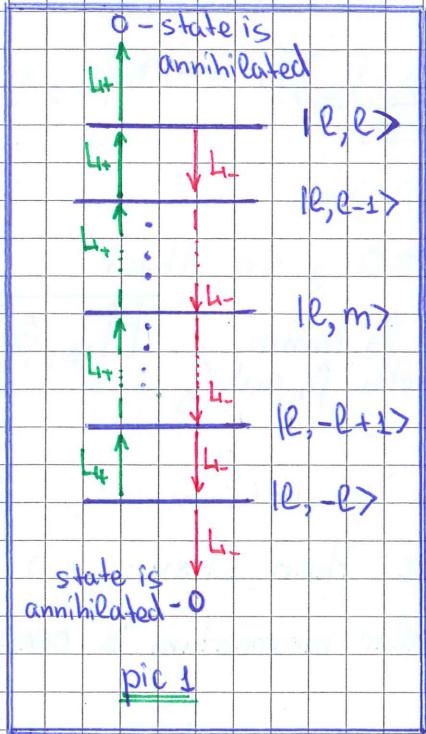
$$|l, m\rangle \sim Y_{lm}(\theta, \varphi). \text{ Indeed we have seen on previous class } \hat{L}^2 Y_{lm} = -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \cdot \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right) Y_{lm} =$$

$$= \hbar^2 l(l+1) Y_{lm}; \text{ and } L_z Y_{lm} = m Y_{lm} \text{ which coincides with equations above.}$$

- Another useful formulas are action of L_{\pm} operators on $|l, m\rangle$ state. In particular:

$L_+ l, m\rangle = \hbar \sqrt{l(l+1) - m(m+1)} l, m+1\rangle;$
$L_- l, m\rangle = \hbar \sqrt{l(l+1) - m(m-1)} l, m-1\rangle;$

③ These relations can be treated as ladder operators. In particular, we have ladder of $(2l+1)$ states with angular momentum "l": $|l, m\rangle$, $-l \leq m \leq l$; And using \hat{L}_\pm operator we are able to move between them (see pic. 1). This picture is similar to the



one we had in harmonic oscillator. The only difference is that now we have so called "highest weight state" $|l, l\rangle$ which is annihilated by \hat{L}_+ operator. While in h.o. we have only vacuum state $|0\rangle$ annihilated by \hat{a} (analog in our case is $|l, -l\rangle$ state annihilated by \hat{L}_-) but there were no state annihilated by \hat{a}^* operator (ladder was unbounded from above).

Problem I Show that:

$$[\hat{L}_z, \hat{x}] = i\hbar y; \quad [\hat{L}_z, \hat{y}] = -i\hbar x; \quad [\hat{L}_z, \hat{z}] = 0;$$

$$[\hat{L}_z, \hat{p}_x] = i\hbar \hat{p}_y; \quad [\hat{L}_z, \hat{p}_y] = -i\hbar \hat{p}_x; \quad [\hat{L}_z, \hat{p}_z] = 0;$$

• First of all derivation rule of commutator:

$$[AB, C] = ABC - CAB = A[B, C] + [A, C]B, \text{ and canonical}$$

commutator $[\hat{p}_i, \hat{x}_j] = -i\hbar \delta_{ij}$ will be usefull for us.

$$\begin{aligned} \bullet \quad [\hat{L}_z, \hat{x}] &\equiv [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{x}] = [\hat{x}\hat{p}_y, \hat{x}] - [\hat{y}\hat{p}_x, \hat{x}] = \\ &= [\text{using derivation property}] = \hat{x}[\hat{p}_y, \hat{x}] + \hat{p}_y[\cancel{\hat{x}}, \hat{x}] - \hat{y}[\hat{p}_x, \hat{x}] - \end{aligned}$$

$$[\cancel{\hat{x}}, \hat{x}] \hat{p}_x = -i\hbar \hat{y}; \Rightarrow [\hat{L}_z, \hat{x}] = i\hbar \hat{y}, \text{ q.e.d.}$$

$$\begin{aligned} \bullet \quad [\hat{L}_z, \hat{y}] &\equiv [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{y}] = [\hat{x}\hat{p}_y, \hat{y}] - [\hat{y}\hat{p}_x, \hat{y}] = [\text{derivation}] = \\ &= \hat{x}[\hat{p}_y, \hat{y}] + [\cancel{\hat{x}}, \hat{y}] \hat{p}_y - \hat{y}[\cancel{\hat{x}}, \hat{y}] - [\cancel{\hat{y}}, \hat{y}] \hat{p}_x = -i\hbar \hat{x}, \text{ so that} \end{aligned}$$

$$[\hat{L}_z, \hat{y}] = -i\hbar \hat{x}, \text{ q.e.d.}$$

- ④ • $[\hat{L}_z, \hat{z}] \equiv [\hat{x}\hat{p}_y, \hat{z}] - [\hat{y}\hat{p}_x, \hat{z}] = 0, \Rightarrow [\hat{L}_z, \hat{z}] = 0, \text{ q.e.d.}$
- $[\hat{L}_z, \hat{p}_x] \equiv [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{p}_x] = [\hat{x}\hat{p}_y, \hat{p}_x] - [\hat{y}\hat{p}_x, \hat{p}_x] =$
 $= \hat{x}[\cancel{\hat{p}_y, \hat{p}_x}]_0 + [\hat{x}, \hat{p}_x]\hat{p}_y - \hat{y}[\cancel{\hat{p}_x, \hat{p}_x}]_0 - [\cancel{\hat{y}, \hat{p}_x}]_0\hat{p}_x = i\hbar \hat{p}_y$
- hence: $[\hat{L}_z, \hat{p}_x] = i\hbar \hat{p}_y;$
- $[\hat{L}_z, \hat{p}_y] \equiv [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{p}_y] = -[\hat{y}, \hat{p}_y]\hat{p}_x = -i\hbar \hat{p}_x, \text{ so that:}$
 $[\hat{L}_z, \hat{p}_y] = -i\hbar \hat{p}_x;$
- $[\hat{L}_z, \hat{p}_z] = [\hat{x}\hat{p}_y, \hat{p}_z] - [\hat{y}\hat{p}_x, \hat{p}_z] = 0, \text{ so that}$
 $\text{as } \hat{p}_z \text{ comm. with both } \hat{x} \text{ and } \hat{p}_y \quad \text{as } \hat{p}_z \text{ comm. with both } \hat{p}_x \text{ and } \hat{y} \quad [\hat{L}_z, \hat{p}_z] = 0;$

Problem II Consider the potential $V(\vec{r})$

① If $V(\vec{r})$ is spherically symmetric then show

$$\frac{\partial}{\partial t} \langle \vec{L} \rangle = 0; \text{ i.e. the angular momentum is conserved.}$$

• Hamiltonian for 3d particle in potential $V(\vec{r})$ is given by:

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + V(\vec{r}) = -\frac{\hbar^2}{2\mu} \Delta + V(\vec{r}) \text{ which in spherical coordinates is}$$

$$\Delta = \underbrace{\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)}_{-\frac{1}{\hbar^2} \hat{L}^2} + \underbrace{\frac{1}{r^2} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right)}_{-\frac{1}{\hbar^2} \hat{p}_r^2}$$

$$\text{So that Hamiltonian is given by: } \hat{H} = \frac{\hat{p}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} + V(\vec{r});$$

• Now we can use Heisenberg equation describing time evolution of operators expectation value:

$$\frac{\partial}{\partial t} \langle \vec{L} \rangle = -\frac{i}{\hbar} \langle [\vec{L}, \hat{H}] \rangle; \text{ Let's now find commutator}$$

$[\vec{L}, \hat{H}]$ standing on the r.h.s. of the Heisenberg equation.

It has 3 components:

$$* \frac{1}{2\mu} [\vec{L}, \hat{p}_r] = 0 \text{ since } \vec{L} \text{ is operator acting on}$$

(5) angular variables (and thus contains only θ and φ -dependence as it can be seen from explicit expressions)

$$*\frac{1}{2\mu} \left[\hat{L}_z, \frac{\hat{L}^2}{r^2} \right] = \begin{bmatrix} \text{using derivation} \\ \text{property of} \\ \text{commutator} \end{bmatrix} = \frac{1}{2\mu} [\hat{L}_z, \hat{L}^2] \frac{1}{r^2} +$$

$$+ \frac{1}{2\mu} \hat{L}^2 [\hat{L}_z, \frac{1}{r^2}] ; \text{ while}$$

$[\hat{L}_z, \hat{L}^2] = 0$, as all components of \hat{L} commute with \hat{L}^2 operator (see "theory" part)

$$[\hat{L}_z, \frac{1}{r^2}] = 0 \text{ by the very same reason as } [\hat{L}_z, \hat{p}_r] = 0.$$

So we get: $\boxed{\frac{1}{2\mu} [\hat{L}_z, \frac{\hat{L}^2}{r^2}] = 0;}$

* Finally $[\hat{L}_z, V(\vec{r})]$. If potential is spherically symmetric then $V(\vec{r}) = V(r)$; (part @ of the problem)

$[\hat{L}_z, V(r)] = 0$ by the same reason as $[\hat{L}_z, \hat{p}_r] = 0$, i.e. \hat{L}_z depends on φ and θ (including derivatives $\frac{\partial}{\partial \varphi}, \frac{\partial}{\partial \theta}$), and $V(r)$ is just function of r so they should commute.

If now $V(\vec{r})$ is not spherically symmetric:

$$\begin{aligned} [\hat{L}_z, V(\vec{r})] \psi(\vec{r}) &\equiv -i\hbar [\vec{r} \times \vec{\nabla}, V(\vec{r})] \psi(\vec{r}) = -i\hbar \vec{r} \times \vec{\nabla} (V(\vec{r}) \psi(\vec{r})) + \\ &+ i\hbar V(\vec{r}) \vec{r} \times \vec{\nabla} \psi(\vec{r}) = -i\hbar V(\vec{r}) \cdot \vec{r} \times (\vec{\nabla} \psi) - i\hbar \vec{r} \times (\vec{\nabla} V(\vec{r})) \psi + \\ &+ i\hbar V(\vec{r}) \cancel{\vec{r} \times \vec{\nabla}} \psi(\vec{r}) = -i\hbar \vec{r} \times (\vec{\nabla} V) \cdot \psi, \text{ so we have got:} \end{aligned}$$

$$[\hat{L}_z, V(\vec{r})] \psi = -i\hbar \vec{r} \times (\vec{\nabla} V) \psi \text{ thus } \boxed{[\hat{L}_z, V(\vec{r})] = -i\hbar \vec{r} \times \vec{\nabla} V = i\hbar \vec{T}}$$

where \vec{T} is the torque which is given by

$$\boxed{\vec{T} \equiv \vec{r} \times (-\vec{\nabla} V)}$$

Summing up we get:

$$\boxed{[\hat{L}_z, \hat{H}] = i\hbar \vec{T}} \text{ notice that in the case of spherically symmetric potential } V(r) \text{ we automatically get } \vec{T} = 0 \Rightarrow$$

$$[\hat{L}_z, \hat{H}] = 0;$$

- Now substituting this result into Heisenberg eq.

⑥ we get

$$\boxed{\frac{\partial}{\partial t} \langle \bar{L} \rangle = \langle \bar{T} \rangle}$$

which in case of spherically symmetric potential turns into

$$\boxed{\frac{\partial}{\partial t} \langle \bar{L} \rangle = 0}, \text{ QED.}$$

Problem III Consider the 3-degenerate states with $\ell=1$ orbital angular momentum in a spherically symmetric potential ($V(\vec{r}) = V(r)$). Suppose that the Hamiltonian has an extra piece ΔH which breaks the degeneracy:

$$\Delta H = 2(L_+^2 + L_-^2), \Delta > 0$$

① Find all energy eigenvalues of ΔH for the $\ell=1$ states.

- As basis of states for this problem it is useful to use $|l, m\rangle$ states with $\ell=1$:

$$|1, -1\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}; \quad |1, 0\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}; \quad |1, 1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix};$$

Let's use this basis to write down \hat{H} in form of matrix.

We will use following formulas for ladder operators:

$$\hat{L}_+ |l, m\rangle = \hbar \sqrt{l(l+1) - m(m+1)} |l, m+1\rangle;$$

$$\hat{L}_- |l, m\rangle = \hbar \sqrt{l(l+1) - m(m-1)} |l, m-1\rangle;$$

- in particular for the states we have, we get:

$$\hat{L}_+ |1, 1\rangle = 0; \quad \hat{L}_+ |1, 0\rangle = \sqrt{2}\hbar |1, 1\rangle; \quad \boxed{\hat{L}_+^2 |1, 0\rangle = 0. \hat{L}_+ |1, 1\rangle = 0};$$

$$\hat{L}_+ |1, -1\rangle = \sqrt{2}\hbar |1, 0\rangle; \quad \boxed{\hat{L}_+^2 |1, -1\rangle = 2\hbar^2 |1, 1\rangle};$$

$$\hat{L}_- |1, 1\rangle = \hbar \sqrt{2} |1, 0\rangle; \quad \hat{L}_-^2 |1, 1\rangle = \sqrt{2}\hbar \hat{L}_- |1, 0\rangle = 2\hbar^2 |1, -1\rangle; \quad \text{so that}$$

$$\boxed{\hat{L}_-^2 |1, 1\rangle = 2\hbar^2 |1, -1\rangle};$$

$$\hat{L}_- |1, 0\rangle = \sqrt{2}\hbar |1, -1\rangle; \quad \boxed{\hat{L}_-^2 |1, 0\rangle = \hat{L}_- \sqrt{2}\hbar |1, -1\rangle = 0}; \quad \boxed{\hat{L}_-^2 |1, 0\rangle = 0};$$

$$\text{Finally } \hat{L}_- |1, -1\rangle = 0;$$

As we see only nonzero matrix elements of \hat{L}_+^2 and \hat{L}_-^2 operators are

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- For \hat{L}_+^2 : $\langle 1, 1 | \hat{L}_+^2 | 1, -1 \rangle = 2\hbar^2$, thus

$$\hat{L}_+^2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} 2\hbar^2;$$

- For \hat{L}_-^2 : $\langle 1, -1 | \hat{L}_-^2 | 1, 1 \rangle = 2\hbar^2$, thus:

$$\hat{L}_-^2 = 2\hbar^2 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix};$$

Thus for Hamiltonian operator we get:

$$\Delta H = 2\lambda\hbar^2 \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix};$$

- Now we can find eigenvalues and eigenstates of ΔH operator:

$$0 = \det [\Delta H - E \cdot \mathbb{1}] = \begin{vmatrix} E & 0 & 2\lambda\hbar^2 \\ 0 & E & 0 \\ 2\lambda\hbar^2 & 0 & E \end{vmatrix} = E^3 - E^4 \lambda^3 \hbar^4 = E(E - 2\lambda\hbar^2)(E + 2\lambda\hbar^2)$$

So we get 3 eigenvalues:

$$E_0 = 0; E_+ = 2\lambda\hbar^2; E_- = -2\lambda\hbar^2;$$

- ⑥ Find the normalized eigenstates in terms of eigenstates of \hat{L}_z .

Notice that eigenstates of \hat{L}_z are exactly $|l, m\rangle$ states that we have used as the basis.

- $E_0 = 0$ state equation for eigenstate

$$|\Psi_0\rangle = \begin{bmatrix} a \\ b \\ c \end{bmatrix} \text{ is: } 2\lambda\hbar^2 \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = 0 \text{ so that } a=0, c=0,$$

while b can be any number. Normalized eigenstate is then given by

$$|\Psi_0\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = |1, 0\rangle; E_0 = 0$$

- $E_+ = 2\lambda\hbar^2$ state is defined by equation

$$2\lambda\hbar^2 \begin{bmatrix} -1 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = 0 \Rightarrow \begin{array}{l} a=c \\ b=0 \end{array} \text{ then normalized eigenstate}$$

⑧ Is given by:

$$\Psi_+ = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} (|1,1\rangle + |1,-1\rangle); E_+ = 2\omega\hbar^2;$$

• Finally we consider $E_- = -2\omega\hbar^2$ eigenstate $|\Psi_-\rangle = \begin{bmatrix} 0 \\ b \\ c \end{bmatrix}$.

Equation it should satisfy is given by:

$$2\omega\hbar^2 \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ b \\ c \end{bmatrix} = 0 \Rightarrow \begin{aligned} a &= -c; \text{ so that normalized eigenstate:} \\ b &= 0; \end{aligned}$$

$$|\Psi_-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}} (|1,1\rangle - |1,-1\rangle); E_- = -2\omega\hbar^2;$$

(c) What is probability that a measurement of \hat{L}_z in the \hat{z} direction for the highest energy state will be \hbar ? What is the probability that it will be $0\hbar$?

Probability will be given by the inner product of corresponding \hat{L}_z and $\Delta\hat{H}$ eigenstates:

• Highest energy state is $|\Psi_+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$; and probability is

$$P_{+\hbar} = |\langle 1,1 | \Psi_+ \rangle|^2 = \frac{1}{2} \left| \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \right|^2 = \frac{1}{2};$$

$$P_0 = |\langle 1,0 | \Psi_+ \rangle|^2 = \frac{1}{2} \left| \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \right|^2 = 0;$$

• So we have got

$$P_{+\hbar} = \frac{1}{2}; P_0 = 0;$$

⑨ What is the expectation value for L_z for the highest energy state?

By the definition expectation value is given by:

$$\langle \hat{L}_z \rangle_+ \equiv \langle \Psi_+ | \hat{L}_z | \Psi_+ \rangle = \frac{1}{\sqrt{2}} [1 0 1] \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{2} [1 0 1] \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} = 0;$$

Where we have used matrix representation of \hat{L}_z

operator. Note that $|1,\pm 1\rangle$ and $|1,0\rangle$ are eigenstates of \hat{L}_z so only diagonal terms:

$$\langle 1,1 | \hat{L}_z | 1,1 \rangle = +1; \langle 1,0 | \hat{L}_z | 1,0 \rangle = 0; \langle 1,-1 | \hat{L}_z | 1,-1 \rangle = -1; \text{ are}$$

relevant, and we then conclude $\hat{L}_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$,

$$\langle \hat{L}_z \rangle_+ = 0;$$

⑨ Problem IV Consider a particle with mass μ that is constrained to move on a 2d sphere of radius R , but is otherwise free to move on the sphere. Assuming that the lowest energy state is 0, find the energies and degeneracies for all states.

- Hamiltonian in our case is usual 3d Hamiltonian with

$$\hat{H} = \frac{\hat{p}_r^2}{2\mu} + \frac{\hat{l}^2}{2\mu r^2} + V(r). \text{ In particular in our case } V(R) = V_0, \text{ i.e. on}$$

sphere potential is just constant chosen so that ground state has zero energy ($E=0$); and everywhere except sphere it's " ∞ ". We can write it in a form:

$$V(r) = \begin{cases} V_0, & r \in [R - \Delta R, R + \Delta R] \text{ in the limit} \\ \infty, & \text{everywhere else} \quad \Delta R \rightarrow 0; \end{cases}$$

- Due to the form of potential there is no movement transverse to the sphere i.e. $\psi(r)=0$ if $r \neq R$, and thus we can neglect $\frac{\hat{p}_r^2}{2\mu}$ term in Hamiltonian, and Schrödinger equation takes form:

$$\frac{\hat{l}^2}{2\mu r^2} \psi(\bar{r}) = (E - V_0) \psi(\bar{r})$$

This is just equation for the eigenvalues of \hat{l}^2 operator, and we know that solutions of these are spherical harmonics, i.e.

$$\boxed{\Psi(\bar{r}) = Y_{lm}(\theta, \phi); \quad -l \leq m \leq l}$$

With the angular momentum squared eigenvalues given by:

$$\hat{l}^2 Y_{lm} = +\hbar^2 l(l+1) Y_{lm}. \text{ That means for us:}$$

$E_l = V_0 + \frac{\hbar^2}{2\mu R^2} l(l+1)$, in order for ground state to have zero energy ($E_0=0$), we choose $V_0=0$, so that

$$\boxed{E_l = \frac{\hbar^2}{2\mu R^2} l(l+1)}; \text{ Now as } E_l \text{ doesn't depend on } m, \text{ there are } (2l+1) \text{ different w.f. (i.e. spherical)}$$

⑩ harmonics Y_{lm} with the same l) corresponding to energy level E_l, i.e:

$$N_l = 2l+1 \text{ - degeneracy of level } E_l$$

Problem II

Consider 3d h.o.:

$$V(r) = \frac{1}{2} \mu \omega^2 (x^2 + y^2 + z^2) = \frac{1}{2} \mu \omega^2 r^2;$$

① Separating the variables, find the allowed energy levels and degeneracies for this system.

This part of the problem was solved in (problem set 10, problem N2)

Upshot of the solution

- Using separation of variables $\Psi(x, y, z) = X(x) Y(y) Z(z)$

we reduced 3d h.o. problem to 3 1d h.o.-problems:

$$-\frac{\hbar^2}{2\mu} \frac{\partial^2 X}{\partial x^2} + \frac{1}{2} \mu \omega^2 x^2 X(x) = E_x X(x); \text{ + the same equations for } Y(y), Z(z).$$

- Then we get spectrum given by eigenstates

$|n_1, n_2, n_3\rangle$ with energies:

$$E_n = \hbar \omega \left(n + \frac{3}{2}\right), \text{ where } n = n_1 + n_2 + n_3$$

as we see different combinations of n_1, n_2, n_3 give the same E_n . Degeneracy of level n is given by:

$$D = \frac{1}{2} (n+1)(n+2); E_n = \hbar \omega \left(n + \frac{3}{2}\right);$$

② Since the potential also has spherical symmetry, it is possible to separate the system into radial coordinates as well. Find the 8₀ energy levels. With this information and the result from part (a) what value of l does the first excited level have?

We have already done separation into radial and angular

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variables in (problem 3 of set 10)

Upshot of radial-angular separation:

- We used usual separation formula

$$\psi(\vec{r}) = R(r) Y_{lm}(\theta, \phi);$$

- For angular part we have observed as usually:

$$\hat{L}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}$$

- Then equation for the radial part of w.f. turns out to be:

$$-\frac{\hbar^2}{2\mu} u_e'' + \left(\frac{\hbar^2 l(l+1)}{2\mu r^2} + \frac{1}{2} \mu \omega^2 r^2 \right) u_e = E u_e \text{ where}$$

$u_e(r) = R_e(r) \cdot r$ and satisfies boundary condition

$$u_e(0) = 0.$$

You can see explicit solution to this problem in the corresponding scan. But here we don't even need to solve it in general case. We should concentrate only on the case $l=0$, when radial Schrödinger equation turns into:

$$\boxed{-\frac{\hbar^2}{2\mu} u_0'' + \frac{1}{2} \mu \omega^2 r^2 u_0 = E u_0}, \text{ which is just the usual}$$

Schrodinger equation for 1d harmonic oscillator.

Thus spectrum of energy is given by the usual expression

$$\boxed{E_{\tilde{n}} = \hbar \omega \left(\tilde{n} + \frac{1}{2} \right), \quad \tilde{n} = \text{odd}}$$

Note that \tilde{n} should be odd

in order for $u_0(r)$ be odd function

so that $u_0(0) = 0$ is satisfied

Let's compare it with the one we had before, i.e.:

$$E_n = \hbar \omega \left(n + \frac{1}{2} \right)$$

• if $\tilde{n} = 1$, $E_{\tilde{n}} = \frac{3}{2} \hbar \omega \Rightarrow n = 0$ - ground state.

• if $\tilde{n} = 3$, $E_{\tilde{n}} = \frac{7}{2} \hbar \omega \Rightarrow n = 2$ so we see that first excited level with $n = 1$ has $l \neq 0$, thus it should

have $l=1$. Notice that degeneracy of the state with orbital angular momentum $l=1$ is $D = 2l+1 = 3$ which coincide with degeneracy obtained before:

$$D = \frac{(n+1)(n+2)}{2} = \frac{2 \cdot 3}{2} = 3.$$

①

Seminar 12 (Hydrogen atom)

Theory

- Electrons in the atom are moving in the electric field of atom nucleus $V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$. So that Schrödinger equation turns out to be:

$$\hat{H} = \frac{1}{2\mu} \hat{p}_r^2 + \frac{\hat{l}^2}{2\mu r^2} - \frac{Ze^2}{4\pi\epsilon_0 r}, \text{ where } \mu = \frac{m \cdot M_n}{m + M_n} \text{ is}$$

electron's reduced mass.

- Now if we use separation of variables in spherical coordinates $\Psi(r, \theta, \varphi) = R_{ne}(r) Y_{lm}(\theta, \varphi)$; Then:
 - for $Y_{lm}(\theta, \varphi)$ we get standard spherical harmonics.
 - for $R_{ne}(r)$ we get:

$$\left(\frac{\hat{p}_r^2}{2\mu} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r) \right) R_{ne}(r) = E \cdot R_{ne}(r);$$

- as usually for radial part of the w.f. we introduce $U_{ne}(r) = \frac{R_{ne}(r)}{r}$ with the boundary conditions at zero $U_{ne}(0) = 0$; and at infinity $U_{ne}(\infty) = 0$;

Then equation for U_{ne} takes form:

$$-\frac{\hbar^2}{2\mu} U_{ne}''(r) + V_{eff}(r) U_{ne}(r) = E_{ne} U_{ne}(r).$$

- If we now introduce $g = \alpha \cdot r$ where $\alpha = \sqrt{-\frac{2\mu E}{\hbar^2}}$;

then equation turns into:

$$\frac{d^2}{dg^2} U_e(r) = \left(1 - \frac{2\lambda}{g} + \frac{l(l+1)}{g^2} \right) U_e(r)$$

- For $g \gg 1$ equation turns into $\frac{d^2}{dg^2} U_e(r) = U_e(r)$ so that

$$U_{ne}(r) = A e^{-\beta}, \beta \gg 1;$$

- We take full ansatz in form $U_{ne}(r) = g^{l+1} e^{-\beta} \cdot g_e(g)$.

Then we get equation:

$$g \cdot g_e''(g) + 2(l+1-g) g_e'(g) + 2(\lambda - l - 1) g_e(g) = 0;$$

Now we take $g_e(g)$ in the form of polynomial:

$$g_e(g) = \sum_{k=0}^{\infty} c_k g^k = c_0 + c_1 g + \dots + c_n g^n$$

Substituting this into equation above is

(2) We get recursive relation for c_k coefficients:

$$c_{k+1} = \frac{2(k+l+1-\lambda)}{(k+1)(k+2l+2)} c_k. \text{ Then we want this}$$

polynomial to be of final power, i.e. should

be such k so that $c_{k+1}=0$. For this to be satisfied

we want $\lambda=k+l+1$. λ is integer n and so that

$n \geq l+1$, in fact if $n=1, l=0$; $n=2, l=0, 1$; $n=3, l=0, 1, 2$; etc.

- Solutions of Schrödinger equation are:

$$R_{nl}(r) = r^l e^{-\frac{r}{a_n}} g_{nl}(r); \text{ where } g_{nl}(r) \text{ are Laguerre polynomials}$$

- Degeneracy of n^{th} level is calculated as following:

- As we have said for each n defining energy

$$\text{Level } E_n = -\frac{Z_1^2}{2n^2} \frac{e^2}{4\pi\epsilon_0 a_n}; a_n = \frac{n}{2c\mu}; \text{ we have } l \leq n+1 \text{ so}$$

l run through all values $0, 1, 2, \dots, n-1$;

- and for each l we have $(2l+1)$ states with different m . So degeneracy is $D = \sum_{l=0}^{n-1} (2l+1) = \frac{1}{2}n(1+2n-1) = n^2$; $D=n^2$

- One useful formula for this session is

$$\int_0^\infty dt t^n e^{-t} = \lim_{\lambda \rightarrow 1} (-1)^n \frac{d^n}{dt^n} \int_0^\infty e^{-\lambda t} = \lim_{\lambda \rightarrow 1} (-1)^n \frac{d^n}{dt^n} \frac{1}{\lambda} = n!; \Rightarrow$$

$$\Rightarrow \int_0^\infty dt t^n e^{-t} = n!$$

③

Problem I (Compendium 14)

Consider the $n=1$ level of the hydrogen atom. The normalized w.f. is

$$\Psi_{100}(r, \theta, \varphi) = \frac{2}{\sqrt{4\pi}} \left(\frac{1}{a_1}\right)^{3/2} e^{-r/a_1};$$

- (a) Find the expectation value for x^2 for this state.
- By definition expectation value should be given by

$$\langle x^2 \rangle = \int d^3x |\Psi_{100}|^2 x^2 = \underbrace{\int d\cos\theta \int d\varphi}_{\text{coming from } d^3x} \int dr \cdot r^2 \underbrace{\frac{1}{\pi} \frac{1}{a_1^3} e^{-2r/a_1} \cdot r^2 \sin^2\theta \cdot \cos\varphi}_{\text{from } |\Psi|^2}$$

$$\begin{aligned} &= \left[\begin{array}{l} \text{with the change of} \\ \text{variable } \cos\theta = t \end{array} \right] = \int_{-1}^1 dt (1-t^2) \cdot \frac{1}{\pi} \int_0^\infty dr \frac{r^4}{a_1^3} e^{-2r/a_1} \int_0^{2\pi} d\varphi \frac{1}{2} (1 + \cos 2\varphi) = \\ &= \left[\begin{array}{l} \text{change of variable} \\ y = 2r/a_1 \Rightarrow r = a_1 y/2 \end{array} \right] = \int_{-1}^1 dt (1-t^2) \cdot \left(\pi + \frac{1}{4} \sin 2\varphi \Big|_0^{2\pi} \right) \cdot \frac{a_1^2}{2^5} \int_0^\infty dy y^4 e^{-y} = \\ &= \frac{4}{3} \cdot \pi \cdot \frac{a_1^2}{2^5} \cdot 4! = a_1^2; \quad \left(t - \frac{1}{3} t^3 \right) \Big|_{-1}^1 = \frac{4}{3}; \end{aligned}$$

$$\text{so } \boxed{\langle x^2 \rangle = a_1^2}$$

- Other way to solve the problem is to use symmetry of the problem:

as w.f. doesn't depend on angles θ and φ , i.e.

spherically symmetric we conclude that:

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle \text{ and by the definition}$$

$$\langle r^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle; \Rightarrow \boxed{\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{1}{3} \langle r^2 \rangle};$$

Indeed let's check that this 2 results coincide:

$$\langle r^2 \rangle = \int d^3r |\Psi_{100}|^2 r^2 = \underbrace{\int d\cos\theta \int d\varphi}_{4\pi} \int dr r^2 \frac{1}{\pi} \frac{1}{a_1^3} e^{-2r/a_1} \cdot r^2 =$$

$$\begin{aligned} &= \left[\begin{array}{l} \text{change of variables} \\ y = 2r/a_1 \end{array} \right] = 4a_1^2 \cdot \frac{1}{2^5} \int_0^\infty dy y^4 e^{-y} = \frac{1}{2^5} \cdot 2^5 \cdot 3a_1^2 = a_1^2; \end{aligned}$$

(4) So we have got $\langle r^2 \rangle = 3a_p^2 \Rightarrow \langle x^2 \rangle = \frac{1}{3} \langle r^2 \rangle = a_p^2$

(5) Find the expectation value for $\langle p_x^2 \rangle$:

Here we will use the same symmetry argument as in the previous part of the problem:

$$\langle \hat{p}_x^2 \rangle = \langle \hat{p}_y^2 \rangle = \langle \hat{p}_z^2 \rangle = \frac{1}{3} \langle \hat{p}^2 \rangle$$

In this case it is especially useful as problem can be solved easily in spherical coordinates ($\psi(r)$) and \hat{p} depend only on radial coordinates "r"), but in cartesian coordinates it will be more complicated problem as $\psi(r)$ still has only r-dependence, while $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ has all dependencies.

$$\langle \hat{p}^2 \rangle = -\hbar^2 \int d^3r \psi_{100}^*(r) (\Delta) \psi_{100}(r), \text{ here } \Delta = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta_{\theta, \varphi}$$

is Laplace operator and $\Delta_{\theta, \varphi}$ is angle-dependent part of Laplace operator. We know (see theory for this class and

class 11) $\Delta_{\theta, \varphi} \psi_{nlm} = -\frac{l^2}{\hbar^2} \psi_{nlm} = -\frac{1}{\hbar^2} l(l+1) \psi_{nlm}$; So that in

our case $\Delta^2 \psi_{100} = 0$ and $\Delta \psi_{100} = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \psi_{100} =$

$$= \frac{1}{\sqrt{\pi}} \frac{1}{a_p^{3/2}} \cdot \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} e^{-\frac{r}{a_p}} = -\frac{1}{\sqrt{\pi}} \frac{1}{a_p^{3/2}} \frac{1}{a_p} \cdot \frac{1}{r^2} \frac{\partial}{\partial r} r^2 e^{-\frac{r}{a_p}} =$$

$$= \frac{1}{\sqrt{\pi} a_p^{3/2}} \left(\frac{1}{a_p^2} e^{-\frac{r}{a_p}} - \frac{2}{r a_p} e^{-\frac{r}{a_p}} \right) \text{ So that:}$$

$$\langle p^2 \rangle = -\frac{\hbar^2}{\pi a_p^3} \int d^3r \left(\frac{1}{a_p^2} - \frac{2}{r a_p} \right) e^{-\frac{2r}{a_p}} = -\frac{\hbar^2}{\pi a_p^5} \int d\Omega \int dr \cdot r^2 \left(1 - \frac{2r}{a_p} \right) e^{-\frac{2r}{a_p}} =$$

$$= \left[\begin{array}{l} \text{Changing Variable:} \\ \frac{2r}{a_p} = t \end{array} \right] = \frac{-\hbar^2}{8\pi a_p^2} \cdot \underbrace{\int d\Omega \int_0^\infty dt}_{4\pi} t^2 \left(1 - \frac{t}{4} \right) e^{-t}, \text{ using integrals:}$$

$$\int_0^\infty dt \cdot t^2 \cdot e^{-t} = 2! \quad \text{and} \quad \int dt \cdot t \cdot e^{-t} = 1; \quad \int d\Omega = 4\pi; \quad \text{so that:}$$

$$\langle p^2 \rangle = -\frac{\hbar^2}{2a_p^2} \cdot (2-4) = \frac{\hbar^2}{a_p^2}; \text{ and thus}$$

$$\boxed{\langle p_x^2 \rangle = \frac{1}{3} \langle p^2 \rangle = \frac{\hbar^2}{a_p^2}}$$

⑤ ⑥ Show that Δx and Δp from ④ and ⑤ are consistent with Heisenberg uncertainty.

As system is rotationally invariant we have

$\langle x \rangle = \langle p_x \rangle = 0$; Indeed there is no preferable direction

so the only possibility is $\langle x \rangle = \langle p_x \rangle = 0$; Thus:

$$\sigma_x^2 \equiv \langle x^2 \rangle - \langle x \rangle^2 = \langle x^2 \rangle = a_p^2;$$

$$\sigma_{p_x}^2 \equiv \langle p_x^2 \rangle - \langle p_x \rangle^2 = \langle p_x^2 \rangle = \frac{\hbar^2}{3a_p^2}; \text{ So that:}$$

$$\boxed{\sigma_x^2 \cdot \sigma_{p_x}^2 = \frac{\hbar^2}{3} > \frac{\hbar^2}{4}} \quad \text{so that Heisenberg identity is satisfied.}$$

Problem N 2 (Compendium N 15)

Consider simple hydrogenic atom with potential $V(r) = -\frac{Z e^2}{4\pi\epsilon_0 r}$;

The normalized radial w.f. for the 1s and 2p states

are:

$$R_{10}(r) = 2 \left(\frac{Z}{a_p} \right)^{3/2} e^{-Zr/a_p}; \quad R_{21}(r) = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_p} \right)^{3/2} \frac{Zr}{a_p} e^{-Zr/2a_p};$$

① Compute the expectation value $\langle 1s | \hat{r} | 1s \rangle$

• Wave function for the state $|nlm\rangle$ is $\Psi_{nlm} = R_{nl}(r) Y_{lm}(\theta, \phi)$

so that average is given by:

$$\langle nlm | \hat{r} | nlm \rangle = \int d^3r \cdot r \cdot |R_{nl}(r)|^2 \cdot |Y_{lm}|^2 = \int dr \cdot r^3 |R_{nl}(r)|^2 \int d\Omega |Y_{lm}(\theta, \phi)|^2$$

as $\int d\Omega |Y_{lm}|^2 = 1$ due to normalization so that:

$$\langle nlm | \hat{r} | nlm \rangle = \int_0^\infty dr \cdot r^3 |R_{nl}(r)|^2;$$

• In particular:

$$\langle 1s | \hat{r} | 1s \rangle = \int_0^\infty dr \cdot r^3 \cdot 4 \left(\frac{Z}{a_p} \right)^3 e^{-2Zr/a_p} = \left[\begin{array}{l} \text{changing variables} \\ t = \frac{2Zr}{a_p} \end{array} \right] =$$

$$= \frac{a_p}{4Z} \int_0^\infty dt \cdot t^3 \cdot e^{-t} = \frac{3! a_p}{4Z} = \frac{3}{2} \frac{a_p}{2} \quad \text{so that} \quad \boxed{\langle 1s | \hat{r} | 1s \rangle = \frac{3}{2} \frac{a_p}{2}};$$

② Compute the expectation value $\langle 2p | \hat{r} | 2p \rangle$. In the same way we have:

$$\textcircled{6} \quad \langle 2p | \hat{r} | 2p \rangle = \int_0^{\infty} dr \cdot r^3 \cdot \frac{1}{3} \left(\frac{Z}{2a_0} \right)^3 \left(\frac{Zr}{a_0} \right)^2 \cdot \exp\left(-\frac{Zr}{2a_0}\right) =$$

= [changing variable:
 $t = \frac{Zr}{a_0}$] $= \frac{1}{3 \cdot 8} \frac{a_0^5}{Z^5} \int_0^{\infty} dt t^5 e^{-t} = \frac{5!}{3 \cdot 8} \frac{a_0^5}{Z^5} = \frac{5! a_0^5}{Z^5}$, so

We have got $\boxed{\langle 2p | \hat{r} | 2p \rangle = \frac{5! a_0^5}{Z^5}}$

③ Now assume that there is small perturbation to the Hamiltonian, $H' = \lambda r$. Compute first order corrections to the energies of the 1s and 2p states.

We haven't yet studied perturbation theory but still we can calculate at least first order correction using general considerations. Energy of the system is given by the expectation value:

$\langle H \rangle \equiv \langle \psi | \hat{H}_0 + \hat{H}' | \psi \rangle$ where \hat{H}_0 is unperturbed hamiltonian (in our case simply: hydrogen atom hamiltonian) so that $\langle \psi | \hat{H}_0 | \psi \rangle$ is nonperturbed energy of the state and $\langle \psi | \hat{H}' | \psi \rangle$ is first order correction. Here you should ask why we don't consider back reaction of Hamiltonian perturbation on the state of the system, i.e. changing $|\psi\rangle \rightarrow |\psi^{(0)}\rangle + |\psi^{(1)}\rangle$ where $\hat{H}_0 |\psi^{(0)}\rangle = E_0 |\psi^{(0)}\rangle$ - eigenstate of unperturbed Hamiltonian. By the moment we omit this important question and postpone it to the corresponding class (problem set N 15). So that first order correction will simply be given by:

$$E_{1s}^{(1)} = \lambda \langle \hat{r} \rangle_{1s} = \frac{3 \lambda a_0}{Z};$$

$$E_{2p}^{(1)} \equiv \langle 2p | \hat{H} | 2p \rangle = \lambda \langle \hat{r} \rangle_{2p} = \frac{5 \lambda a_0}{Z};$$

(7)

Problem III (Compendium 16)

An electron in the ground state of tritium, for which the nucleus consists of 1 proton (charge +e) and 2 neutrons (charge 0). A nuclear reaction instantaneously changes the nucleus to He^3 which consists of two protons and one neutron (hence total charge +2e)

@ Find the probability that the electron is in the ground state of He^3

- First let's write down w.f. of electrons in Tritium and Helium. For the ground state we have

$$\Psi_{100}(r, \theta, \phi) = R_{10}(r, Z) Y_{00}(\theta, \phi) \quad \text{where}$$

• $R_{10}(r, Z) = 2 \left(\frac{Z}{a_n} \right)^{3/2} \exp\left(-\frac{Zr}{a_n}\right)$; and for Tritium we should take $Z=1$ (charge of the nucleus is +e) while for Helium we take $Z=2$ (charge of the nucleus is +2e)

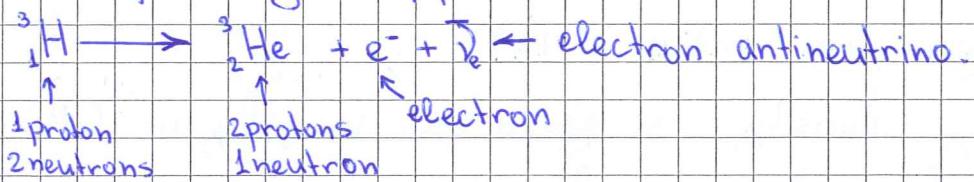
For $2p$ state we have

$$\Psi_{21m} = R_{21}(r, Z) Y_{1m}(\theta, \phi); \quad \text{where}$$

$$R_{21}(r, Z) = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_n} \right)^{3/2} \left(\frac{Z \cdot r}{a_n} \right) \exp\left(-\frac{Z \cdot r}{2a_n}\right); \quad \text{with the same}$$

values of Z for Tritium and Helium atoms.

- Now β -decay happens:



and the electron is forced to change state to one of the eigenstates of ${}^3_2\text{He}$ atom. In particular probability to jump into $1s$ state is given by inner product:

$$P(1s \rightarrow 1s) = |\langle \Psi_{100}^{Z=1} | \Psi_{100}^{Z=2} \rangle|^2 \equiv \int dr \cdot r^2 \cdot (R_{10}^*(r, Z=1) \cdot R_{10}(r, Z=2)) *$$

$$\textcircled{8} * \int d\Omega |Y_{00}(\theta, \varphi)|^2 |^2 \text{ as } \int d\Omega |Y_{00}(\theta, \varphi)|^2 = 1 \text{ by}$$

normalization, we get:

$$P(1s \rightarrow 1s) = \left| \int_0^\infty dr \cdot r^2 \cdot 4 \cdot \frac{2^{3/2}}{a_p^3} e^{-\frac{3r}{a_p}} \right|^2 = \left[\text{using change of var. } t = \frac{3r}{a_p} \right] =$$

$$= \left| \int_0^\infty dt \cdot 4\sqrt{8} \frac{1}{3^3} t^2 e^{-t} \right|^2 = \left| 8\sqrt{2} \cdot \frac{1}{3^3} \cdot 2! \right|^2 = \frac{8^3}{3^3} \Rightarrow$$

$$\Rightarrow P(1s \rightarrow 1s) = \left(\frac{8}{3} \right)^3 \quad \text{- this number is very close to 1.}$$

\textcircled{6} What is the probability that the electron is in the $2p(l=1)$ state of ${}^3\text{He}$

In analogy, this probability is given by the following inner product:

$$P(1s \rightarrow 2p) \equiv |\langle \Psi_{100}(Z=1) | \Psi_{21m}(Z=2) \rangle|^2 = \\ = \left| \int dr \cdot r^2 R_{10}^*(Z=1, r) R_{21}(Z=2, r) \int d\Omega Y_{00}^*(\theta, \varphi) Y_{1m}(\theta, \varphi) \right|^2 \text{ as}$$

$$\int d\Omega Y_{0m}^* Y_{0m} = \delta_{mm} \text{ we get}$$

$$\boxed{P(1s \rightarrow 2p) = 0;}$$

Problem N4 Find the probability that an electron in the ground state is inside the proton in a hydrogen atom. Assume that the proton radius $b \ll a_p$. Using $b = 10^{-15} \text{ m}$, what is this probability? What is the probability if the electron is in (210) state? ($a_p = 0.5 \cdot 10^{-10} \text{ m}$ - Bohr radius is of order of what we call hydrogen atom radius $\sim 1 \text{ \AA}$)

• Probability density is given (as usually in QM) by the square of electron's w.f.:

$g(\bar{x}) = |\Psi_{nem}(\bar{x})|^2$ and corresponding probability for the electron to be found inside nucleus is then:

$$P(nlm) = \underbrace{\int dr \cdot r^2 |R_{nl}(r)|^2}_{\text{due to the normalization}} \underbrace{\int d\Omega |Y_{lm}(\theta, \varphi)|^2}_{\text{}} = \int dr \cdot r^2 |R_{nl}(r)|^2;$$

- ⑤ So for ground state (1s) we get:

$$P(1s) = \int_0^{\infty} dr \cdot r^2 |R_{10}(r)|^2 = \int_0^{\infty} dr \cdot r^2 \cdot \frac{4}{\alpha_n^3} e^{-2r/\alpha_n}$$

In general case this integral is hard to evaluate but we can notice that in the region $0 < r < b$ we have $e^{-2r/\alpha_n} \approx 1$ as $b \ll \alpha_n$; and integral is simple under this assumption:

$$P(1s) = \int_0^b dr \cdot r^2 \frac{4}{\alpha_n^3} = \frac{4}{3} \left(\frac{b}{\alpha_n}\right)^3 \Rightarrow P(1s) = \frac{4}{3} \left(\frac{b}{\alpha_n}\right)^3 \approx 10^{-14};$$

- In the same way for (210) state we get

$$P(210) = \int_0^{\infty} dr \cdot r^2 |R_{21}(r)|^2 = \int_0^{\infty} dr \cdot r^2 \frac{1}{3} \frac{1}{8\alpha_n^3} \frac{1}{\alpha_n^2} e^{-r/\alpha_n} \approx [\text{again using }] \approx$$

$$\approx \frac{1}{24\alpha_n^5} \int_0^{\infty} dr \cdot r^4 = \frac{1}{5 \cdot 24} \left(\frac{b}{\alpha_n}\right)^5 \text{ so finally } P(2p) = \frac{1}{120} \left(\frac{b}{\alpha_n}\right)^5 \approx 2,5 \cdot 10^{-26};$$

Problem I Consider the hydrogen atom w.f.

$\Psi = \frac{1}{\sqrt{2}} \Psi_{211} + \frac{1}{\sqrt{2}} \Psi_{21-1}$. Find the expectation values $\langle x^2 \rangle$, $\langle y^2 \rangle$, and $\langle z^2 \rangle$ for this state.

- First let's write down explicit view of the state Ψ :

$$\Psi = \frac{1}{\sqrt{2}} (\Psi_{211} + \Psi_{21-1}) \equiv \frac{1}{\sqrt{2}} R_{21} (\Psi_{111} + \Psi_{1-1}), \text{ and then we}$$

use explicit expressions for spherical harmonics,

$$\Psi_{111} = -\sqrt{\frac{3}{8\pi}} \sin\theta \cdot e^{i\varphi}; \quad \Psi_{1-1} = \sqrt{\frac{3}{8\pi}} \sin\theta \cdot e^{-i\varphi}; \text{ so that:}$$

$$\Psi = \frac{1}{\sqrt{2}} \sqrt{\frac{3}{8\pi}} \cdot R_{21} \cdot \sin\theta (e^{-i\varphi} - e^{i\varphi}) = -i \sqrt{\frac{3}{4\pi}} R_{21} \cdot \sin\theta \cdot \sin\varphi; \Rightarrow$$

$$\Rightarrow \Psi = -i \sqrt{\frac{3}{4\pi}} R_{21}(r) \sin\theta \cdot \sin\varphi;$$

$$R_{21}(r) = \frac{1}{\sqrt{3}} r \left(\frac{Zr}{\alpha_n}\right) \left(\frac{Z_1}{2\alpha_n}\right)^{3/2} \cdot \exp\left(-\frac{Zr}{2\alpha_n}\right);$$

- Now we can find the expectation values:

$$\langle x^2 \rangle = \int_{-1}^1 d\cos\theta \int_0^{2\pi} d\varphi \int_0^{\infty} dr \cdot r^2 \cdot \underbrace{r^2 \sin^2\theta \cos^2\varphi}_{x^2} \underbrace{|R_{21}|^2}_{|\Psi|^2} \underbrace{\frac{3}{4\pi} \sin^2\theta \sin^2\varphi}_{A} =$$

$$= \frac{3}{4\pi} \int d\cos\theta \cdot \sin^4\theta \cdot \int_0^{2\pi} d\varphi \cdot \sin^2\varphi \cdot \cos^2\varphi \underbrace{\int_0^{\infty} dr \cdot r^4 |R_{21}|^2}_{C} = \frac{3}{4\pi} A \cdot B \cdot C;$$

$$\textcircled{10} \quad \langle y^2 \rangle \equiv \int d\cos\theta \int_0^{2\pi} d\varphi \int_0^\infty dr \cdot r^2 \cdot r^2 \cdot \sin^2\theta \cdot \sin^2\varphi \cdot |R_{21}|^2 \frac{3}{4\pi} \sin^2\theta \cdot \sin^2\varphi =$$

$$= \frac{3}{4\pi} \underbrace{\int d\cos\theta \cdot \sin^4\theta}_{A} \underbrace{\int d\varphi \sin^4\varphi}_{B} \underbrace{\int_0^\infty dr \cdot r^4 |R_{21}|^2}_{C} = \frac{3}{4\pi} A \cdot B \cdot C;$$

$$\langle z^2 \rangle \equiv \int d\cos\theta \int_0^{2\pi} d\varphi \int_0^\infty dr \cdot r^2 \cdot \cos^2\theta \cdot |R_{21}|^2 \cdot \frac{3}{4\pi} \sin^2\theta \cdot \sin^2\varphi =$$

$$= \frac{3}{4\pi} \underbrace{\int d\cos\theta \cdot \cos^2\theta \cdot \sin^2\theta}_{E} \underbrace{\int d\varphi \cdot \sin^4\varphi}_{F} \underbrace{\int_0^\infty dr \cdot r^4 |R_{21}|^2}_{C} = \frac{3}{4\pi} E \cdot F \cdot C;$$

• Let's now calculate all the integrals we have got:

$$* \underline{A} = \int d\cos\theta \cdot \sin^4\theta = [\cos\theta = t] = \int_{-1}^1 dt \cdot (1-t^2)^2 = \int_{-1}^1 dt \cdot (1-2t^2+t^4) = \left(t - \frac{2}{3}t^3 + \frac{1}{4}t^4\right) \Big|_{-1}^1 = \frac{16}{15};$$

$$* \underline{B} = \int_0^{2\pi} d\varphi \cdot \sin^2\varphi \cdot \cos^2\varphi = \int_0^{2\pi} d\varphi \cdot \frac{1}{4} \sin^2 2\varphi = \int_0^{2\pi} d\varphi \cdot \frac{1}{8} (1 - \cos 4\varphi) = \frac{\pi}{4} - \frac{1}{32} \sin 4\varphi \Big|_0^{2\pi} = \frac{\pi}{4};$$

$$* \underline{C} = \int_0^\infty dr \cdot r^4 \cdot |R_{21}|^2 = \frac{1}{3} \cdot \frac{1}{8a_p^3} \cdot \frac{1}{a_p^2} \int_0^\infty dr \cdot r^6 e^{-\frac{r}{a_p}} = \left[\frac{r}{a_p} - t\right] = \frac{1}{24} a_p^2 \int_0^\infty dt \cdot t^6 e^{-t} = \frac{6!}{24} a_p^2 = 30a_p^2;$$

$$* \underline{D} = \int_0^{2\pi} d\varphi \sin^4\varphi = \int_0^{2\pi} d\varphi \cdot \frac{1}{4} (1 - \cos 2\varphi)^2 = \frac{1}{4} \int_0^{2\pi} d\varphi (1 - 2\cos 2\varphi + \cos^2 2\varphi) =$$

$$= \frac{1}{4} \int_0^{2\pi} d\varphi (1 - 2\cos 2\varphi + \frac{1}{2} + \frac{1}{2} \cos 4\varphi) = \frac{1}{4} \left(\frac{3}{2} \cdot 2\pi - \sin 2\varphi \Big|_0^{2\pi} + \frac{1}{8} \sin 4\varphi \Big|_0^{2\pi} \right) = \frac{3\pi}{4};$$

$$* \underline{E} = \int d\cos\theta \cdot \cos^2\theta \cdot \sin^2\theta = [\cos\theta = t] = \int_{-1}^1 dt \cdot t^2 \cdot (1-t^2) = \left(\frac{1}{3}t^3 - \frac{1}{5}t^5\right) \Big|_{-1}^1 = \frac{4}{15};$$

$$* \underline{F} = \int_0^{2\pi} d\varphi \cdot \sin^2\varphi = \frac{1}{2} \int_0^{2\pi} d\varphi (1 - \cos 2\varphi) = \frac{1}{2} (2\pi - \frac{1}{2} \sin 2\varphi \Big|_0^{2\pi}) = \pi;$$

So we get:

$$\langle x^2 \rangle = \frac{3}{4\pi} A \cdot B \cdot C = \frac{3}{4\pi} \cdot \frac{16}{15} \cdot \frac{\pi}{4} \cdot 30a_p^2 = 6a_p^2;$$

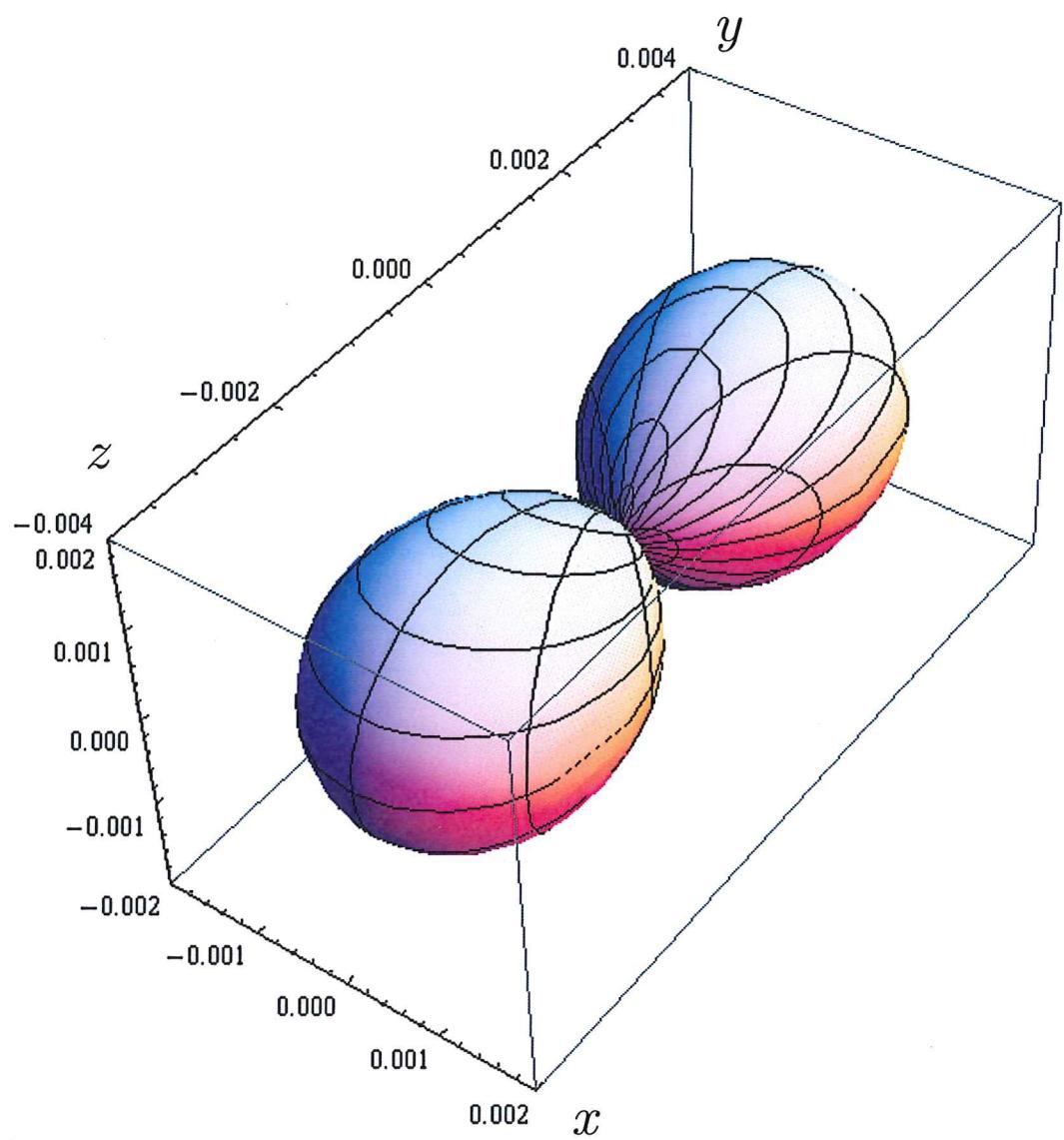
$$\langle y^2 \rangle = \frac{3}{4\pi} A \cdot B \cdot C = \frac{3}{4\pi} \cdot \frac{16}{15} \cdot \frac{3\pi}{4} \cdot 30a_p^2 = 18a_p^2;$$

$$\langle z^2 \rangle = \frac{3}{4\pi} E \cdot F \cdot C = \frac{3}{4\pi} \cdot \frac{4}{15} \cdot \pi \cdot 30a_p^2 = 6a_p^2;$$

So $\boxed{\langle x^2 \rangle = \langle z^2 \rangle = 6a_p^2; \langle y^2 \rangle = 18a_p^2;}$

This is consistent with the probability density $|\psi|^2$ plot

which peaks in larger y -values than x and z , which leads to larger expectation value (see the picture below)



① Seminar 13 (Generalized Angular Momentum)

Theory • On one of the previous classes we have considered angular momentum operator \hat{L} , which was taking only integer values. But from real world we know that particles can have half-integer momentum. For this purpose we introduce generalized angular momentum \hat{J} that obeys the same commutation relation as orbital angular momentum:

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z; \quad [\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x; \quad [\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y;$$

$$[\hat{J}_z, \hat{J}_{\pm}] = \pm \hbar \hat{J}_{\pm}; \quad \text{and} \quad [\hat{J}, \hat{J}^2] = 0;$$

- In the same way as in the case of orbital angular momentum we should describe all states in the basis of eigenvalues of commuting operators \hat{J}_z and \hat{J}^2 : $|j, m\rangle$; such that:

$$\hat{J}^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle;$$

$$J_z |j, m\rangle = \hbar m |j, m\rangle;$$

- Assume we want to add 2 angular momenta $\hat{\vec{J}} = \hat{\vec{J}}_1 + \hat{\vec{J}}_2$. We assume $[J_1, J_2] = 0$ i.e. momenta of 2 particles are independent and we can find simultaneous eigenstate of $\hat{J}_{1z}, \hat{J}_1^2, \hat{J}_{2z}, \hat{J}_2^2$: $|j_1, m_1; j_2, m_2\rangle$

- At the same time we can find the following commutators to be "0":

$[\hat{J}_1^2, \hat{J}_1^2] = [\hat{J}_2^2, \hat{J}_2^2] = 0; \quad [J_2, \hat{J}_1^2] = [\hat{J}_2, J_1^2] = 0$; but at the same time $[\hat{J}^2, J_{1z}] \neq 0$ and $[\hat{J}^2, J_{2z}] \neq 0$; so the state can be taken in the basis of simultaneous eigenstates of $\hat{J}^2, J_z, \hat{J}_1^2, \hat{J}_2^2$: $|j, m; j_1, j_2\rangle$

- ② • note that:

$$\begin{aligned}\hat{J}_z |j_1, m_1; j_2, m_2\rangle &\equiv (\hat{j}_{1z} + \hat{j}_{2z}) |j_1, m_1; j_2, m_2\rangle = \\ &= (m_1 + m_2) |j_1, m_1; j_2, m_2\rangle \quad \text{thus we say that} \\ |m = m_1 + m_2| \text{ always.}\end{aligned}$$

• Now assume we want to solve the following problem: express our states $|j, m; j_1, j_2\rangle$ through the states $|j_1, m_1; j_2, m_2\rangle$; For this we follow algorithm:

① Write down highest weight state $|j_1, j_1; j_2, j_2\rangle = |j, j; j_1, j_2\rangle$ which is annihilated by the operator $\hat{J}_+ = \hat{J}_{1+} + \hat{J}_{2+}$:

$$\hat{J}_+ |j, j; j_1, j_2\rangle = (\hat{j}_{1+} + \hat{j}_{2+}) |j_1, j_1; j_2, j_2\rangle = 0;$$

② Starting from the highest weight state and acting with the lowering operator

$$J_- |j, j; j_1, j_2\rangle = (J_{1-} + J_{2-}) |j_1, j_1; j_2, j_2\rangle \quad \text{and formulas:}$$

$$J_{\pm} |j, m\rangle = \hbar \sqrt{j(j \pm 1) - m(m \pm 1)} |j, m \pm 1\rangle$$

in this way we get all the states $|j, m; j_1, j_2\rangle$ with $-j \leq m \leq j$

③ Then we get state $|j-1, j-1; j_1, j_2\rangle = \sum_{\substack{\text{all} \\ m_1+m_2=j}} a_i |j_i, m_i; j_2, m_2\rangle$

tuning a_i so that the state $|j-1, j-1; j_1, j_2\rangle$ is orthogonal to all states $|j, m; j_1, j_2\rangle$;

④ Then starting with $|j-1, j-1; j_1, j_2\rangle$ we get all states $|j-t, m; j_1, j_2\rangle$ acting with lowering operator J_- .

⑤ Repit this algorith untill we get all the states with $|j_1-j_2| \leq j \leq j_1+j_2$ and all possible $j, m \leq j$

In total there should be:

$$\begin{aligned}N &= \sum_{j_1+j_2}^{j_1+j_2} (2j+1) = \left[\begin{array}{l} \text{Using formula for the} \\ \text{summ of arithm. progression} \end{array} \right] = \frac{1}{2} \underbrace{(j_1+j_2-j_1+j_2+1)}_{\# \text{ of terms in progression}} \times \\ &\times (2j_1+2j_2+2j_1-2j_2+1+1) = (2j_1+1)(2j_2+1)\end{aligned}$$

③

So that $N = (2j_1+1)(2j_2+1)$

- Another way to derive this is to consider $|j_1, m_1; j_2, m_2\rangle$ states. As $-j_1 \leq m_1 \leq j_1$ and $-j_2 \leq m_2 \leq j_2$ so that total number of states is $N = (2j_1+1)(2j_2+1)$ which coincides with expression obtained previously.

Problem I (Compendium N12)

Consider 2 particles, one with $s = \frac{3}{2}$ and the other with $s = \frac{1}{2}$. Recall that $J_z |j, m\rangle = \hbar \sqrt{j(j+1) - m(m\pm1)} |j, m\pm1\rangle$ and $J_z |j, m\rangle = m\hbar |j, m\rangle$

④ What are allowed values for total angular momentum?

We sum up $s = \frac{1}{2}$ and $s = \frac{3}{2}$ so that total angular momentum is $|s_1 - s_2| \leq j \leq s_1 + s_2$, so that in our case it turns to be $1 \leq j \leq 2$ now as momentum takes only integer values $j=1, 2$.

⑤ What is total number of different spin states for the combined system?

As we have discussed in theory part, total number of states is given by:

$$N = (2j_1+1)(2j_2+1) = (2 \cdot \frac{1}{2} + 1)(2 \cdot \frac{3}{2} + 1) = 8. \text{ So in total we get } N = 8 \text{ states.}$$

⑥ Find normalized eigenstates of the total angular momentum $|j, m; j_1, j_2\rangle$ in terms of the eigenstates of the individual spins $|\frac{3}{2}, m_1; \frac{1}{2}, m_2\rangle$

Let's follow the algorithm described in theoretical part:

① Highest weight state in our case is

$$|2, 2; \frac{3}{2}, \frac{1}{2}\rangle = |\frac{3}{2}, \frac{3}{2}; \frac{1}{2}, \frac{1}{2}\rangle;$$

④ ② Now we will apply lowering operator $\hat{J}_- = \hat{J}_-^{(1)} + \hat{J}_-^{(2)}$ to this state. It is useful to write down all possible actions of the lowering operator:

$$\bullet \hat{J}_-^{(1)} |2, 2; \frac{3}{2}, \frac{1}{2}\rangle = \hbar \sqrt{2 \cdot 3 - 2 \cdot 1} |2, 1; \frac{3}{2}, \frac{1}{2}\rangle = 2\hbar |2, 1; \frac{3}{2}, \frac{1}{2}\rangle; \quad (1)$$

$$\hat{J}_-^{(1)} |2, 1; \frac{3}{2}, \frac{1}{2}\rangle = \hbar \sqrt{2 \cdot 3 - 0} |2, 0; \frac{3}{2}, \frac{1}{2}\rangle = \sqrt{6} \hbar |2, 0; \frac{3}{2}, \frac{1}{2}\rangle; \quad (2)$$

$$\hat{J}_-^{(1)} |2, 0; \frac{3}{2}, \frac{1}{2}\rangle = \hbar \sqrt{2 \cdot 3 - 0} |2, -1; \frac{3}{2}, \frac{1}{2}\rangle = \sqrt{6} \hbar |2, -1; \frac{3}{2}, \frac{1}{2}\rangle; \quad (3)$$

$$\hat{J}_-^{(1)} |2, -1; \frac{3}{2}, \frac{1}{2}\rangle = \hbar \sqrt{2 \cdot 3 - (-1)(-2)} |2, -2; \frac{3}{2}, \frac{1}{2}\rangle = 2\hbar |2, -2; \frac{3}{2}, \frac{1}{2}\rangle; \quad (4)$$

$$\bullet \hat{J}_-^{(2)} |1, 1; \frac{3}{2}, \frac{1}{2}\rangle = \hbar \sqrt{2 - 0} |1, 0; \frac{3}{2}, \frac{1}{2}\rangle = \sqrt{2} \hbar |1, 0; \frac{3}{2}, \frac{1}{2}\rangle; \quad (5)$$

$$\hat{J}_-^{(2)} |1, 0; \frac{3}{2}, \frac{1}{2}\rangle = \hbar \sqrt{2 - 0} |1, -1; \frac{3}{2}, \frac{1}{2}\rangle = \sqrt{2} \hbar |1, -1; \frac{3}{2}, \frac{1}{2}\rangle; \quad (6)$$

$$\bullet \hat{J}_-^{(1)} | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, m\rangle = \hbar \sqrt{\frac{3}{2} \cdot \frac{5}{2} - \frac{3}{2} \cdot \frac{1}{2}} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, m\rangle = \sqrt{3} \hbar | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, m\rangle \quad (7)$$

$$\hat{J}_-^{(1)} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, m\rangle = \hbar \sqrt{\frac{3}{2} \cdot \frac{5}{2} - \frac{1}{2}(-\frac{1}{2})} | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, m\rangle = 2\hbar | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, m\rangle \quad (8)$$

$$\hat{J}_-^{(1)} | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, m\rangle = \hbar \sqrt{\frac{3}{2} \cdot \frac{5}{2} + \frac{1}{2}(-\frac{3}{2})} | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, m\rangle = \sqrt{3} \hbar | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, m\rangle \quad (9)$$

In equations (7) - (9) $m = \pm \frac{1}{2}$ as $\hat{J}_-^{(1)}$ acts only on first spin

$$\bullet \hat{J}_-^{(2)} | \frac{3}{2}, m; \frac{1}{2}, \frac{1}{2}\rangle = \hbar \sqrt{\frac{1}{2} \cdot \frac{3}{2} - \frac{1}{2}(-\frac{1}{2})} | \frac{3}{2}, m; \frac{1}{2}, -\frac{1}{2}\rangle = \hbar | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2}\rangle; \quad (10)$$

here $-\frac{3}{2} \leq m \leq \frac{3}{2}$ as $\hat{J}_-^{(2)}$ acts only on $S_2 = \frac{1}{2}$ spin

• Now we can start acting with \hat{J}_- on the highest weight state:

$$\bullet \hat{J}_- |2, 2; \frac{3}{2}, \frac{1}{2}\rangle = (\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, \frac{1}{2}\rangle$$

↓ using eq (1), (7) and (10)

$$2 |2, 1; \frac{3}{2}, \frac{1}{2}\rangle = \sqrt{3} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle + | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle;$$

$$|2, 1; \frac{3}{2}, \frac{1}{2}\rangle = \frac{\sqrt{3}}{2} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle + \frac{1}{2} | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2}\rangle;$$

$$\bullet \hat{J}_- |2, 1; \frac{3}{2}, \frac{1}{2}\rangle = \frac{\sqrt{3}}{2} (\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle + \frac{1}{2} (\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2}\rangle$$

↓ using eq. (2), (8), (7) and (10)

$$\sqrt{6} |2, 0; \frac{3}{2}, \frac{1}{2}\rangle = \frac{\sqrt{3}}{2} (2 | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle + | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle) +$$

$$+ \frac{1}{2} \cdot \sqrt{3} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle + 0 \rightarrow \text{last term "0" is from } \hat{J}_-^{(2)} | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2}\rangle = 0$$

(5)

So we get:

$$|2,0; \frac{3}{2}, \frac{1}{2}\rangle = \frac{1}{\sqrt{2}} (| \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle + | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle)$$

• $\hat{J}_- |2,0; \frac{3}{2}, \frac{1}{2}\rangle = \frac{1}{\sqrt{2}} ((\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle + (\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle)$

\Downarrow using eq. (3), (9), (10), (7)

$$\begin{aligned} \sqrt{6} |2,-1; \frac{3}{2}, \frac{1}{2}\rangle &= \frac{1}{\sqrt{2}} (\sqrt{3} | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, \frac{1}{2}\rangle + | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle + \\ &+ 2 | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle) \text{ so that} \end{aligned}$$

$$|2,-1; \frac{3}{2}, \frac{1}{2}\rangle = \frac{1}{2} | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, \frac{1}{2}\rangle + \frac{\sqrt{3}}{2} | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle;$$

- Now we act one more (the last) time:

$$\begin{aligned} \hat{J}_- |2,-1; \frac{3}{2}, \frac{1}{2}\rangle &= \frac{1}{2} ((\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, \frac{1}{2}\rangle + \\ &+ \sqrt{3} (\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle) \end{aligned}$$

\Downarrow using (4), (10) and (9)

$$2 |2,-2; \frac{3}{2}, \frac{1}{2}\rangle = \frac{1}{2} | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, -\frac{1}{2}\rangle + \frac{\sqrt{3}}{2} \cdot \sqrt{3} | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, -\frac{1}{2}\rangle;$$

$$|2,-2; \frac{3}{2}, \frac{1}{2}\rangle = | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, -\frac{1}{2}\rangle;$$

Note 1: This is the lowest weight state (state annihilated by \hat{J}_- : $\hat{J}_- |1\rangle = 0$) and it is exactly of the expected form. Due to $m = m_1 + m_2$ condition, the only possibility to have $m = -2$ is $m_1 = -\frac{3}{2}; m_2 = -\frac{1}{2}$. This is cross check that we did everything right if we end up with the desired expression.

Note 2: Another cross check is normalization: note that all states we get are automatically normalized.

③ So we have finished with all $j=2$ states (5 of them in total) and now should proceed with $j=1$ states.

- Highest weight state for $j=1$ is

$$|1,1; \frac{3}{2}, \frac{1}{2}\rangle = ?$$

- As $m = m_1 + m_2 = 1$ we have just 2 opportunities:

$$m_1 = \frac{1}{2}, m_2 = \frac{1}{2} \text{ (state } | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle \text{) and } m_1 = \frac{3}{2}, m_2 = -\frac{1}{2}$$

⑥ with corresponding state $| \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2} \rangle$. Thus

$j=1$ highest weight state is

$$| 1, 1; \frac{3}{2}, \frac{1}{2} \rangle = a | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \rangle + b | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2} \rangle$$

• This state should be orthogonal to all states

we have built. But as $\langle j_1, m_1; j_2, m_2 | j'_1, m'_1; j'_2, m'_2 \rangle = \delta_{j_1 j'_1} \delta_{j_2 j'_2} \delta_{m_1 m'_1} \delta_{m_2 m'_2}$

this state will automatically be orthogonal to all the states with $m \neq 1$ (as $m = m_1 + m_2$ this is true). So really we should just check

$$\langle 2, 1; \frac{3}{2}, \frac{1}{2} | 1, 1; \frac{3}{2}, \frac{1}{2} \rangle = 0 - ?$$

Substituting explicit expression for $| 2, 1; \frac{3}{2}, \frac{1}{2} \rangle$ and our ansatz for $| 1, 1; \frac{3}{2}, \frac{1}{2} \rangle$ we get:

$$\left(\frac{\sqrt{3}}{2} \langle \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} | + \frac{1}{2} \langle \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2} | \right) (a | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \rangle + b | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2} \rangle) = \\ = \frac{\sqrt{3}}{2} a + \frac{1}{2} b = 0 \Rightarrow b = -\sqrt{3} a \text{ so normalized state is:}$$

$$| 1, 1; \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{2} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \rangle - \frac{\sqrt{3}}{2} | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2} \rangle;$$

⑦ Now we act with lowering operator $\hat{J}_- = \hat{J}_-^{(1)} + \hat{J}_-^{(2)}$:

$$\bullet \hat{J}_- | 1, 1; \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{2} (\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \rangle - \frac{\sqrt{3}}{2} (\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, \frac{3}{2}; \frac{1}{2}, -\frac{1}{2} \rangle; \\ \Downarrow \text{using eq. (5), (7), (8), (10)}$$

$$\sqrt{2} | 1, 0; \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{2} \cdot 2 | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \rangle + \frac{1}{2} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2} \rangle - \frac{\sqrt{3}}{2} \sqrt{3} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2} \rangle;$$

$$| 1, 0; \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{\sqrt{2}} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \rangle - \frac{1}{\sqrt{2}} | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2} \rangle;$$

$$\bullet \hat{J}_- | 1, 0; \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{\sqrt{2}} ((\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2} \rangle - (\hat{J}_-^{(1)} + \hat{J}_-^{(2)}) | \frac{3}{2}, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2} \rangle) \\ \Downarrow \text{using (6), (9), (8) and (10)}$$

$$\sqrt{2} | 1, -1; \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{\sqrt{2}} (\sqrt{3} | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, \frac{1}{2} \rangle + | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2} \rangle - 2 | \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2} \rangle)$$

$$| 1, -1; \frac{3}{2}, \frac{1}{2} \rangle = \frac{\sqrt{3}}{2} | \frac{3}{2}, -\frac{3}{2}; \frac{1}{2}, \frac{1}{2} \rangle - \frac{1}{2} | \frac{3}{2}, -\frac{1}{2}; \frac{1}{2}, -\frac{1}{2} \rangle$$

Note that all states we get are orthogonal (you can check it)

This is another good cross-check that everything is done right.

⑦ So we have got all 8 states !!!

Problem II (Compendium 13)

Consider 3 distinguishable (nonidentical) spin $\frac{1}{2}$ particles with a Hamiltonian given by

$$H = \lambda (\vec{s}_1 \cdot \vec{s}_2 + \vec{s}_2 \cdot \vec{s}_3 + \vec{s}_1 \cdot \vec{s}_3)$$

ⓐ Find all eigenstates of the total angular momentum J^2 in terms of the individual spins. Each state should be normalized and its J_z eigenvalue given.

- Let's denote individual spin states as:

- spin up $| \frac{1}{2}, \frac{1}{2} \rangle = |+\rangle$;

- spin down $| \frac{1}{2}, -\frac{1}{2} \rangle = |- \rangle$;

- Now we can write down highest weight state:

$$| \frac{3}{2}, \frac{3}{2} \rangle = |+++ \rangle$$

- Before going to algorithm let's define how many states do we have in total?

- First we add 2 spins $\frac{1}{2}$ which gives us

$$|\vec{s}_1 - \vec{s}_2| \leq j \leq |\vec{s}_1 + \vec{s}_2| \Rightarrow j = 1, 0.$$

- Then we add $\vec{s}_3 \equiv \vec{s}_1 + \vec{s}_2$ and \vec{s}_3 . There are 2 possibilities:

ⓐ $j_1 = 1$ then $|j_1 - s_3| \leq j \leq j_1 + s_3 \Rightarrow \frac{1}{2} \leq j \leq \frac{3}{2}; j = \frac{1}{2}; j = \frac{3}{2};$

ⓑ $j_1 = 0$ then $|j_1 - s_3| \leq j \leq j_1 + s_3 \Rightarrow j = \frac{1}{2};$

So we conclude that total angular momentum take values $j = \frac{1}{2}; j = \frac{3}{2};$

- Now we go through the algorithm:

① Highest weight state is $| \frac{3}{2}, \frac{3}{2} \rangle = |++,+\rangle$;

② Now we can act with the lowering operator

$$\hat{J}_- = \hat{J}_-^{(1)} + \hat{J}_-^{(2)};$$

⑧ Let's first write following actions:

$$\hat{J}_- | \frac{3}{2}, \frac{3}{2} \rangle = \hbar \sqrt{\frac{3}{2} \cdot \frac{5}{2} - \frac{3}{2} \cdot \frac{1}{2}} | \frac{3}{2}, \frac{1}{2} \rangle = \sqrt{3} \hbar | \frac{3}{2}, \frac{1}{2} \rangle; \quad (1)$$

$$\hat{J}_- | \frac{3}{2}, \frac{1}{2} \rangle = \hbar \sqrt{\frac{3}{2} \cdot \frac{5}{2} - \frac{1}{2} \cdot (-\frac{1}{2})} | \frac{3}{2}, -\frac{1}{2} \rangle = 2\hbar | \frac{3}{2}, -\frac{1}{2} \rangle; \quad (2)$$

$$\hat{J}_- | \frac{3}{2}, -\frac{1}{2} \rangle = \hbar \sqrt{\frac{3}{2} \cdot \frac{5}{2} + \frac{1}{2} \cdot (-\frac{3}{2})} | \frac{3}{2}, -\frac{3}{2} \rangle = \sqrt{3} \hbar | \frac{3}{2}, -\frac{3}{2} \rangle; \quad (3)$$

$$\hat{J}_- | + \rangle = \hat{J}_- | \frac{1}{2}, \frac{1}{2} \rangle = \hbar \sqrt{\frac{1}{2} \cdot \frac{3}{2} - \frac{1}{2} \cdot (-\frac{1}{2})} | \frac{1}{2}, -\frac{1}{2} \rangle = \hbar | \frac{1}{2}, -\frac{1}{2} \rangle = \hbar | - \rangle; \quad (4)$$

Now we act:

$$\bullet \hat{J}_- | \frac{3}{2}, \frac{3}{2} \rangle = (\hat{J}_-^{(1)} + \hat{J}_-^{(2)} + \hat{J}_-^{(3)}) | + + + \rangle$$

↓ using (1) and (4)

$$\sqrt{3} | \frac{3}{2}, \frac{1}{2} \rangle = | - + + \rangle + | + - + \rangle + | + + - \rangle \text{ so that:}$$

$$| \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{\sqrt{3}} (| - + + \rangle + | + - + \rangle + | + + - \rangle);$$

$$\bullet \hat{J}_- | \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{\sqrt{3}} (\hat{J}_-^{(1)} + \hat{J}_-^{(2)} + \hat{J}_-^{(3)}) (| - + + \rangle + | + - + \rangle + | + + - \rangle);$$

↓ using (2) and (4)

$$2 | \frac{3}{2}, -\frac{1}{2} \rangle = \frac{1}{\sqrt{3}} (| - - + \rangle + | - + - \rangle + | - - + \rangle + | + - - \rangle + | - + - \rangle + | + - - \rangle)$$

$$| \frac{3}{2}, -\frac{1}{2} \rangle = \frac{1}{\sqrt{3}} (| + - \rangle + | - + \rangle + | - - + \rangle);$$

$$\bullet \hat{J}_- | \frac{3}{2}, -\frac{1}{2} \rangle = \frac{1}{\sqrt{3}} (\hat{J}_-^{(1)} + \hat{J}_-^{(2)} + \hat{J}_-^{(3)}) (| + - \rangle + | - + \rangle + | - - + \rangle)$$

↓ using (3) and (4)

$$\sqrt{3} | \frac{3}{2}, -\frac{3}{2} \rangle = \frac{1}{\sqrt{3}} (| - - - \rangle) \text{ so that:}$$

$$| \frac{3}{2}, -\frac{3}{2} \rangle = | - - - \rangle; \text{ this is what we expect}$$

lowest weight state to be.

⑨ Now we should built state $| \frac{1}{2}, \frac{1}{2} \rangle$ which is orthogonal to all the states we have built.

As $m = m_1 + m_2 + m_3 = \frac{1}{2}$ we have following possibilities:

$$m_1 = \frac{1}{2}; m_2 = \frac{1}{2}; m_3 = -\frac{1}{2}$$

$$m_1 = \frac{1}{2}; m_2 = -\frac{1}{2}; m_3 = \frac{1}{2}; \text{ so that:}$$

$$m_1 = -\frac{1}{2}; m_2 = \frac{1}{2}; m_3 = \frac{1}{2}$$

$$| \frac{1}{2}, \frac{1}{2} \rangle = a | + + - \rangle + b | + - + \rangle + c | - + + \rangle;$$

As usually this state is automatically orthogonal to any

③ state with $m \neq \frac{1}{2}$ so we check $\langle \frac{1}{2}, \frac{1}{2} | \frac{3}{2}, \frac{1}{2} \rangle = 0$
 So that: $\langle \frac{1}{2}, \frac{1}{2} | \frac{3}{2}, \frac{1}{2} \rangle = (a^* \langle -+ + | + b^* \langle +- + | + c^* \langle ++ - |)$
 $\cdot \frac{1}{\sqrt{3}} (\langle -++ | + \langle +-+ | + \langle ++- |) = \frac{1}{\sqrt{3}} (a^* + b^* + c^*) = 0$
 As you can see there is only 1 relation for 3 variables
 and we have freedom of choice. This freedom of
 choice is related to the fact that we obtain $j=\frac{1}{2}$ in
 2 ways: either summing s_1 and s_2 to $j_z=1$ and
 then s_3 so that resulting state has $j=\frac{1}{2}$, second
 way is to sum up s_1 and s_2 to $j_z=0$ and
 then add s_3 to get total spin $j=\frac{1}{2}$; This really
 just choice of basis and doesn't matter. So we will
 choose for example $a=-b, c=0$

$$|\frac{1}{2}, \frac{1}{2}\rangle = \frac{1}{\sqrt{2}} (\langle -++ | - \langle +-+ |)$$

④ Now acting on this state with the lowering
 operator \hat{J}_- we get:

$$\hat{J}_- |\frac{1}{2}, \frac{1}{2}\rangle = \frac{1}{\sqrt{2}} (\hat{J}_-^{(1)} + \hat{J}_-^{(2)} + \hat{J}_-^{(3)}) (\langle -++ | - \langle +-+ |)$$

↓ using eq. (4)

$$|\frac{1}{2}, -\frac{1}{2}\rangle = \frac{1}{\sqrt{2}} (\langle -+- | + \langle -+- | - \langle --+ | - \langle +-+ |) \text{ so that}$$

$$|\frac{1}{2}, -\frac{1}{2}\rangle = \frac{1}{\sqrt{2}} (\langle -+- | - \langle --+ |)$$

Note: Physically our choice of $|\frac{1}{2}, \frac{1}{2}\rangle$ state corresponds
 to the case when 2 first spins sum to 0 and we
 add 3rd spin. To build another $|\frac{1}{2}, \frac{1}{2}\rangle$ state we
 take the same ansatz but demand it to be orthogonal
 to $|\frac{3}{2}, \frac{1}{2}\rangle$ and $|\frac{1}{2}, \frac{1}{2}\rangle$ that we have obtained.

Final answer is (obtain it yourself):

$$|\frac{1}{2}, \frac{1}{2}\rangle_2 = \frac{1}{\sqrt{6}} (\langle -++ | - 2 \langle +-+ | + \langle ++- |)$$

$$|\frac{1}{2}, -\frac{1}{2}\rangle_2 = \frac{1}{\sqrt{6}} (\langle -+- | - 2 \langle --+ | + \langle +-+ |)$$

(10) (b) Find the normalized eigenstates and energies of the Hamiltonian.

- Let's first rewrite the Hamiltonian in the form more useful. Total angular momentum is:

$$\vec{J} = \vec{s}_1 + \vec{s}_2 + \vec{s}_3 \Rightarrow J^2 = s_1^2 + s_2^2 + s_3^2 + 2(\underbrace{\vec{s}_1 \cdot \vec{s}_2 + \vec{s}_2 \cdot \vec{s}_3 + \vec{s}_3 \cdot \vec{s}_1}_{\frac{1}{2}H})$$

thus
$$H = \frac{\alpha}{2} (J^2 - s_1^2 - s_2^2 - s_3^2)$$

Note that $[J^2, s_i^2] = 0$, $i=1,2,3$ so that we can write down states $|j, m; j_1, j_2, j_3\rangle$ (which we have actually found in part (a) of the problem). These states will exactly be eigenstates of Hamiltonian. Indeed:

$$\begin{aligned} \hat{H} |j, m; s_1, s_2, s_3\rangle &= \frac{\alpha}{2} (J^2 |j, m; s_1, s_2, s_3\rangle - s_1^2 |j, m; s_1, s_2, s_3\rangle - \\ &- s_2^2 |j, m; s_1, s_2, s_3\rangle - s_3^2 |j, m; s_1, s_2, s_3\rangle) = \\ &= \frac{\alpha}{2} \hbar^2 ((j(j+1) - s_1(s_1+1) - s_2(s_2+1) - s_3(s_3+1))) |j, m; s_1, s_2, s_3\rangle = \\ &= \frac{\alpha}{2} \hbar^2 (j(j+1) - 3 \cdot \frac{3}{4}) \end{aligned}$$

In particular:

- For $|3/2, m\rangle$ states $-\frac{3}{2} \leq m \leq \frac{3}{2}$: 4 states

$$\hat{H} |3/2, m\rangle \equiv E |3/2, m\rangle = \frac{\alpha \hbar^2}{2} \left(\frac{15}{4} - \frac{9}{4} \right) = \frac{3}{4} \alpha \hbar^2$$

$E_{j=3/2} = \frac{3}{4} \alpha \hbar^2$ - 4-degenerate state

- For $|1/2, \pm 1/2\rangle$ (2 states)

$$\hat{H} |1/2, \pm 1/2\rangle = -2 \cdot \frac{3}{4} \cdot \frac{\alpha \hbar^2}{2} = -\frac{3}{4} \alpha \hbar^2; \text{ so that:}$$

$E_{j=1/2} = -\frac{3}{4} \alpha \hbar^2$; -2 degenerate state.

(11) Problem III Suppose 2 spin $\frac{1}{2}$ particles form a singlet state (their total angular momentum is 0, so there is only one state). Let $\hat{S}^{(1)}$ and $\hat{S}^{(2)}$ be the spin operators for the first and second particle respectively. Find the expectation value of $S_x^{(1)} (\cos\theta \cdot S_x^{(2)} + \sin\theta \cdot S_y^{(2)})$ as a function of θ .

- Singlet state is given by:

$$|0,0; \frac{1}{2}, \frac{1}{2}\rangle = \frac{1}{\sqrt{2}} (|+\rightarrow -\leftarrow +\rangle) \quad (\text{see lecture notes})$$

- We can write \hat{S}_x and \hat{S}_y operators as the following:

$$\hat{S}_x = \frac{1}{2} (\hat{S}_+ + \hat{S}_-); \quad \hat{S}_y = -\frac{i}{2} (\hat{S}_+ - \hat{S}_-);$$

- We know how \hat{S}_{\pm} acts on $| \pm \rangle \equiv | \frac{1}{2}, \pm \frac{1}{2} \rangle$ states:

$$\hat{S}_{\pm} | \pm \rangle = 0; \quad S_{\pm} | \mp \rangle = \pm | \pm \rangle; \quad (\text{see previous problem})$$

- Using expressions for \hat{S}_x and \hat{S}_y we can rewrite

$$\hat{A} \equiv \hat{S}_x^{(1)} (\cos\theta \cdot \hat{S}_x^{(2)} + \sin\theta \cdot \hat{S}_y^{(2)}) = \frac{1}{4} (\hat{S}_+^{(1)} + \hat{S}_-^{(1)}) (\hat{S}_+^{(2)} e^{-i\theta} + \hat{S}_-^{(2)} e^{i\theta})$$

- Now we are able to find expectation value:

$$\begin{aligned} & \frac{1}{4} (\hat{S}_+^{(1)} + \hat{S}_-^{(1)}) (e^{-i\theta} \hat{S}_+^{(2)} + e^{i\theta} \hat{S}_-^{(2)}) \frac{1}{\sqrt{2}} (|+\rightarrow -\leftarrow +\rangle) = \\ & = \frac{\hbar}{4\sqrt{2}} (\hat{S}_+^{(1)} + \hat{S}_-^{(1)}) (e^{-i\theta} |+\rightarrow -\rangle - e^{i\theta} |-\rightarrow \rangle) = \\ & = \frac{\hbar^2}{4\sqrt{2}} (-e^{i\theta} |+\rightarrow \rangle + e^{-i\theta} |-\rightarrow \rangle) \end{aligned}$$

Finally

$$\begin{aligned} \langle \hat{A} \rangle &= \frac{\hbar^2}{4\sqrt{2} \cdot \sqrt{2}} (\langle +|- \rangle - \langle -|+ \rangle) (-e^{i\theta} |+\rightarrow \rangle + e^{-i\theta} |-\rightarrow \rangle) = \\ & = \frac{\hbar^2}{8} (-e^{i\theta} - e^{-i\theta}) = -\frac{\hbar^2}{4} \cos\theta; \quad \text{So that} \end{aligned}$$

$$\boxed{\langle \hat{S}_x^{(1)} (\cos\theta \cdot \hat{S}_x^{(2)} + \sin\theta \cdot \hat{S}_y^{(2)}) \rangle_{\text{singlet}} = -\frac{\hbar^2}{4} \cos\theta;}$$

① Seminar 14 (QM of more than one particle)

- Before we always were considering quantum mechanics of only one particle. But there are some interesting properties of many-particle states in QM.

- Let's describe many-particle wave-function as product of single-particle w.f.'s:

$$\Psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N) = \Psi_{k_1}(\bar{r}_1) \Psi_{k_2}(\bar{r}_2) \cdots \Psi_{k_N}(\bar{r}_N);$$

$\Psi_{k_i}(\bar{r}_i)$ is w.r.t. particle k_i at position \bar{r}_i

- Now let's examine how this w.f. transforms under permutation of the positions of particles. For this purpose we introduce permutation operator \hat{P}_{12} that acts on the multiparticle w.f. in the following way:

$\hat{P}_{12} \Psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N) = \Psi(\bar{r}_2, \bar{r}_1, \dots, \bar{r}_N)$. As we consider identical particles interchange of 2 of them shouldn't effect physics, i.e. shouldn't effect any probability distribution given by $|\Psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N)|^2$, i.e. all we can obtain is additional phase:

$$\hat{P}_{12} \Psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N) = e^{i\phi} \Psi(\bar{r}_2, \bar{r}_1, \dots, \bar{r}_N);$$

If we now apply permutation operator one more time we get the same w.f. back. That means we are left with only 2 possibilities:

$$\hat{P}_{12} \Psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N) = \pm \Psi(\bar{r}_2, \bar{r}_1, \dots, \bar{r}_N);$$

- There are 2 kinds of particles in nature:
 - bosons are symmetric under interchanging particles
 - fermions are antisymmetric under permutation
- Let's consider simpler example of 2 particles wave function

$$\Psi(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}} (\Psi_1(\bar{r}_1) \Psi_2(\bar{r}_2) \pm \Psi_2(\bar{r}_1) \Psi_1(\bar{r}_2))$$

② Where "+" sign corresponds to bosons and "-" sign to fermions.

- From here we can see work of Pauli exclusion principle, that state: 2 identical spinless fermions can't be putted in one point. Indeed if we put $\vec{r}_1 = \vec{r}_2$ in the expression above we get $\Psi(\vec{r}_1, \vec{r}_2) = 0$;

- Above we have considered spinless particle. Now we can put spin into play. Overall w.f. is then product of spin and spatial parts of w.f.:

$$\Psi_{S=0}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left[(\Psi_+(\vec{r}_1) \Psi_-(\vec{r}_2) + \Psi_-(\vec{r}_1) \Psi_+(\vec{r}_2)) \frac{1}{\sqrt{2}} (|1\uparrow\rangle - |1\downarrow\rangle) \right] - \text{singlet state}$$

symmetric

$$\Psi_{S=1}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left[(\Psi_+(\vec{r}_1) \Psi_+(\vec{r}_2) - \Psi_-(\vec{r}_1) \Psi_-(\vec{r}_2)) \frac{1}{\sqrt{2}} (|1\uparrow\rangle + |1\downarrow\rangle) \right] + \text{triplet state}$$

antisymmetric.

$$+ \frac{1}{\sqrt{2}} (|1\downarrow\rangle + |1\uparrow\rangle)$$

symmetric.

So how we can put 2 fermions at one point, provided they are in the singlet state.

Problem I

Consider 5 identical spin $\frac{1}{2}$ noninteracting fermions with mass μ in a 3-dimensional cubic box of size L . Find the first 5 energy levels and their degeneracies for this system.

We have found spectrum of particle inside 3d box in the problem I of set 10. Let's shortly remember how this spectrum looks like:

- Energy for the particle in the box is:

$$E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2m L^2} (n_1^2 + n_2^2 + n_3^2), \quad n_1, n_2, n_3 = 1, 2, 3, \dots$$

- Hereby we summarize levels together with degeneracies:

$\{n_1, n_2, n_3\}$	$n_1^2 + n_2^2 + n_3^2$	D(degeneracies)
{1,1,1}	3	2
{2,1,1}	6	6
{2,2,1}	9	6
{3,1,1}	11	6
{2,2,2}	12	2
{1,2,3}	14	12

Table 1

- Note that we twiced degeneracy of each level in comparison to problem 1 from the problem set 10. This happened because we can put spin of the particle either up or down not affecting it's energy.

- Now for the purpose of solving problem let's introduce the following notation:

$n_1, n_2, n_3, n_4, n_5, n_6$ is the case when there are n_1 fermions on the level {1,1,1}, n_2 fermions on {2,1,1} level and so on. So in terms of this states we can find out how should we fill levels with 5 fermions:

① Lowest energy configuration

- First we fill level {1,1,1} with 2 particles (maximal number available) and remaining 3 we put for the next energy level {2,1,1} so we get:

$$\begin{array}{|c|c|c|c|c|c|} \hline 2 & 3 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad E_1 = \frac{\pi^2 \hbar^2}{2mL^2} (3 \cdot 2 + 6 \cdot 3) \Rightarrow E_1 = \underline{\underline{\frac{12\pi^2 \hbar^2}{mL^2}}}$$

- Now we should find degeneracy of the state. Degeneracy here comes out because in total there are 6 possib. to put fermion on the level {2,1,1} and we put only 3 of them. This is typical problem about combinatorics.

(4) In particular we should find all possible ways to choose 3 single states out of 6. (or more general m single states of n if we put m fermions on the level with degeneracy in). The answer is given by binomial coefficient $\binom{6}{3}$ (or $\binom{n}{m} = \frac{n!}{m!(n-m)!}$). So, in

$$\text{our case degeneracy is } D = \binom{6}{3} = \frac{6!}{3! \cdot 3!} = \frac{4 \cdot 5 \cdot 6}{6} = 20$$

2	3	0	0	0	0
---	---	---	---	---	---

$$; E_1 = \frac{12\pi^2 h^2}{m L^2}; D = 20;$$

② First excited state.

To excite level minimally we should move only 1 particle to the closest unoccupied level. There are 2 possibilities to do this:

2	2	1	0	0	0
1	4	0	0	0	0

$$\Rightarrow E_2 = \frac{27\pi^2 h^2}{2mL^2};$$

$$D = 120;$$

$$E_2 = \frac{\pi^2 h^2}{2mL^2} (2 \cdot 3 + 2 \cdot 6 + 1 \cdot 9) = \frac{\pi^2 h^2}{2mL^2} (13 + 4 \cdot 6) \Rightarrow$$

Degeneracy in this case will be given by the sum of degeneracies of this 2 states

$$D = \binom{2}{2} \binom{6}{2} \binom{6}{1} + \binom{2}{1} \binom{6}{4} = \left[\begin{array}{l} \text{using } \binom{6}{2} = \frac{6!}{2!4!} = 15 \\ (\binom{6}{4}) = 15; (\binom{2}{1}) = 2 \end{array} \right] =$$

from from from
 {1,1,1} {2,1,1} {2,2,1}

level level level

$$= 1 \cdot 15 \cdot 6 + 2 \cdot 15 = 8 \cdot 15 = 120;$$

③ Second excited level

Next excited level can be obtained by throwing particle from the level {2,1,1} onto level {2,2,1}

2	2	0	1	0	0
---	---	---	---	---	---

$$E_3 = \frac{29\pi^2 h^2}{2mL^2};$$

$$D = 90;$$

$$E_3 = \frac{\pi^2 h^2}{2mL^2} (2 \cdot 3 + 2 \cdot 6 + 1 \cdot 11); \text{ thus}$$

$$\text{Degeneracy is given by: } D = \binom{2}{2} \binom{6}{2} \binom{8}{1} = 1 \cdot 15 \cdot 6 = 90$$

(5)

④ Third excited level

There are 4 different ways to obtain next excited level:

1 3 1 0 0 0 ;
2 1 2 0 0 0 ;
0 5 0 0 0 0 ;
2 2 0 0 1 0 ;
$E_4 = \frac{15\pi^2 h^2}{mL^2}$;
$D = 366$;

• Energy of this level is

$$E_4 = \frac{\pi^2 h^2}{2mL^2} (1 \cdot 3 + 3 \cdot 6 + 1 \cdot 9) =$$

$$= \frac{\pi^2 h^2}{2mL^2} (2 \cdot 3 + 6 + 2 \cdot 9) = \frac{\pi^2 h^2}{2mL^2} 5 \cdot 6 =$$

$$= \frac{\pi^2 h^2}{2mL^2} (2 \cdot 3 + 2 \cdot 6 + 12) = \frac{15\pi^2 h^2}{mL^2}$$

• Degeneracy is given by:

$$\underline{D} = \binom{2}{1} \binom{6}{3} \binom{6}{1} + \binom{2}{2} \binom{6}{1} \binom{6}{2} + \binom{6}{5} + \binom{2}{2} \binom{6}{2} \binom{2}{1} = \\ = 2 \cdot 20 \cdot 6 + 1 \cdot 6 \cdot 15 + 6 + 1 \cdot 15 \cdot 2 = \underline{366}$$

Where we have used $\binom{6}{3} = \frac{6!}{3!3!} = \frac{4 \cdot 6 \cdot 5}{6} = 20$;

⑤ Forth excited level

This state can be obtained in 3 ways:

2 2 0 0 0 1 ;
2 1 1 1 0 0 ;
1 3 0 1 0 0 ;
$E_5 = \frac{16\pi^2 h^2}{mL^2}$;
$D = 636$;

• Energy of the level is

$$E_5 = \frac{\pi^2 h^2}{2mL^2} (2 \cdot 3 + 2 \cdot 6 + 1 \cdot 14) = \frac{\pi^2 h^2}{2mL^2} (2 \cdot 3 + 1 \cdot 6 + 1 \cdot 9 + 1 \cdot 11) =$$

$$= \frac{\pi^2 h^2}{2mL^2} (1 \cdot 3 + 3 \cdot 6 + 1 \cdot 11) = \frac{16\pi^2 h^2}{mL^2};$$

• Degeneracy is given by:

$$\underline{D} = \binom{2}{2} \binom{6}{2} \binom{12}{1} + \binom{2}{2} \binom{6}{1} \binom{6}{1} \binom{6}{1} + \binom{2}{1} \binom{6}{3} \binom{6}{1} = \\ = \underline{636};$$

• That are all energy levels we were asked to find.

④ Problem II

Consider N noninteracting spinless particles with mass m in the 2-dimensional potential $V(x,y)$, where:

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

① Assuming that the particles are unidentical, find the ground state energy.

Assuming that particles are unidentical, we should allow all of them to occupy the lowest energy level possible. We remind that using separation of variables in cartesian coordinates we reduce problem to 2 1-d. h.o. thus energy spectrum is given by:

$$E_{n_1, n_2} = \hbar\omega (n_1 + n_2 + 1) \quad n_1, n_2 = 0, 1, 2, \dots$$

So if all N particles occupy lowest energy level $E = \hbar\omega$ the energy will be given by $E = N\hbar\omega$

② Assuming that the particles are identical bosons, find the ground state energy.

The story with the bosons are the same as with unidentical particles. As bosons can be put on the same energy level all of them will go to the ground state $E_0 = \hbar\omega$ (this phenomenon is known as Bose-Einstein condensation)

and ground state energy of the system is again $E = N\hbar\omega$

③ Assuming that the particles are identical fermions and $N \gg 1$ find a reasonable approximation to the ground state energy.

- For each state labeled by the pair $\{n_1, n_2\}$ we can put 1 fermion as there is no spin. So that we can find $n_{\max} = n_1 + n_2$ which still will be occupied. All states with the higher n will be empty. To find n_{\max} we write down

$$\sum_{n_1, n_2}^{n_{\max}} 1 = N$$

$$\text{We rewrite } \sum_{n_1, n_2}^{n_{\max}} 1 = \sum_{n_1=0}^{n_{\max}} \sum_{n_2=0}^{n_{\max}-n_1} 1 = \sum_{n_1=0}^{n_{\max}} (n_{\max} - n_1 + 1) =$$

$$\textcircled{7} \quad = \left[\begin{array}{l} \text{using standard} \\ \text{formula for the} \\ \text{summ of arithm. progr.} \end{array} \right] = (n_m + 1)^2 - \frac{1}{2} n_m^2 = \frac{1}{2} n_m^2 + \text{subleading terms}$$

So we get $\frac{1}{2} n_{\max}^2 = N \Rightarrow n_{\max} = \sqrt{2N};$

- Now we can calculate total energy by simply summing energy of all filled energy levels:

$$E = \sum_{n=0}^{n_m} E_n = \sum_{n_1=0}^{n_m} \sum_{n_2=0}^{n_m-n_1} \hbar\omega(n_1+n_2+1) \quad \text{Now as } N \gg 1 \text{ it is}$$

natural to go to continuous limit and substitute integrals

instead of sums:

$$\begin{aligned} E &= \int dn_1 \int dn_2 \hbar\omega(n_1+n_2+1) = \int dn_1 \hbar\omega(n_1 n_2 + \frac{1}{2} n_2^2 + n_2) \Big|_0^{n_m-n_1} = \\ &= \int dn_1 \hbar\omega(n_1(n_m-n_1) + \frac{1}{2}(n_m-n_1)^2 + n_m n_1) = \\ &= \hbar\omega \int dn_1 (n_m - n_1) \frac{1}{2} (n_m + n_1 + 1) = \frac{1}{2} \hbar\omega \int dn_1 (n_m^2 - n_1^2 + n_m - n_1) = \\ &= \frac{1}{2} \hbar\omega (n_m^3 - \frac{1}{3} n_m^3 + n_m^2 - \frac{1}{2} n_m^2) = \frac{1}{3} \hbar\omega n_m^3 + O(n_m^2) = \frac{1}{3} \hbar\omega (2N)^{3/2} \end{aligned}$$

So that

$$E = \frac{1}{3} \hbar\omega (2N)^{3/2}$$
 is the ground state of the system

Problem II Suppose that there are $N \gg 1$ noninteracting spin- $\frac{1}{2}$ fermions with mass μ in a cubic box of size L

(a) Find the Fermi energy and the total energy

In the same way as previously we first find maximal occupation number. Energy levels are given by

$$E = \frac{\pi^2 \hbar^2}{2m L^2} (n_1^2 + n_2^2 + n_3^2), \quad \text{Now we should sum over}$$

all states with $n^2 < n_m^2$, where $n^2 = n_1^2 + n_2^2 + n_3^2$. This

corresponds to the integration of one eights interior of the ball. (one eights is due to positiveness of

n_1, n_2, n_3) so we get

factor of 2
is coming from spin
each level \Rightarrow
2 possible states

$$2 \sum_{n_1, n_2, n_3}^{n^2 < n_m^2} 1 = 2 \sum_{n_1=0}^{n_m} \sum_{n_2=0}^{n_m-n_1} \sum_{n_3=0}^{n_m-n_1-n_2} 1 = N. \quad \text{As } N \gg 1 \text{ we , as in the}$$

previous problem go from the sum to integral

$$\sum_{n_1=0}^{n_m} \sum_{n_2=0}^{n_m-n_1} \sum_{n_3=0}^{n_m-n_1-n_2} 1 = \int dn_1 \int dn_2 \int dn_3. \quad \text{As we integrate over the}$$

⑧ part of ball interior it is natural to go to spherical coordinates:

$$\begin{aligned} n_1 &= n \cdot \sin\theta \cdot \cos\varphi, \text{ as } n_1 \geq 0, \quad \varphi \in [0, \pi/2] \\ n_2 &= n \cdot \sin\theta \cdot \sin\varphi \quad \begin{cases} n_2 \geq 0 \\ n_3 \geq 0 \end{cases} \Rightarrow \theta \in [0; \pi/2] \\ n_3 &= n \cdot \cos\theta \end{aligned}$$

Then we get usual spherical integral:

$$N = 2 \int_0^{n_m} dn \cdot n^2 \int_0^{\pi/2} d\cos\theta \int_0^{\pi/2} d\varphi = 2 \cdot \frac{1}{3} n_m^3 \cdot \frac{\pi}{2} \cdot 1 = \frac{\pi}{3} n_m^3 \text{ so maximal}$$

occupation number is given by

$$n_m = \left(\frac{3N}{\pi} \right)^{1/3}$$

- and Fermi energy then is given by

$$E_F = \frac{\pi^2 \hbar^2}{2mL^2} n_m^2 = \frac{\pi^2 \hbar^2}{2mL^2} \left(\frac{3N}{\pi} \right)^{2/3} = \frac{\hbar^2}{2m} \left(\frac{3N\pi^2}{4^3} \right)^{2/3} \text{ so that}$$

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3N\pi^2}{4^3} \right)^{2/3}$$

- To obtain total energy we should summ energies of all filled levels, i.e.

$$E = \sum_{n_1}^{n_m} \sum_{n_2}^{(n_m - n_1)} \sum_{n_3}^{(h_m^2 - n_1^2 - n_2^2)} \cdot \frac{\hbar^2 \pi^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2) \text{ going once again from}$$

the summ to the integral we get:

$$E = 2 \int_0^{n_m} dn \cdot n^2 \int_0^{\pi/2} d\varphi \int_0^{\pi/2} d\cos\theta \frac{\hbar^2 \pi^2}{2mL^2} n^2 = 2 \frac{\hbar^2 \pi^2}{2mL^2} \cdot \frac{1}{5} n_m^5 \cdot \frac{\pi}{2} \cdot 1 = \frac{\hbar^2 \pi^3}{10mL^2} n_m^5 \text{ so that}$$

$$E = \frac{\hbar^2 \pi^3}{10mV^{4/3}} n_m^5;$$

⑨ Find Fermi pressure $-\frac{dE}{dV}$:

Taking derivative of obtained energy we get:

$$P_F = -\frac{dE}{dV} = \frac{2}{3} \frac{\hbar^2 \pi^3}{10mV^{5/3}} n_m^5, \text{ so that}$$

$$P_F = \frac{\hbar^2 \pi^3}{15mV^{5/3}} n_m^5;$$

⑩ Assume that the fermions are electrons, that $N = 10^{23}$ and that $L = 1 \text{ cm}$. What is Fermi pressure?

$$P_F = \frac{(1,05 \cdot 10^{-27} \text{ erg} \cdot \text{s})^2 \cdot \pi^3}{15 \cdot 9 \cdot 10^{-28} \text{ gm} \cdot 1 \text{ cm}^{5/3}} \left(\frac{3 \cdot 10^{23}}{\pi} \right)^{5/3} \approx 5 \cdot 10^{11} \frac{\text{dyne}}{\text{cm}^2} = 5 \cdot 10^6 \frac{\text{N}}{\text{cm}^2}$$

①

Seminar 15 (Non-degenerate perturbation theory)

Theory: • Unfortunately there are not so many exactly solvable (i.e. you can find full solution of Sch. eq.). Thus to solve quantum systems we should develop some approximate methods. One of them is perturbation theory.

- The sense of perturbation theory is to devide

Hamiltonian : $H = H_0 + \varepsilon H_1$ where

- H_0 is main Hamiltonian for which we know the solution, i.e. we know all it's eigenstates and eigenvalues:

$$H_0 |\Psi_n^{(0)}\rangle = E_n^{(0)} |\Psi_n^{(0)}\rangle \quad (\text{On this lesson we assume spectrum to be non-degenerate})$$

↑
eigenstate ↓
eigenvalue.

- εH_1 is small perturbation of the Hamiltonian. ($\varepsilon \ll 1$)

Our goal is to find how this small additional part modifies spectrum of Hamiltonian.

- We expand E_n and $|\Psi_n\rangle$ in the series of ε :

$$E_n = E_n^{(0)} + \varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)} + O(\varepsilon^3);$$

$$|\Psi_n\rangle = |\Psi_n^{(0)}\rangle + \varepsilon |\Psi_n^{(1)}\rangle + \varepsilon^2 |\Psi_n^{(2)}\rangle + O(\varepsilon^3);$$

- Then Sch. eq. turns into:

$$(H_0 + \varepsilon H_1)(|\Psi_n^{(0)}\rangle + \varepsilon |\Psi_n^{(1)}\rangle + \varepsilon^2 |\Psi_n^{(2)}\rangle) = (E_n^{(0)} + \varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)}) (|\Psi_n^{(0)}\rangle + \varepsilon |\Psi_n^{(1)}\rangle + \varepsilon^2 |\Psi_n^{(2)}\rangle). \text{ Writing eq. order by order we get:}$$

$$\underline{\varepsilon^0}: \hat{H}_0 |\Psi_n^{(0)}\rangle = E_n^{(0)} |\Psi_n^{(0)}\rangle \quad - \text{ordinary Sch. eq.}$$

$$\underline{\varepsilon^1}: \hat{H}_0 |\Psi_n^{(1)}\rangle + \hat{H}_1 |\Psi_n^{(0)}\rangle = E_n^{(1)} |\Psi_n^{(0)}\rangle + E_n^{(0)} |\Psi_n^{(1)}\rangle;$$

$$\underline{\varepsilon^2}: \hat{H}_0 |\Psi_n^{(2)}\rangle + \hat{H}_1 |\Psi_n^{(1)}\rangle = E_n^{(2)} |\Psi_n^{(1)}\rangle + E_n^{(1)} |\Psi_n^{(2)}\rangle + E_n^{(0)} |\Psi_n^{(0)}\rangle;$$

- If we consider (ε^1) equation and multiply it with bra

$\langle \Psi_m^{(0)} |$ we get

$$E_m^{(0)} \langle \Psi_m^{(0)} | \underbrace{\langle \Psi_m^{(0)} | \hat{H}_0 | \Psi_n^{(1)} \rangle}_{* \text{ if } m=n \text{ we get: } E_n^{(1)} = \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle} + \langle \Psi_m^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle = E_n^{(1)} \langle \Psi_m^{(0)} | \Psi_n^{(0)} \rangle + E_n^{(0)} \langle \Psi_m^{(0)} | \Psi_n^{(1)} \rangle$$

* if $m=n$ we get: $E_n^{(1)} = \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle$

* if $m \neq n$ equation turns into:

$$② \langle \Psi_m^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle = (E_n^{(0)} - E_m^{(0)}) \langle \Psi_m^{(0)} | \Psi_n^{(0)} \rangle$$

If we now as usually expand $|\Psi_n^{(1)}\rangle$ in terms of complete basis $|\Psi_k^{(0)}\rangle$ of states we get:

$$|\Psi_n^{(1)}\rangle = \sum_k C_{nk}^{(1)} |\Psi_k^{(0)}\rangle \text{ so that}$$

$$\langle \Psi_m^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle = (E_n^{(0)} - E_m^{(0)}) \sum_k \underbrace{\langle \Psi_m^{(0)} | \Psi_k^{(0)} \rangle}_{\delta_{mk}} C_{nk}^{(1)}$$

$$\text{so that } C_{nk}^{(1)} = \frac{\langle \Psi_m^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \text{ so that:}$$

$$|\Psi_n^{(1)}\rangle = \sum_{k \neq n} \frac{\langle \Psi_k^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} |\Psi_k^{(0)}\rangle;$$

- finally if we multiply equation of order ② with $\langle \Psi_n^{(0)} |$ state we get:

$$E_n^{(0)} \langle \Psi_n^{(0)} | \Psi_n^{(2)} \rangle + \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(1)} \rangle = E_n^{(0)} \langle \Psi_n^{(0)} | \Psi_n^{(2)} \rangle + E_n^{(1)} \langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle + \\ + E_n^{(2)} \underbrace{\langle \Psi_n^{(0)} | \Psi_n^{(0)} \rangle}_1$$

Substituting $E_n^{(1)} = \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle$ and obtained expression for $|\Psi_n^{(1)}\rangle$

We get:

$$\langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle = \sum_{k \neq n} \frac{\langle \Psi_k^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} \underbrace{\langle \Psi_n^{(0)} | \Psi_k^{(0)} \rangle}_{\delta_{nk}} = 0 \text{ as } n \neq k;$$

$$\langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(1)} \rangle = \sum_{k \neq n} \frac{\langle \Psi_k^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_k^{(0)} \rangle = \sum_{k \neq n} \frac{|\langle \Psi_k^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

So that:

$$E_n^{(2)} = \sum_{k \neq n} \frac{|\langle \Psi_k^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}}; \text{ - second order correction to the energy.}$$

- Note that levels "repel" each other, let's consider

contribution to $E_n^{(2)}$ from only one particular k^{th} level:

$$E_n^{(2)} = \frac{|\langle \Psi_k^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \text{ note that}$$

- $E_n^{(2)} > 0$ for $E_n^{(0)} > E_k^{(0)}$ (level n higher than level k)

- $E_n^{(2)} < 0$ for $E_n^{(0)} < E_k^{(0)}$ (level n is lower than level k)

So corrections tends to make gaps between level larger (higher levels become higher, lowest - lower)

③ Problem I (Compendium 17)

Consider the 4-state system with states given by.

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \quad |2\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}; \quad |3\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}; \quad |4\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix};$$

and a Hamiltonian $H=H_0+H_1$ where

$$H_0 = \omega \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix}; \quad H_1 = \omega \begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix};$$

where $\omega > 0$, $\omega > 0$ and $\omega \gg \lambda$;

① Find the eigenvalues and normalized eigenstates of H_0 ;

- Secular equation is given by

$$\det(H_0 - \varepsilon \mathbb{I}) = \begin{vmatrix} -\varepsilon & \omega & 0 & 0 \\ \omega & -\varepsilon & 0 & 0 \\ 0 & 0 & -\varepsilon & 0 \\ 0 & 0 & 0 & 3\omega - \varepsilon \end{vmatrix} = \begin{array}{l} \text{[expanding in last]} \\ \text{row we get]} \end{array} =$$

$$=(3\omega - \varepsilon)(-\varepsilon^3 + \varepsilon \omega^2) = (\varepsilon - 3\omega)(\varepsilon - \omega)(\varepsilon + \omega)\varepsilon$$

So there are 4 levels:

$$\varepsilon_1^{(0)} = -\omega; \quad \varepsilon_2^{(0)} = 0; \quad \varepsilon_3^{(0)} = \omega; \quad \varepsilon_4^{(0)} = 3\omega; \quad \text{notice there are no degeneracies.}$$

- Now we can find corresponding eigenvalues:

① $\varepsilon_1^{(0)} = -\omega$; Equation for the eigenstate taken in general form

$$|\Psi_1\rangle = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

, where $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$ (normalisation condition)

$$\omega \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow \begin{array}{l} a = -b \\ c = d = 0 \end{array} \Rightarrow \begin{array}{l} a = \frac{1}{\sqrt{2}} \\ b = -\frac{1}{\sqrt{2}} \end{array} \text{ so that}$$

$$\boxed{\varepsilon_1^{(0)} = -\omega; \quad |\Psi_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle);}$$

② $\varepsilon_2^{(0)} = 0$; Equation for the eigenstate is

$$\omega \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow \begin{array}{l} a = b = d = 0 \\ \text{Then choose } c = 1 \end{array} \Rightarrow$$

$$\boxed{|\Psi_2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}; \quad \varepsilon_2^{(0)} = 0;}$$

④ ③ $E_3^{(0)} = \lambda$; Equation for the eigenstate is

$$\lambda \begin{bmatrix} -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow a=b; \quad \text{So that:}$$

$$c=d=0; \quad E_3^{(0)} = \lambda; \quad |\psi_3\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle);$$

④ $E_4^{(0)} = 3\lambda$; Equation for the eigenstate is

$$\lambda \begin{bmatrix} -3 & 1 & 0 & 0 \\ 1 & -3 & 0 & 0 \\ 0 & 0 & -3 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow b=3a; \quad a=3b \Rightarrow a=b=0$$

$c=0; \quad d = \text{any (we choose } d=1 \text{ for the proper normalization)}$

So we get:

$$E_4^{(0)} = 3\lambda; \quad |\psi_4\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = |4\rangle;$$

⑤ Treating H_2 as a perturbation of H_0 , find the correction to the energy of the ground state up to second order in perturb. theory.

- Ground state is $E_1^{(0)} = -\lambda$, $|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix}$; First order correction is given by

$$\delta E_1^{(1)} \equiv \langle \psi_1^{(0)} | H_2 | \psi_1^{(0)} \rangle = \frac{\lambda}{2} [1 - 1 \ 0 0] \begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix} = \frac{\lambda}{2} [3 - 3 \ 1 - 1] \begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix} =$$

$= 3\lambda$; So we have got

$$\boxed{\delta E_1^{(1)} = 3\lambda};$$

- Now we go to the second order correction, which is

given by: $\delta E_1^{(2)} = \sum_{k \neq n} \frac{|\langle \psi_n^{(0)} | H_2 | \psi_k^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}}$

The common object presented in all terms of the summ

is $\langle \psi_1^{(0)} | \hat{H}_2 | \psi_1^{(0)} \rangle = \frac{\lambda}{\sqrt{2}} [1 - 1 \ 0 0] \begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix} = \frac{\lambda}{\sqrt{2}} [3 - 3 \ 1 - 1];$

Then:

- $\langle \psi_1^{(0)} | \hat{H}_2 | \psi_2^{(0)} \rangle = \frac{\lambda}{\sqrt{2}} [3 - 3 \ 1 - 1] \cdot \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \frac{\lambda}{\sqrt{2}};$
- $\langle \psi_1^{(0)} | \hat{H}_2 | \psi_3^{(0)} \rangle = \frac{\lambda}{\sqrt{2}} [3 - 3 \ 1 - 1] \cdot \frac{1}{\sqrt{2}} \cdot \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} = 0;$
- $\langle \psi_1^{(0)} | \hat{H}_2 | \psi_4^{(0)} \rangle = \frac{\lambda}{\sqrt{2}} [3 - 3 \ 1 - 1] \cdot \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = -\frac{\lambda}{\sqrt{2}};$

(5)

So that second order correction is given by:

$$\delta E_1^{(2)} = \frac{|\langle \Psi_1^{(0)} | \hat{H}_1 | \Psi_2^{(0)} \rangle|^2}{E_1^{(0)} - E_2^{(0)}} + \frac{|\langle \Psi_1^{(0)} | \hat{H}_2 | \Psi_4^{(0)} \rangle|^2}{E_1^{(0)} - E_4^{(0)}} \Rightarrow$$

$$\Rightarrow \underline{\delta E_1^{(2)}} = \frac{\lambda^2}{2} \left(\frac{1}{-2-\lambda} + \frac{1}{-2-3\lambda} \right) = -\frac{\lambda^2}{2} \left(1 + \frac{1}{4} \right) = -\frac{5}{8} \frac{\lambda^2}{2};$$

So that ground state energy up to λ^2 order is:

$$E_1 \equiv E_1^{(0)} + \delta E_1^{(1)} + \delta E_1^{(2)} \Rightarrow \boxed{E_1 = -\lambda + 3\lambda - \frac{5}{8} \frac{\lambda^2}{2}};$$

Problem II (Compendium 18)

Consider the Hamiltonian $H = H_0 + H_1$, where

$$H_0 = \frac{\hbar\omega}{2} (\hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger); \quad \hat{H}_1 = \lambda (\hat{a}^\dagger + \hat{a}); \quad \text{where}$$

\hat{a}^\dagger and \hat{a} are the h.o. creation and annihilation operators

which satisfy the relation $[\hat{a}, \hat{a}^\dagger] = 1$

Assuming that \hat{H}_1 is a small perturbation of \hat{H}_0 , find the energy of the ground state to second order in λ .

- When you deal with the corrections to the ground state level of h.o. $|0\rangle$ it is optimal to normal order Hamiltonian correction \hat{H}_1 .

Normal order means that all lowering operators \hat{a} are to the right of all creation operators \hat{a}^\dagger . It is useful as we know that $\hat{a}|0\rangle = 0$. Note else that this is

useful for the ground state only otherwise you should just use relations: $\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$; $\hat{a} |n\rangle = \sqrt{n} |n-1\rangle$;

- Let's find $\hat{H}_1 |0\rangle$ using normal ordering:

$$\begin{aligned} \hat{H}_1 |0\rangle &= \lambda (\hat{a}^\dagger + \hat{a})^2 (\hat{a}^\dagger + \hat{a}) |0\rangle = [\text{as } \hat{a}|0\rangle = 0] = \lambda (\hat{a}^\dagger + \hat{a})^2 (\hat{a}^\dagger + \hat{a}) \hat{a}^\dagger |0\rangle = \\ &= \lambda (\hat{a}^\dagger + \hat{a})^2 ((\hat{a}^\dagger)^2 + \hat{a} \hat{a}^\dagger) |0\rangle = \left[\text{using } \hat{a} \hat{a}^\dagger = \hat{a}^\dagger \hat{a} + \frac{1}{2} [\hat{a}, \hat{a}^\dagger] \right] = \end{aligned}$$

$$= \lambda (\hat{a}^\dagger + \hat{a})^2 ((\hat{a}^\dagger)^2 + 1 + \hat{a}^\dagger \hat{a}) |0\rangle = \lambda (\hat{a}^\dagger + \hat{a}) ((\hat{a}^\dagger)^2 + 1) |0\rangle =$$

$$= \lambda (\hat{a}^\dagger + \hat{a}) (\hat{a}^\dagger + \hat{a}) ((\hat{a}^\dagger)^2 + 1) |0\rangle = \left[\text{further it will be useful to remember } [\hat{a}, (\hat{a}^\dagger)^n] = n (\hat{a}^\dagger)^{n-1}; \hat{a} (\hat{a}^\dagger)^n = (\hat{a}^\dagger)^n \hat{a} + [\hat{a}, (\hat{a}^\dagger)^n] \right]$$

$$= \lambda (\hat{a}^\dagger + \hat{a}) ((\hat{a}^\dagger)^2 + \hat{a}^\dagger + \hat{a} (\hat{a}^\dagger)^2 + \hat{a}) |0\rangle = \lambda (\hat{a}^\dagger + \hat{a}) ((\hat{a}^\dagger) + 3 \hat{a}^\dagger + ((\hat{a}^\dagger)^2 + 1) \hat{a}) |0\rangle =$$

$$\textcircled{6} = \lambda ((\hat{a}^+)^4 + 3(\hat{a}^+)^2 + \hat{a}(\hat{a}^+)^3 + 3\hat{a}\hat{a}^+) |0\rangle = \begin{bmatrix} \text{using } \hat{a} \\ \hat{a}(\hat{a}^+)^3 = (\hat{a}^+)^3 \hat{a} + 3(\hat{a}^+)^2 \\ \hat{a}\hat{a}^+ = 1 + \hat{a}^+\hat{a} \end{bmatrix} =$$

$$= \lambda ((\hat{a}^+)^4 + 6(\hat{a}^+)^2 + 3) |0\rangle = \begin{bmatrix} \text{using definition} \\ \text{of } |n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}} \end{bmatrix} =$$

$$= \lambda (\sqrt{4!} |4\rangle + 6\sqrt{2!} |2\rangle + 3|0\rangle) \text{ so we have got:}$$

$$\boxed{\hat{H}_2 |0\rangle = \lambda (2\sqrt{6} |4\rangle + 6\sqrt{2} |2\rangle + 3|0\rangle);}$$

- Another way to find $\hat{H}_2 |0\rangle$ is more straightforward:

$$\hat{H}_2 = \lambda (\hat{a}^+ + \hat{a})(\hat{a}^+ + \hat{a})(\hat{a}^+ + \hat{a})(\hat{a}^+ + \hat{a}) = \begin{bmatrix} \text{note you should always} \\ \text{care about order of operators} \end{bmatrix} =$$

$$= \lambda ((\hat{a}^+)^2 + \hat{a}^2 + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+) ((\hat{a}^+)^2 + \hat{a}^2 + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+) = \begin{bmatrix} \text{using } \hat{a}\hat{a}^+ = \hat{a}^+\hat{a} + 1 \end{bmatrix} =$$

$$= \lambda ((\hat{a}^+)^2 + \hat{a}^2 + 2\hat{a}^+\hat{a} + 1) ((\hat{a}^+)^2 + \hat{a}^2 + 2\hat{a}^+\hat{a} + 1) =$$

$$= \lambda ((\hat{a}^+)^4 + (\hat{a}^+)^2\hat{a}^2 + 2(\hat{a}^+)^3\hat{a} + (\hat{a}^+)^2\hat{a}^2 + \hat{a}^2(\hat{a}^+)^2 + \hat{a}^4 + 2\hat{a}^2\hat{a}^+\hat{a} + \hat{a}^2 + 2\hat{a}^+\hat{a}(\hat{a}^+)^2 + 2\hat{a}^+\hat{a}^3 + 4\hat{a}^+\hat{a}\hat{a}^+\hat{a} + 2\hat{a}^+\hat{a} + (\hat{a}^+)^2 + \hat{a}^2 + 2\hat{a}^+\hat{a} + 1)$$

as $\hat{a}|0\rangle = 0$ we omit all terms with \hat{a} standing to the right of everything the we are left with:

$$\hat{H}_2 |0\rangle = \lambda ((\hat{a}^+)^4 + (\hat{a}^+)^2 + \hat{a}^2(\hat{a}^+)^2 + 2\hat{a}^+\hat{a}(\hat{a}^+)^2 + (\hat{a}^+)^2 + 1) |0\rangle$$

Using commutation relations:

$$\cdot \hat{a}^2(\hat{a}^+)^2 = \hat{a}(\hat{a}^+)^2\hat{a} + \hat{a}[\hat{a}, (\hat{a}^+)^2] = (\hat{a}^+)^2\hat{a}^2 + [\hat{a}, (\hat{a}^+)^2]\hat{a} + \hat{a}[\hat{a}, (\hat{a}^+)^2] =$$

$$= (\hat{a}^+)^2\hat{a}^2 + 2(\hat{a}^+\hat{a} + \hat{a}\hat{a}^+) \Rightarrow \underline{\hat{a}^2(\hat{a}^+)^2 = (\hat{a}^+)^2\hat{a}^2 + 4\hat{a}^+\hat{a} + 2}$$

$$\cdot \underline{\hat{a}^+\hat{a}(\hat{a}^+)^2} = (\hat{a}^+)^3\hat{a} + \hat{a}^+[\hat{a}, (\hat{a}^+)^2] = (\hat{a}^+)^3\hat{a} + 2(\hat{a}^+)^2. \text{ So that:}$$

$$\hat{H}_2 |0\rangle = \lambda ((\hat{a}^+)^4 + (\hat{a}^+)^2 + 2 + 4(\hat{a}^+)^2 + (\hat{a}^+)^2 + 1) |0\rangle = \lambda ((\hat{a}^+)^4 + 6(\hat{a}^+)^2 + 3) |0\rangle$$

which coincides with expression we have observed previously.

This method is more useful if we consider

$\hat{H}_2 |n\rangle$ ($n \neq 0$). Then using formulas $\hat{a}^+|n\rangle = \sqrt{n+1} |n+1\rangle$; $\hat{a}|n\rangle = \sqrt{n} |n-1\rangle$; we can derive $\hat{H}_2 |n\rangle$, for example:

$$\hat{a}(\hat{a}^+)^2\hat{a}|n\rangle = \hat{a}(\hat{a}^+)^2\sqrt{n} |n-1\rangle = \sqrt{n} \cdot \sqrt{n} \cdot \sqrt{n+1} \hat{a}|n+1\rangle = n(n+1)|n\rangle$$

and similar for all the terms.

- Now using obtained expression for $\hat{H}_2 |0\rangle$ we conclude that only nonzero matrix elements are:

(7)

- $\langle 0 | \hat{H}_1 | 10 \rangle = 3\lambda;$
- $\langle 2 | \hat{H}_1 | 10 \rangle = 6\sqrt{2}\lambda;$
- $\langle 4 | \hat{H}_1 | 10 \rangle = 2\sqrt{6}\lambda;$

Now we can calculate energy of oscillator:

① For the ground state of usual h.o.:

$$\underline{E_0^{(0)} = \frac{1}{2}\hbar\omega};$$

② First order correction

$$\underline{\delta E_0^{(1)} = \langle 0 | \hat{H}_1 | 10 \rangle = 3\lambda}$$

③ Second order correction

$$\delta E_0^{(2)} = \sum_{n \neq 0} \frac{|\langle n | \hat{H}_1 | 10 \rangle|^2}{E_0^{(0)} - E_n^{(0)}} = \frac{|\langle 2 | \hat{H}_1 | 10 \rangle|^2}{E_0^{(0)} - E_2^{(0)}} + \frac{|\langle 4 | \hat{H}_1 | 10 \rangle|^2}{E_0^{(0)} - E_4^{(0)}}$$

as $E_n^{(0)} = \hbar\omega(n + \frac{1}{2})$ we get: $E_0^{(0)} - E_2^{(0)} = -2\hbar\omega; E_0^{(0)} - E_4^{(0)} = -4\hbar\omega$

$$\text{So we get: } \underline{\delta E_0^{(2)} = \left(\frac{36 \cdot 2}{2} + \frac{6 \cdot 4}{4}\right) \frac{\lambda^2}{\hbar\omega} = -42 \frac{\lambda^2}{\hbar\omega}};$$

So the energy of the ground state up to order λ^2 is given by:

$$\boxed{E_0 = \frac{1}{2}\hbar\omega + 3\lambda - 42 \frac{\lambda^2}{\hbar\omega};}$$

Problem III (Compendium 1g)

Consider a particle with mass m in the sd potential:

$$V(x) = V_0(x) + V_1(x), \text{ where: } V_0(x) = \frac{1}{2}mc^2x^2; V_1 = \lambda|x|;$$

① Assuming that $V_1(x)$ is a small perturbation to $V_0(x)$, compute the first order correction to the energy of the ground state.

W.l.f. for the ground state of unperturbed h.o. (\hat{H}_0) is

$$\Psi_0^{(0)}(x) = \frac{\sqrt{2}}{\pi^{1/4}} e^{-\lambda^2 x^2/2} \quad \text{where } \lambda = \sqrt{\frac{mc^2}{\hbar}};$$

Then first order correction in λ to the ground state of h.o. $E_0^{(0)} = \frac{\hbar\omega}{2}$ is given by:

$$\begin{aligned} \delta E_0^{(1)} &\equiv \langle \Psi_0^{(0)} | \hat{H}_1 | \Psi_0^{(0)} \rangle = \int_{-\infty}^{+\infty} dx (\Psi_0^{(0)}(x))^* \hat{H}_1 \Psi_0^{(0)}(x) = \int_{-\infty}^{+\infty} dx \frac{\lambda}{\sqrt{\pi}} e^{-\lambda^2 x^2} \lambda|x| = \\ &= \frac{2\lambda^2}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dx x e^{-\lambda^2 x^2} = \left[\text{changing variable } t = \lambda^2 x^2 \right] = \frac{2\lambda^2}{\sqrt{\pi}} \frac{1}{2\lambda^2} \int_{-\infty}^{+\infty} dt e^{-t} = \frac{\lambda}{2\sqrt{\pi}}; \end{aligned}$$

$$⑧ \text{ So } \boxed{\delta E_0^{(1)} = \frac{\lambda}{2\sqrt{\pi}};}$$

⑥ Now we can calculate first order correction to first excited level:

$$\delta E_1^{(1)} = \langle \Psi_1^{(0)} | \hat{H}_2 | \Psi_1^{(0)} \rangle = \int_{-\infty}^{+\infty} dx (\Psi_1^{(0)})^* \hat{H}_2 \Psi_1^{(0)}, \text{ using expression for}$$

the w.f. of the first excited level of h.o.:

$$\Psi_1^{(0)} = \frac{\sqrt{2}}{\pi^{1/4}} \cdot 2^{-1/2} \cdot x \cdot e^{-x^2/2} \text{ then:}$$

$$\delta E_1^{(1)} = \int_{-\infty}^{+\infty} dx \frac{1}{\pi^{1/4}} \cdot 2^{-1/2} \cdot x^2 e^{-x^2/2} \cdot \lambda |x| = \int_0^{\infty} dx \cdot x^2 e^{-x^2/2} \cdot 4 \frac{x^3 \lambda}{\sqrt{\pi}} = \left[\begin{array}{l} \text{using change of} \\ \text{variable } x^2 = t^2 \end{array} \right] =$$

$$= 4 \frac{x^3 \lambda}{\sqrt{\pi}} \cdot \frac{1}{2} \frac{1}{2^4} \int_0^{\infty} dt + e^{-t} = \frac{2\lambda}{2\sqrt{\pi}}; \text{ so } \boxed{\delta E_1^{(1)} = \frac{2\lambda}{2\sqrt{\pi}};}$$

Problem IV (Compendium 20)

Hyperfine splitting of the $l=0$ energy levels of a hydrogenic atom are due to an interaction between the spin \vec{S} of the electron and the spin \vec{I} of the nucleus. The eigenvalue of \vec{I}^2 is $\hbar^2 I(I+1)$, where I can be integer or half-integer, depending on the number of protons and neutrons in the nucleus. For our purposes, the contribution to the Hamiltonian of this hyperfine interaction has the form:

$$H' = \lambda \cdot \vec{S} \cdot \vec{I} \delta^3(\vec{r});$$

The δ -function satisfies: $\int_0^{\infty} r^2 dr \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \delta^3(\vec{r}) f(\vec{r}) = f(0)$

Normalized 1s w.f. is given by:

$$\Psi_{100}(r) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \cdot \exp(-Zr/a_0);$$

To first order in λ find the splitting of the degeneracy of the 1s level (in other words find the difference in the perturbed energies) as a function of I .

- Let's clarify what we are asked to find in this problem. We add spins of nucleus and electron:

$$\vec{J} = \vec{I} + \vec{S} \quad \text{as } S = \frac{1}{2} \text{ we have 2 possibilities:}$$

$j = I \pm \frac{1}{2}$; Now we should find first order in λ corrections to

④

the energies of states with $j = I \pm \frac{1}{2}$;

- Notice that now we deal with degenerate spectrum, i.e.

initial Hamiltonian of the electron in the atom

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + V(r), \text{ where } V(r) = -\frac{e^2}{4\pi\varepsilon_0 r} \text{ hasn't had any}$$

dependence on spins and hasn't distinguished between states with different j . Before proceeding with the solution let's refresh our knowledge about degenerate perturbation theory:

- Now we don't have some particular state $|\psi_n^{(0)}\rangle$ in the leading order, but set of states (say $|\psi_n^{(0)}\rangle$) and any linear combinations of them. Then we have:

$$|\psi\rangle = \sum_{n''} b_{n'n''} |\psi_n^{(0)}\rangle + \sum_{k=1}^{\infty} \varepsilon_k |\psi^{(k)}\rangle; \text{ Then substituting this state into Sch. eq. we get:}$$

$$\sum_{n''} H'_{n'n''} b_{n'n''} = \Delta E_n b_{n'n} \text{ where } H'_{n'n''} = \langle \psi_{n''}^{(0)} | H' | \psi_{n''}^{(0)} \rangle.$$

This is just secular equation in the basis of states $|\psi_n^{(0)}\rangle$;

- So to find the corrections to the degenerate levels we should find eigenstates and eigenvalues of Hamiltonian correction:

- Eigenstates correspond to real "0-order" states
- Eigenvalues are corrections to the energy corrections
- As different states will get different corrections degeneracy will be reduced by perturbation.

- Now we can solve our problem:

First of all we rewrite Hamiltonian correction as

$$H' = \lambda \delta^{(3)}(\vec{r}) (\vec{S} \cdot \vec{I}) = \lambda \delta^{(3)}(\vec{r}) ((\vec{S} + \vec{I})^2 - S^2 - I^2) \cdot \frac{1}{2} = \\ = \frac{1}{2} \lambda \delta^{(3)}(\vec{r}) (\vec{J}^2 - \vec{S}^2 - \vec{I}^2);$$

$$H' = \frac{1}{2} \lambda \delta^{(3)}(\vec{r}) (\vec{J}^2 - \vec{S}^2 - \vec{I}^2);$$

(10) • Next step we should do is the best choice of basis.

As for our Hamiltonian \hat{H}_1 we already know its eigenvalues. Indeed if we take state with:

① Total angular momentum $j = I + \frac{1}{2}$ i.e. $|I + \frac{1}{2}, m; I, \frac{1}{2}\rangle$

we obtain immediately:

$$\hat{H}' |I + \frac{1}{2}, m; I, \frac{1}{2}\rangle = \frac{1}{2} \lambda \delta^{(3)}(\vec{r}) (\hat{J}^2 - \hat{s}^2 - \hat{I}^2) |I + \frac{1}{2}, m; I, \frac{1}{2}\rangle =$$

↑
can be
any of $-|I| \leq m \leq I + \frac{1}{2}$

$$= \frac{1}{2} \lambda \delta^{(3)}(\vec{r}) (\hbar^2 (I + \frac{1}{2}) (I + \frac{3}{2}) - \hbar^2 I (I + 1) - \hbar^2 \frac{1}{2} \cdot \frac{3}{2}) |I + \frac{1}{2}, m; I, \frac{1}{2}\rangle =$$

$$= \frac{1}{2} \lambda \delta^{(3)}(\vec{r}) \hbar^2 I |I + \frac{1}{2}, m; I, \frac{1}{2}\rangle;$$

② Total angular momentum $j = I - \frac{1}{2}$ i.e. $|I - \frac{1}{2}, m; I, \frac{1}{2}\rangle$

we obtain:

$$\hat{H}' |I - \frac{1}{2}, m; I, \frac{1}{2}\rangle = \frac{1}{2} \lambda \delta^{(3)}(\vec{r}) (\hat{J}^2 - \hat{s}^2 - \hat{I}^2) |I - \frac{1}{2}, m; I, \frac{1}{2}\rangle =$$

$$= \frac{1}{2} \lambda \delta^{(3)}(\vec{r}) \hbar^2 ((I - \frac{1}{2}) (I + \frac{1}{2}) - I (I + 1) - \frac{3}{4}) |I - \frac{1}{2}, m; I, \frac{1}{2}\rangle =$$

$$= -\frac{1}{2} \lambda \delta^{(3)}(\vec{r}) \hbar^2 (I + 1) |I - \frac{1}{2}, m; I, \frac{1}{2}\rangle;$$

• So corrections to energy and corresponding "zero-order" states are given by:

$$\Delta E_+ = \langle \Psi_{100}; I + \frac{1}{2}, m; I, \frac{1}{2} | \hat{H}' | \Psi_{100}; I + \frac{1}{2}, m; I, \frac{1}{2} \rangle =$$

$$= \int d^3 r \Psi_{100}^*(r) \frac{1}{2} \lambda \delta^{(3)}(\vec{r}) \hbar^2 I \Psi_{100}(\vec{r}) = \frac{1}{2} \lambda \hbar^2 I \int d^3 r \delta^{(3)}(\vec{r}) |\Psi_{100}(r)|^2 =$$

$$= \frac{1}{2} \lambda \hbar^2 I |\Psi_{100}(0)|^2 = \frac{1}{2} \lambda \hbar^2 I \frac{1}{\pi} \left(\frac{Z}{a_0}\right)^3; \text{ for } |\Psi_{100}; I + \frac{1}{2}, m; I, \frac{1}{2}\rangle \text{ state}$$

• In analogy:

$$\Delta E_- = \langle \Psi_{100}; I - \frac{1}{2}, m; I, \frac{1}{2} | \hat{H}' | \Psi_{100}; I - \frac{1}{2}, m; I, \frac{1}{2} \rangle =$$

$$= \int d^3 r \Psi_{100}^*(r) \frac{1}{2} \lambda \delta^{(3)}(\vec{r}) (-\hbar^2 (I + 1)) \Psi_{100}(\vec{r}) = -\frac{1}{2} \lambda \hbar^2 (I + 1) |\Psi_{100}(0)|^2 =$$

$$= -\frac{1}{2} \lambda \hbar^2 (I + 1) \frac{1}{\pi} \left(\frac{Z}{a_0}\right)^3 \text{ for the state } |\Psi_{100}; I - \frac{1}{2}, m; I, \frac{1}{2}\rangle$$

• Finally difference we were asked to find is given

by: $\Delta E = \Delta E_+ - \Delta E_- = \frac{\lambda \hbar^2}{2\pi} \left(\frac{Z}{a_0}\right)^3 (2I + 1)$. Thus we see the

splitting of the level (100) (picture below)



$$\boxed{\Delta E = \frac{\lambda \hbar^2}{2\pi} \left(\frac{Z}{a_0}\right)^3 (2I + 1);}$$

(11) Problem II (Compendium 2)

Consider the case of 2 coupled h.o.

$H = H_0 + H'$, where

$$H_0 = \frac{\hbar\omega_1}{2} (\hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger) + \frac{\hbar\omega_2}{2} (\hat{b}^\dagger \hat{b} + \hat{b} \hat{b}^\dagger) \text{ and:}$$

$$H' = \lambda (\hat{a}^\dagger)^2 \hat{b}^2 + (\hat{b}^\dagger)^2 \hat{a}^2$$

The oscillators satisfy comm. relations

$$[\hat{a}, \hat{a}^\dagger] = 1; [\hat{b}, \hat{b}^\dagger] = 1; [\hat{a}, \hat{b}] = [\hat{a}, \hat{b}^\dagger] = 0;$$

and the ground state $|0,0\rangle$ satisfies:

$$\hat{a}|0,0\rangle = \hat{b}|0,0\rangle = 0;$$

Assume that $\omega_1 \neq \omega_2$ so that there are no degeneracies.

Find the energy of the normalized state $|2,0\rangle = \frac{1}{\sqrt{2}} (\hat{a}^\dagger)^2 |0\rangle$ to 2nd order in λ .

- First of all "zero-order" energy is given by

$$\begin{aligned} \hat{H}_0 |2,0\rangle &= \left(\hbar\omega_1 \left(\hat{N}_1 + \frac{1}{2} \right) + \hbar\omega_2 \left(\hat{N}_2 + \frac{1}{2} \right) \right) |2,0\rangle = \\ &= \left(\hbar\omega_1 \left(2 + \frac{1}{2} \right) + \hbar\omega_2 \cdot \frac{1}{2} \right) |2,0\rangle \text{ so} \end{aligned}$$

$$E^{(0)} = \hbar \left(\frac{5}{2}\omega_1 + \frac{1}{2}\omega_2 \right);$$

Here $\hat{N}_1 = \hat{a}^\dagger \hat{a}$ and $\hat{N}_2 = \hat{b}^\dagger \hat{b}$ are usual h.o. "number operators" such that $\hat{N}_1 |n_1, n_2\rangle = n_1 |n_1, n_2\rangle$ and $\hat{N}_2 |n_1, n_2\rangle = n_2 |n_1, n_2\rangle$; (we have basically 2 independent h.o. with the usual rules for both of them)

- Now we turn on coupling term. Let's find how it acts on $|2,0\rangle$ term. Using rules:

$$\begin{aligned} \hat{a}^\dagger |n_1, n_2\rangle &= \sqrt{n_1+1} |n_1+1, n_2\rangle; \quad \hat{b}^\dagger |n_1, n_2\rangle = \sqrt{n_2+1} |n_1, n_2+1\rangle; \\ \hat{b} |n_1, n_2\rangle &= \sqrt{n_2} |n_1, n_2-1\rangle; \quad \hat{a} |n_1, n_2\rangle = \sqrt{n_1} |n_1-1, n_2\rangle; \end{aligned}$$

We derive:

$$\hat{H}' |2,0\rangle = \lambda (\hat{a}^\dagger)^2 \hat{b}^2 |2,0\rangle + (\hat{b}^\dagger)^2 \hat{a}^2 |2,0\rangle \quad \text{as } \hat{b}|0\rangle = 0$$

$$\hat{H}' |2,0\rangle = \lambda \underbrace{(\hat{b}^\dagger)^2}_{\hat{a}^\dagger} \hat{a} |2,0\rangle = \lambda \sqrt{2} \cdot \sqrt{1} |1,1\rangle = \lambda \sqrt{2} \sqrt{1} |0,2\rangle =$$

$$\Rightarrow \hat{H}' |2,0\rangle = 2\lambda |0,2\rangle$$

- So that only nonzero matrix element is:

$$(12) \quad \langle 0,2 | \hat{H}' | 2,0 \rangle = 2\alpha ;$$

• Thus first order correction to energy is

$$\underline{\delta E_{2,0}^{(1)} = \langle 2,0 | \hat{H}' | 2,0 \rangle = 0};$$

• Second order correction to energy is given by

$$\delta E^{(2)} = \sum_{(m,n) \neq (2,0)} \frac{|\langle m,n | \hat{H}' | 2,0 \rangle|^2}{E_{2,0}^{(0)} - E_{m,n}^{(0)}} = \frac{|\langle 0,2 | \hat{H}' | 2,0 \rangle|^2}{E_{2,0}^{(0)} - E_{0,2}^{(0)}}$$

Now

$$E_{2,0}^{(0)} = \hbar\omega_1(2 + \frac{1}{2}) + \hbar\omega_2(0 + \frac{1}{2}) = \hbar(\frac{5}{2}\omega_1 + \frac{1}{2}\omega_2);$$

$$E_{0,2}^{(0)} = \hbar\omega_1(0 + \frac{1}{2}) + \hbar\omega_2(2 + \frac{1}{2}) = \hbar(\frac{1}{2}\omega_1 + \frac{5}{2}\omega_2);$$

$$\text{Thus } E_{2,0}^{(0)} - E_{0,2}^{(0)} = 2\hbar\omega_1 - 2\hbar\omega_2 \text{ and}$$

$$\delta E^{(2)} = \frac{4\alpha^2}{2\hbar(\omega_1 - \omega_2)}; \Rightarrow \boxed{\delta E^{(2)} = \frac{2\alpha^2}{\hbar(\omega_1 - \omega_2)}}$$

①

Seminar 16 (Realistic Hydrogen Atom)

Theory:

- Hydrogen atom physics includes not only Coulomb potential which defines energy levels, but some small corrections to the Hamiltonian (spin-orbit interaction, relativistic corrections, etc.). As hydrogen atom levels are highly degenerate we should use degenerate perturbation theory to find corrections to all of these levels.

Short reminder about perturbation theory:

Non-degenerate perturb. theory:

Corrections to the energy level $E_n^{(0)}$ corresponding to $|\Psi_n^{(0)}\rangle$ state is given by:

* First order: $\delta E_n^{(1)} = \langle \Psi_n^{(0)} | \hat{H}' | \Psi_n^{(0)} \rangle$;

* Second order: $\delta E_n^{(2)} = \sum_{m \neq n} \frac{|\langle \Psi_m^{(0)} | \hat{H}' | \Psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$

Degenerate perturb. theory:

To find first order correction and linear combinations of degenerate level w.r.t. we diagonalise \hat{H}' i.e. find its eigenvalues corr. to corrections to energy level and eigenstates (real "zero-order" states).

Problem N1 (Toy model of spin-orbit interaction)

Consider a spin-orbit type coupling applied to the h.o.

$\hat{H}_{so} = \frac{1}{2mc^2} \vec{S} \cdot \vec{L} \frac{1}{r} \frac{dV}{dr}$; where $V(r) = \frac{1}{2} m^2 \omega^2 r^2$. Compute the changes to the energies of the h.o. states from \hat{H}_{so} .

- First let's remember some facts about 3d h.o. which we described in Problem II of set 10:

* Energy levels of 3d. h.o. are given by:

$$E_n = \hbar\omega(n + \frac{3}{2})$$

* Degeneracy of the level with label "n" is given by:

$$(2) \quad D_n = \frac{1}{2} (n+1)(n+2); \quad (\text{or } D_n = (n+1)(n+2) \text{ if particle has spin } s=\frac{1}{2})$$

* For n^{th} level orbital angular momentum take the following values:

① n is even $\Rightarrow 0 \leq l \leq n$ and only even values too, i.e.

$$l=0, 2, 4, \dots, n-2, n;$$

② n is odd $\Rightarrow 0 \leq l \leq n$ taking only odd values, i.e.

$$l=1, 3, 5, \dots, n-2, n;$$

- Now let's consider corrections to the energy levels

due to spin-orbit interaction. Correction Hamiltonian is

$$\text{given by: } \hat{H}_{\text{so}} = \frac{1}{2mc^2} \vec{S} \cdot \vec{L} + \frac{dV}{dr} = \frac{1}{2mc^2} \vec{S} \cdot \vec{L} + m\omega^2 r = \frac{\omega^2}{2mc^2} \vec{S} \cdot \vec{L}$$

- In order to easily diagonalize \hat{H}_{so} , we will rewrite scalar product $\vec{S} \cdot \vec{L}$ in the following way:

$$\vec{S} \cdot \vec{L} = \frac{1}{2} ((\vec{S} + \vec{L})^2 - \vec{S}^2 - \vec{L}^2) = \frac{1}{2} (\vec{J}^2 - \vec{S}^2 - \vec{L}^2) \text{ where } \vec{J}^2 \text{ is}$$

square of total angular momentum.

- So Hamiltonian is now:

$$\hat{H}_{\text{so}} = \frac{\omega^2}{4mc^2} (\vec{J}^2 - \vec{S}^2 - \vec{L}^2)$$

- We already know eigenstates of this hamiltonian: this are the states with particular total angular momentum and angular momentum - $|j, m; s, l\rangle$:

$$(\vec{J}^2 - \vec{S}^2 - \vec{L}^2) |j, m; s, l\rangle = \hbar^2 (j(j+1) - s(s+1) - l(l+1)) |j, m; s, l\rangle$$

Note:

- ① This eigenstates have $(2j+1)$ degeneracy as eigenvalue doesn't depend on m ; and m can take any value $-j \leq m \leq j$.

- ② We consider only angular part of w.f. $|j, m; s, l\rangle$ as perturbation hamiltonian \hat{H}_{so} leaves radial part untouched

- As we add angular momentum l with $s=\frac{1}{2}$ we have 2 possibilities for the resulting angular momentum:

(3)

$j = l \pm \frac{1}{2}$ so that:

$$\textcircled{1} \quad \hat{H}_{\text{so}} |l \pm \frac{1}{2}, m; l, \frac{1}{2}\rangle = \frac{\omega^2}{4mc^2} (\hat{j}^2 - \hat{l}^2 - \hat{s}^2) |l \pm \frac{1}{2}, m; l, \frac{1}{2}\rangle = \\ = \frac{\omega^2 \hbar^2}{4mc^2} ((l \pm \frac{1}{2})(l \pm \frac{3}{2}) - \frac{1}{2}(\frac{1}{2} + 1) - l(l+1)) |l \pm \frac{1}{2}, m; l, \frac{1}{2}\rangle =$$

$$= \frac{\omega^2 \hbar^2}{4mc^2} l |l \pm \frac{1}{2}, m; l, \frac{1}{2}\rangle;$$

$$\textcircled{2} \quad \hat{H}_{\text{so}} |l - \frac{1}{2}, m; l, \frac{1}{2}\rangle = \frac{\omega^2}{4mc^2} (\hat{j}^2 - \hat{l}^2 - \hat{s}^2) |l - \frac{1}{2}, m; l, \frac{1}{2}\rangle = \\ = \frac{\omega^2 \hbar^2}{4mc^2} ((l - \frac{1}{2})(l + \frac{1}{2}) - \frac{1}{2}(\frac{1}{2} + 1) - l(l+1)) |l - \frac{1}{2}, m; l, \frac{1}{2}\rangle = \\ = - \frac{\omega^2 \hbar^2}{4mc^2} (l+1) |l - \frac{1}{2}, m; l, \frac{1}{2}\rangle$$

- So we now got the following situation:

Before perturbation we had degenerate level n with the energy $E_n = \hbar\omega(n + \frac{3}{2})$ and different l 's.

After disturbing system with spin-orbit interaction level is splitted into levels with different j , such

that correction to energy is:

$$\delta E_{l+\frac{1}{2}}^{(1)} = \frac{\omega^2 \hbar^2}{4mc^2} \cdot l; \Leftrightarrow \text{state is } |l \pm \frac{1}{2}, m; l, \frac{1}{2}\rangle;$$

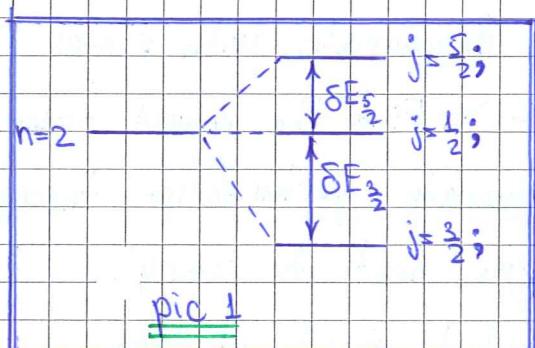
$$\delta E_{l-\frac{1}{2}}^{(1)} = - \frac{\omega^2 \hbar^2}{4mc^2} \cdot (l+1); \Leftrightarrow \text{state is } |l - \frac{1}{2}, m; l, \frac{1}{2}\rangle;$$

• Example:

Let's consider $n=2$ level ($(2+1)(2+2) = 12$ states)

- possible values of l are $l=0$ and $l=2$;

- possible values of j are $j=\frac{1}{2}; j=\frac{3}{2}; j=\frac{5}{2}$;



Note that in total we have got 12 states as it should be.

$| \frac{1}{2}, m; 0, \frac{1}{2}\rangle; \Rightarrow m = \pm \frac{1}{2} \Rightarrow 2 \text{ states};$

$$\delta E_{\frac{1}{2}}^{(1)} = \frac{\omega^2 \hbar^2}{4mc^2} \cdot 0 = 0;$$

$| \frac{3}{2}, m; 2, \frac{1}{2}\rangle; \Rightarrow m = \pm \frac{3}{2}, \pm \frac{1}{2}; 4 \text{ states};$

$$\delta E_{\frac{3}{2}}^{(1)} = - \frac{\omega^2 \hbar^2}{4mc^2} (2+1) = - \frac{3}{4} \frac{\omega^2 \hbar^2}{mc^2};$$

$| \frac{5}{2}, m; 2, \frac{1}{2}\rangle; \Rightarrow m = \pm \frac{5}{2}, \pm \frac{3}{2}, \pm \frac{1}{2}; 6 \text{ states};$

$$\delta E_{\frac{5}{2}}^{(1)} = \frac{\omega^2 \hbar^2}{mc^2} \cdot \frac{2}{4} = \frac{1}{2} \frac{\omega^2 \hbar^2}{mc^2};$$

④ Problem II This problem concerns a physics of phenomenon called the Stark Effect. Consider a hydrogen atom in the presence of an external electric field $\vec{E} = E\hat{z}$. The correction to the Hamiltonian is given by

$$\hat{H}_s = e\vec{r} \cdot \vec{E} = eEr\cos\theta;$$

In this problem you can ignore fine-structure corrections.

- ⓐ Using H_s as a perturbation, show that there is no correction to the ground-state energy to first order in perturbation theory.

- Ground state for the hydrogen atom is (100) state which has the w.f. given by:

$$\Psi_{100}(\vec{r}) = \frac{1}{\sqrt{\pi}} \cdot \frac{1}{a_B^{3/2}} e^{-r/a_B};$$

- There is no degeneracy, so in order to find first order correction to the ground state energy we write:

$$\begin{aligned}\delta E_0^{(1)} &\equiv \langle \Psi_{100} | \hat{H}_s | \Psi_{100} \rangle \equiv \int d^3r \Psi_{100}^*(\vec{r}) \hat{H}_s \Psi_{100}(\vec{r}) = \\ &= \int dr \cdot r^2 \int_0^\pi d\cos\theta \int_0^{2\pi} d\varphi \frac{1}{\pi} \cdot \frac{1}{a_B^3} e^{-2r/a_B} \cdot eE \cdot r \cdot \cos\theta = \\ &= \int dr \cdot r^3 e^{-2r/a_B} \int_0^\pi d\cos\theta \cdot \cos\theta \int_0^{2\pi} d\varphi \cdot \frac{1}{\pi} \cdot \frac{1}{a_B^3} \cdot eE, \text{ note}\end{aligned}$$

$$\text{that } \int d\cos\theta \cdot \cos\theta = \left[\begin{array}{l} \text{change of} \\ \text{variables} \end{array} \right] = \int dt \cdot t = \frac{1}{2}t^2 \Big|_{-1}^1 = 0;$$

So we see that due to this integral

$$\boxed{\delta E_0^{(1)} = 0}, \text{ q.e.d.}$$

- ⓑ First excited state is 4-fold degenerate with states $|2,0,0\rangle, |2,1,1\rangle, |2,1,0\rangle$ and $|2,1,-1\rangle$. Find the lowest order corrections to the energy using degenerate perturbation theory.

For this part of the problem, you need to compute many different matrix elements, but most of them are zero.

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- Now we go to degenerate level $n=2$. It is described by 4 states (i.e. 4-fold degenerate):

$$|2,0,0\rangle \sim R_{20}(r) Y_{00}(\theta, \varphi);$$

$$|2,1,0\rangle \sim R_{21}(r) Y_{10}(\theta, \varphi);$$

$$|2,1,\pm 1\rangle \sim R_{21}(r) Y_{1\pm 1}(\theta, \varphi);$$

Where R_{nlm} and Y_{lm} functions can be found, for example, in Griffiths (Tables 4.3 and 4.7). In particular

- $Y_{00} = \frac{1}{\sqrt{4\pi}}$; $Y_{10} = \sqrt{\frac{3}{4\pi}} \cdot \cos\theta$; $Y_{1\pm 1} = \mp \sqrt{\frac{3}{8\pi}} e^{\pm i\varphi} \cdot \sin\theta$;

- $R_{20}(r) = \frac{1}{\sqrt{2}} \cdot \frac{1}{a_B^{3/2}} \left(1 - \frac{1}{2} \frac{r}{a_B}\right) \exp\left(-\frac{r}{2a_B}\right)$;

$$R_{21}(r) = \frac{1}{\sqrt{24}} \cdot \frac{1}{a_B^{3/2}} \cdot \frac{r}{a_B} \cdot \exp\left(-\frac{r}{2a_B}\right);$$

- Next step is writing down matrix representation of \hat{H}_s in the following basis:

$$|1\rangle = |2,0,0\rangle; |2\rangle = |2,1,-1\rangle; |3\rangle = |2,1,0\rangle; |4\rangle = |2,1,+1\rangle;$$

So we should find all matrix elements of the form $\langle 2l'm' | \hat{H}_s | 2lm \rangle$, but fortunately most of matrix elements are zero:

$$\langle 2l'm' | \hat{H}_s | 2lm \rangle = \int_0^\infty dr \cdot r^2 \int_0^{2\pi} d\cos\theta \int_0^{2\pi} d\varphi \underbrace{eE \cdot r \cdot \cos\theta}_{\hat{H}_s} \cdot \underbrace{R_{2l'm'}^* Y_{l'm'}^*}_{\Psi_{2l'm'}} \underbrace{R_{2l'm}}_{\Psi_{2l'm}}$$

$$= eE \int_0^\infty dr \cdot r^3 R_{2l'm'}^*(r) R_{2l'm}(r) \int_0^{2\pi} d\cos\theta \int_0^{2\pi} d\varphi \cdot \cos\theta Y_{l'm'}^* Y_{lm}$$

- Let's concentrate first on angular part of integrals.

First of all let's consider matrix elements between states with different m :

$$\langle 2l'm' | \hat{H}_s | 2lm \rangle \propto \int_0^{2\pi} d\varphi e^{i(m-m')\varphi} \quad \text{there are 2 cases here}$$

① If $m=m'$ $\int_0^{2\pi} d\varphi e^{i(m-m')\varphi} = \int_0^{2\pi} d\varphi = 2\pi$;

② If now $m \neq m'$ $\int_0^{2\pi} d\varphi e^{i(m-m')\varphi} = \frac{1}{i(m-m')} e^{i(m-m')\varphi} \Big|_0^{2\pi} = 0$ so as

$(m-m')$ is integer. So that

$$\boxed{\int_0^{2\pi} d\varphi e^{i(m-m')\varphi} = 2\pi \delta_{m,m'}}$$

⑥ So we can conclude that matrix elements with different m 's are zero:

$$\langle 2l'm' | \hat{H}_s | 2lm \rangle \sim \delta_{m'm}$$

• Thus we are left with the following possibilities:

① $\langle 200 | \hat{H}_s | 200 \rangle$ Let's consider angular part of integral: $\langle 200 | \hat{H}_s | 200 \rangle \sim \int d\cos\theta \int_0^{2\pi} d\varphi \cos\theta Y_{00}^* Y_{00} \sim \int d\cos\theta \cos\theta = \begin{cases} \text{change} \\ \cos\theta = t \end{cases} = \int dt \cdot t = \frac{1}{2}t^2 \Big|_0^1 = 0$ so that

$$\langle 200 | \hat{H}_s | 200 \rangle = 0$$

② $\langle 21\pm 1 | \hat{H}_s | 21\pm 1 \rangle \sim \int d\cos\theta \int_0^{2\pi} d\varphi \cos\theta Y_{1\pm 1}^* Y_{1\pm 1} \sim \int d\cos\theta \cdot \cos\theta \cdot \sin^2\theta = \begin{cases} \text{change} \\ \cos\theta = t \end{cases} = \int dt \cdot t \cdot (1-t^2) = \left(\frac{1}{2}t^2 - \frac{1}{4}t^4 \right) \Big|_0^1 = 0;$

So again we get $\langle 21\pm 1 | \hat{H}_s | 21\pm 1 \rangle = 0;$

③ $\langle 210 | \hat{H}_s | 210 \rangle \sim \int d\cos\theta \int_0^{2\pi} d\varphi \cos\theta Y_{10}^* Y_{10} \sim \int d\cos\theta \cdot \cos^3\theta = \begin{cases} \text{change} \\ \cos\theta = t \end{cases} = \int dt \cdot t^3 = \frac{1}{4}t^4 \Big|_0^1 = 0,$ so that

$$\langle 210 | \hat{H}_s | 210 \rangle = 0;$$

④ Last possibly nonzero matrix element is:

$$\langle 200 | \hat{H}_s | 210 \rangle = eE \int dr \cdot r^3 R_{20}^*(r) R_{21}(r) \int d\cos\theta \int_0^{2\pi} d\varphi \cos\theta \times$$

$$\times Y_{00}^*(\theta, \varphi) Y_{10}(\theta, \varphi)$$

$$\bullet \int_0^\infty dr \cdot r^3 R_{20}^*(r) R_{21}(r) = \int_0^\infty dr \cdot r^3 \frac{1}{4\sqrt{3}} \frac{1}{a_B^3} \left(1 - \frac{1}{2} \frac{r}{a_B} \right) e^{-r/a_B} =$$

$$= \begin{cases} \text{change} \\ t = \frac{r}{a_B} \end{cases} = \frac{a_B}{4\sqrt{3}} \int_0^\infty dt \cdot t^4 \left(1 - \frac{1}{2}t \right) e^{-t} = \frac{a_B}{4\sqrt{3}} \left(\underbrace{\int_0^\infty dt \cdot t^4 e^{-t} - \frac{1}{2} \underbrace{\int_0^\infty dt \cdot t^5 e^{-t}}_{5!}}_{4!} \right) =$$

$$= \frac{a_B}{4\sqrt{3}} \cdot (4! - \frac{1}{2} 5!) = \frac{a_B}{4\sqrt{3}} (24 - \frac{1}{2} \cdot 24 \cdot 5) = - \frac{9a_B}{\sqrt{3}} = -3\sqrt{3}a_B$$

$$\bullet \int d\cos\theta \int_0^{2\pi} d\varphi \cos\theta Y_{00}^*(\theta, \varphi) Y_{10}(\theta, \varphi) = \int d\cos\theta \cdot \cos\theta \cdot \cos\theta \int_0^{2\pi} d\varphi \frac{\sqrt{3}}{4\pi} =$$

$$= \begin{cases} \text{change} \\ t = \cos\theta \end{cases} = 2\pi \cdot \frac{\sqrt{3}}{4\pi} \cdot \frac{1}{3} t^3 \Big|_0^1 = \frac{1}{\sqrt{3}}$$

(7)

So that

$$\langle 200 | \hat{H}_s | 210 \rangle = -3eE_{ab}$$

- As $\langle 200 | \hat{H} | 210 \rangle = (\langle 210 | \hat{H} | 200 \rangle)^* = -3eE_{ab}$ are only non zero matrix elements we get the following matrix:

$$\hat{H}_s = -3eE_{ab} \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

- Eigenvalues ε_i corresponding to energy levels can be found from secular equation

$$0 = \det(\hat{H}_s - \varepsilon \mathbb{I}) = \begin{vmatrix} -\varepsilon & 0 & -3eE_{ab} & 0 \\ 0 & -\varepsilon & 0 & 0 \\ -3eE_{ab} & 0 & -\varepsilon & 0 \\ 0 & 0 & 0 & -\varepsilon \end{vmatrix} = (-\varepsilon)((-\varepsilon)^3 + \varepsilon \cdot 9e^2 E^2 a_b^2) =$$

$= \varepsilon^2(\varepsilon - 3eE_{ab})(\varepsilon + 3eE_{ab}) = 0$, so that we get following eigenvalues:

$\delta\varepsilon_0^{(1)} = 0$ - doubly degenerate.

$\delta\varepsilon_+^{(1)} = 3eE_{ab}$ - nondegenerate

$\delta\varepsilon_-^{(1)} = -3eE_{ab}$ - nondegenerate

- Find the basis where the first-order matrix elements for the first excited states are diagonalised.

To do this we should find eigenstates of \hat{H}_s .

This eigenstates are "zero-order" states corresponding to different corrections:

- $\delta\varepsilon_0^{(1)} = 0$; equation for the eigenstate is

$$3eE_{ab} \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \text{ where eigenstate is } |\psi_0\rangle = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

so we get: $a=c=0$, b and d can be any, so we

choose

$$|\psi_0^{(1)}\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |2\rangle = |2, 1, -1\rangle; \quad \left. \right\} \text{any normalized linear combination of } |2\rangle \text{ and } |4\rangle \text{ is eigenstate (2-fold degeneracy)}$$

and

$$|\psi_0^{(2)}\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} = |4\rangle = |2, 1, 1\rangle;$$

⑧ ② $\delta E_+^{(0)} = 3eEa_B$; equation for eigenstate is:

$$3eEa_B \begin{bmatrix} -1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow a = -c; b = d = 0.$$

eigenstate is

$$\left| \Psi_+^{(0)} \right\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} (\left| 2,0,0 \right\rangle - \left| 2,1,0 \right\rangle),$$

so that normalized

③ $\delta E_-^{(0)} = -3eEa_B$; equation for eigenstate is:

$$3eEa_B \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow a = c; b = d = 0; \Rightarrow \left| \Psi_-^{(0)} \right\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} (\left| 2,0,0 \right\rangle + \left| 2,1,0 \right\rangle);$$

④ In this diagonal basis, compute the expectation value for the electric dipole moment $\vec{p} = -e\vec{r}$ for these states.

Show that this and results in ⑥ are consistent with an electric dipole in the presence of a constant electric field.

Let's calculate all matrix elements of the form

$\langle \Psi_{\pm,0}^{(0)} | \hat{r} | \Psi_{\pm,0}^{(0)} \rangle$; Once again it will be useful to concentrate on angle integrals:

⑤ $\langle \Psi_+^{(0)} | \hat{r} | \Psi_+^{(0)} \rangle$ Component by component we get:

$$\bullet \langle \Psi_+^{(0)} | \hat{x} | \Psi_+^{(0)} \rangle = \langle \Psi_+^{(0)} | r \cdot \cos\varphi \cdot \sin\theta | \Psi_+^{(0)} \rangle = \frac{1}{2} (\langle 200 | r \cdot \cos\varphi \cdot \sin\theta | 200 \rangle + \langle 210 | r \cdot \cos\varphi \cdot \sin\theta | 200 \rangle + \langle 200 | r \cdot \cos\varphi \cdot \sin\theta | 210 \rangle + \langle 210 | r \cdot \cos\varphi \cdot \sin\theta | 210 \rangle)$$

All expectation values are of the form

$$\langle 2l'0 | r \cdot \cos\varphi \cdot \sin\theta | 2l0 \rangle \sim \int_0^{\pi} d\varphi \cos\varphi = 0 \text{ so we conclude}$$

$$\langle \Psi_+^{(0)} | \hat{x} | \Psi_+^{(0)} \rangle = 0;$$

$$\bullet \langle \Psi_+^{(0)} | \hat{y} | \Psi_+^{(0)} \rangle = \frac{1}{2} (\langle 200 | r \cdot \sin\varphi \cdot \sin\theta | 200 \rangle + \langle 210 | r \cdot \sin\varphi \cdot \sin\theta | 200 \rangle + \langle 200 | r \cdot \sin\varphi \cdot \sin\theta | 210 \rangle + \langle 210 | r \cdot \sin\varphi \cdot \sin\theta | 210 \rangle) = 0 \text{ as}$$

$$\langle 2l'0 | r \cdot \sin\varphi \cdot \sin\theta | 2l0 \rangle \sim \int_0^{\pi} d\varphi \sin\varphi = 0, \text{ so we get}$$

$$\langle \Psi_+^{(0)} | \hat{y} | \Psi_+^{(0)} \rangle = 0;$$

$$\bullet \langle \Psi_+^{(0)} | \hat{z} | \Psi_+^{(0)} \rangle = \langle \Psi_+^{(0)} | r \cdot \cos\theta | \Psi_+^{(0)} \rangle = \frac{1}{eE} \langle \Psi_+^{(0)} | \hat{H}_s | \Psi_+^{(0)} \rangle = \left[\text{as } \hat{H}_s | \Psi_+^{(0)} \rangle = 3eEa_B \right] = \frac{1}{eE} 3eEa_B = \underline{3a_B}$$

①

So that:

$$\boxed{\langle \psi_+^{(o)} | \hat{p}_z | \psi_+^{(o)} \rangle = -3ea_s; \text{ all other components are zero.}}$$

② $\langle \psi_-^{(o)} | \hat{r} | \psi_-^{(o)} \rangle$; By components:

- $\langle \psi_-^{(o)} | \hat{x} | \psi_-^{(o)} \rangle = \langle \psi_-^{(o)} | r \cdot w\varphi \cdot \sin\theta | \psi_-^{(o)} \rangle =$

$$= \frac{1}{2} (\langle 200 | r \cdot w\varphi \cdot \sin\theta | 200 \rangle - \langle 210 | r \cdot w\varphi \cdot \sin\theta | 200 \rangle -$$

$$- \langle 200 | r \cdot w\varphi \cdot \sin\theta | 210 \rangle + \langle 210 | r \cdot w\varphi \cdot \sin\theta | 210 \rangle) = 0$$

By the same reason as $\langle \psi_+^{(o)} | \hat{x} | \psi_+^{(o)} \rangle = 0$,

$$\boxed{\langle \psi_-^{(o)} | \hat{x} | \psi_-^{(o)} \rangle = 0;}$$

- $\langle \psi_-^{(o)} | \hat{y} | \psi_-^{(o)} \rangle = \frac{1}{2} (\langle 200 | r \cdot \sin\varphi \cdot \sin\theta | 200 \rangle -$

$$- \langle 210 | r \cdot \sin\varphi \cdot \sin\theta | 200 \rangle - \langle 200 | r \cdot \sin\varphi \cdot \sin\theta | 210 \rangle +$$

$$+ \langle 210 | r \cdot \sin\varphi \cdot \sin\theta | 210 \rangle) = 0 \text{ by the same reason as}$$

$$\langle \psi_+^{(o)} | \hat{y} | \psi_+^{(o)} \rangle = 0; \text{ so } \boxed{\langle \psi_-^{(o)} | \hat{y} | \psi_-^{(o)} \rangle = 0;}$$

- $\langle \psi_-^{(o)} | \hat{z} | \psi_-^{(o)} \rangle = \frac{1}{eE} \langle \psi_-^{(o)} | \hat{H}_s | \psi_-^{(o)} \rangle = -3a_s$ so that:

$$\boxed{\langle \psi_-^{(o)} | \hat{p}_z | \psi_-^{(o)} \rangle = 3ea_s; \text{ all other components are zero.}}$$

③ Finally $\langle \psi_0^{(o)} | \hat{p} | \psi_0^{(o)} \rangle$ we have here 4 kind of expectation values:

$$\langle 21\pm 1 | \hat{x} | 21\pm 1 \rangle \sim \int_0^{\pi} d\varphi \cdot \cos\varphi = 0;$$

$$\langle 21\pm 1 | \hat{x} | 21\mp 1 \rangle \sim \int_0^{\pi} d\varphi \cdot w\varphi \sin\varphi e^{-2i\varphi} = 0;$$

$$\langle 21\pm 1 | \hat{y} | 21\pm 1 \rangle \sim \int_0^{\pi} d\varphi \cdot \sin\varphi = 0;$$

$$\langle 21\pm 1 | \hat{y} | 21\mp 1 \rangle \sim \int_0^{\pi} d\varphi \cdot \sin\varphi \cdot e^{2i\varphi} = 0;$$

As we see all matrix elements are 0, as for z-component:

$$\langle \psi_0^{(o)} | \hat{z} | \psi_0^{(o)} \rangle = \frac{1}{eE} \langle \psi_0^{(o)} | \hat{H}_s | \psi_0^{(o)} \rangle = 0, \text{ so}$$

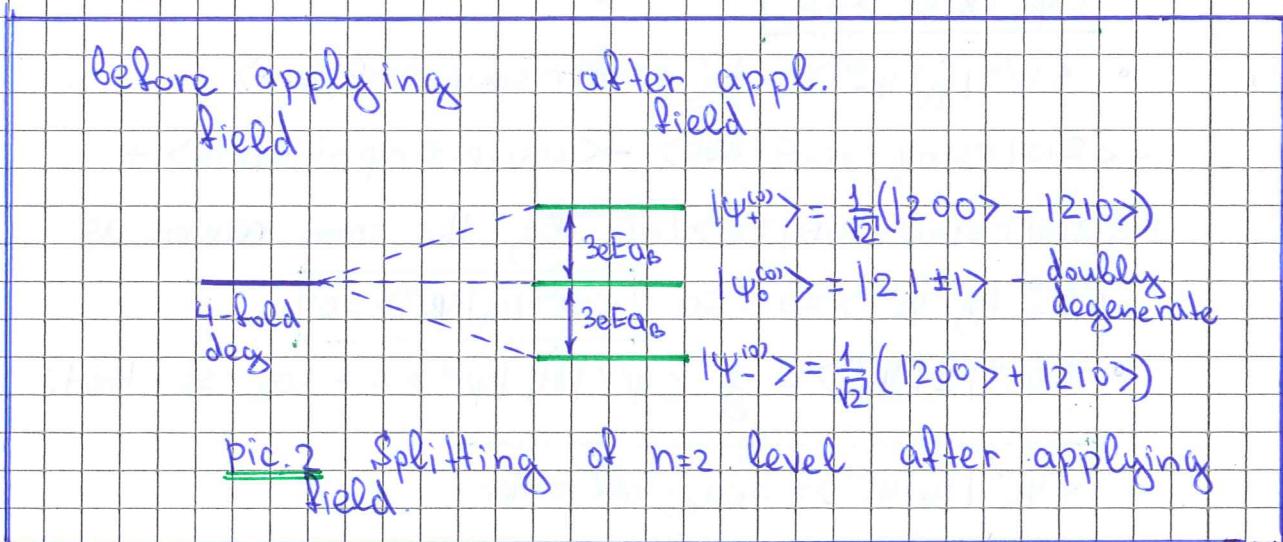
$$\boxed{\langle \psi_0^{(o)} | \hat{p} | \psi_0^{(o)} \rangle = 0}$$

⑩ Let's now make conclusions about the problem.

- Assume we consider first 2 levels of the hydrogen atom

* $n=1$ level is not perturbed if we apply electric field E along Z -axis.

* $n=2$ level which is 4-fold degenerate is splitted into 2 non-degenerate and 1 doubly degenerate level (see picture below)



- Finally we can see problem from the other side.

Atom in diff. states can be considered as electric dipole with the moment given by exp. value $\langle \vec{p} \rangle$. Then the level will get energy shift $\delta E = -\bar{E} \cdot \langle \vec{p} \rangle = -E_z \langle p_z \rangle$ in the external field directed along Z -axis. and indeed.

- ① for $|\Psi_{\pm}^{(0)}\rangle$ states we has got

$$\langle p_z \rangle_{\pm} = \langle \Psi_{\pm}^{(0)} | \hat{p}_z | \Psi_{\pm}^{(0)} \rangle = \mp 3e a_B \text{ so that}$$

$$\underline{\delta E_{\pm} = \pm 3e E a_B} \text{ which coincides with our previous result.}$$

- ② In the same way for $|\Psi_0^{(0)}\rangle$ state:

$$\langle \hat{p}_z \rangle_0 = \langle \Psi_0^{(0)} | \hat{p}_z | \Psi_0^{(0)} \rangle = 0 \text{ so that } \underline{\delta E_0 = 0} \text{ which is}$$

consistent with perturbation theory results too.

① Seminar 17 (Atom and statistics)

Theory: On this lesson we will consider distributions of the electrons on the orbits of atoms, so it will be useful to remember something about statistics:

- ① When we have system of many particles we describe it by the total w.f. depending on the positions of all particles $\{\vec{r}_i\}$:

$\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$ - this w.f. describes the situation when first particle is in position \vec{r}_1 , second - in \vec{r}_2 and so on.

- ② Now the question what happens to the w.f. if we permute 2 particles. There are 2 kind of behaviour:

- Bosons doesn't change w.f. under permutations

$$\Psi(\vec{r}_1, \vec{r}_2) = \Psi(\vec{r}_2, \vec{r}_1)$$

- Fermions change overall sign under permutation

$$\Psi(\vec{r}_1, \vec{r}_2) = -\Psi(\vec{r}_2, \vec{r}_1);$$

- ③ If we consider fermion w.f. for 2 particles, it should look like

$$\Psi(\vec{r}_1, \vec{r}_2) = \Psi_1(\vec{r}_1)\Psi_2(\vec{r}_2) - \Psi_2(\vec{r}_1)\Psi_1(\vec{r}_2);$$

due to antisymmetry under permutation.

- From here we see that if $\vec{r}_1 = \vec{r}_2$, $\Psi = 0$, i.e. we can't put 2 spinless fermions in the same position. This is known as Pauli exclusion principle.

- ④ If we take spin to consideration and consider 2 $s=\frac{1}{2}$ fermions we have 2 possibilities to obtain antisymmetric w.f.

(2)

$$\Psi_{S=0}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}} (\psi_1(\bar{r}_1)\psi_2(\bar{r}_2) + \psi_2(\bar{r}_1)\psi_1(\bar{r}_2)) \cdot \frac{1}{\sqrt{2}} (|1\uparrow\downarrow\rangle - |1\downarrow\uparrow\rangle) \rightarrow \text{singlet state!}$$

symmetric antisymm.

$$\Psi_{S=1}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}} (\psi_1(\bar{r}_1)\psi_2(\bar{r}_2) - \psi_2(\bar{r}_1)\psi_1(\bar{r}_2)) \left\{ \begin{array}{l} \frac{1}{\sqrt{2}} (|1\uparrow\uparrow\rangle + |1\downarrow\uparrow\rangle) \\ |1\downarrow\downarrow\rangle \end{array} \right\} \rightarrow \text{triplet state!}$$

anti symmetric symm.

So now we can see that $\Psi_{S=0}(\bar{r}_1, \bar{r}_2) \neq 0$ for $\bar{r}_1 = \bar{r}_2$
and we can put 2 $s=\frac{1}{2}$ fermions in singlet state in
the same point.

Problem I (Compendium N 25)

Consider 3 identical $s=\frac{1}{2}$ particles of mass m in
3d potential: $V(r) = \frac{1}{2} m\omega^2 r^2$;

a) Assuming that the particles are fermions, find
the ground state energy for this system

- Let's remind some facts about spherically symmetric
3d h.o. spectrum first:

① n^{th} level of h.o. is given by:

$$E_n = \hbar\omega(n + \frac{3}{2});$$

② n^{th} level degeneracy: $D_n = \frac{1}{2}(n+1)(n+2)$;

③ For the level n the following values of
orbital angular momentum l are possible:

- if n is even then $0 \leq l \leq n$ and l is even only too.
- if n is odd then $1 \leq l \leq n$ and l takes odd values only.

(All this facts were derived in Problems II and III of Set 10)

- Let's now fill levels of 3d h.o. with fermions:

① First we fill $n=0$ level which has energy

$$E_0 = \frac{3}{2}\hbar\omega \quad \text{and degeneracy is } D_0 = 1 \quad (\text{or 2 if we})$$

take spin into account) So we can put 2 fermions in
singlet state on this level.

③ ② Now we go to $n=1$ level which has $E_1 = \frac{5}{2}\hbar\omega$ energy with the degeneracy $D_1 = 3$ (or 6 if you take spin into account.). We throw one electron on this level.

③ So total energy of the system is:

$$E = 2 \cdot \frac{3}{2}\hbar\omega + \frac{5}{2}\hbar\omega = \frac{11}{2}\hbar\omega; \text{ So ground state energy is } \boxed{E = \frac{11}{2}\hbar\omega};$$

④ What is the degeneracy of the ground state?

- As first level is completely filled there is no degeneracy there and all degeneracy is coming from the next level.

• Now we consider next level. Its degeneracy is 6 (including spin degree of freedom), as we put only one particle on this level this is degeneracy of our ground state: $D=6$;

⑤ What is the orbital angular momentum of the ground state? What are the allowed values for the total angular momentum of the ground state?

- Using the facts about 3d h.o. from part a we see that particles on $n=0$ level is $l_z=0$ while for the particle on $n=1$, $l_z=1$. So total angular momentum is $L=1$;
- Now we go to spin. First of all we know that electrons on "n=0" level are in singlet state ($S_z=0$). Now we add one more spin $S_z=\frac{1}{2}$ giving total spin being equal to $S=\frac{1}{2}$;
- Finally to obtain total angular momentum adding orbital angular momentum and spin:
 $J=L+S$. Then as we know:

$$④ |l-s| \leq j \leq l+s \Rightarrow l-\frac{1}{2} \leq j \leq l+\frac{1}{2} \Rightarrow$$

$j = \frac{1}{2}; \frac{3}{2}; \dots$ are allowed values of total angular momentum.

Problem II The 2s and 2p states for the hydrogenic atom are degenerate. However, when filling shells the 2s is filled before the 2p. The problem is to understand why this occurs. Suppose we are considering lithium, which has $Z=3$ and 2 electrons in the 1s shell. We now add the third electron which should go into an $n=2$ state. The inner electrons effectively screen the nucleus, so the last electron for the most part sees $Z=1$.

① Find the expectation value $\langle r^2 \rangle$ for the 2s and 2p states, assuming $Z=1$:

- To find r^2 expectation value we should know 2s and 2p states w.f. But before going into details of this state let's consider general state $\Psi_{nem} = R_{ne}(r)Y_{em}(\theta, \phi)$

Then we have:

$$\begin{aligned} \langle r^2 \rangle_{nem} &\equiv \int dr \cdot r^2 R_{ne}^*(r) R_{ne}(r) Y_{em}^*(\theta, \phi) Y_{em}(\theta, \phi) = \\ &= \underbrace{\int d\Omega Y_{em}^*(\theta, \phi) Y_{em}(\theta, \phi)}_{\text{"1" due to normalisation}} \int dr \cdot r^4 |R_{ne}(r)|^2 \Rightarrow \end{aligned}$$

$$\underline{\underline{\langle r^2 \rangle_{nem} = \int_0^\infty dr \cdot r^4 |R_{ne}(r)|^2;}}$$

So we see that we really need only radial part $R_{ne}(r)$ of the w.f. Now we can obtain from the table 4.7. Griffiths

$$R_{20}(r) = 2 \left(\frac{Z}{2a_B} \right)^{3/2} \left(1 - \frac{Zr}{2a_B} \right) e^{-\frac{Zr}{2a_B}};$$

$$R_{21}(r) = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_B} \right)^{3/2} \left(\frac{Zr}{a_B} \right) e^{-\frac{Zr}{2a_B}};$$

(5)

Now using this expressions and substituting $Z_i=1$
 (nucleus charge is screened by 2 inner electrons)
 we can evaluate $\langle r^2 \rangle$ for both 2s and 2p states:

① 2s state

$$\begin{aligned}\underline{\langle r^2 \rangle_{2s}} &= \int_0^\infty dr \cdot r^4 |R_{20}(r)|^2 = \int_0^\infty dr \cdot r^4 \cdot 4 \left(\frac{1}{2a_B}\right)^3 \left(1 - \frac{r}{2a_B}\right)^2 e^{-\frac{r}{a_B}} = \\ &= [\text{using change of variable } t = \frac{r}{a_B}] = a_B^2 \int_0^\infty dt \cdot 4t^4 \frac{1}{8} \left(1 - \frac{t}{2}\right)^2 e^{-t} = \\ &= \frac{1}{2} a_B^2 \int_0^\infty dt \left(t^4 - t^5 + \frac{1}{4}t^6\right) e^{-t} = [\text{using formula we already know } \int_0^\infty dt \cdot t^n e^{-t} = n!] = \\ &= \frac{1}{2} a_B^2 (4! - 5! + \frac{1}{4} 6!) = \frac{24}{2} a_B^2 (1 - 5 + \frac{5}{4} \cdot 6) = 7.6 a_B^2 \approx 42 a_B^2\end{aligned}$$

② 2p state

$$\begin{aligned}\underline{\langle r^2 \rangle_{2p}} &= \int_0^\infty dr \cdot r^4 |R_{21}(r)|^2 = \int_0^\infty dr \frac{r^4}{3} \left(\frac{1}{2a_B}\right)^3 \left(\frac{r}{a_B}\right)^2 e^{-\frac{r}{a_B}} = [t = \frac{r}{a_B}] = \\ &= \frac{a_B^3}{24} \int_0^\infty dt \cdot t^6 \cdot e^{-t} = \frac{a_B^2}{24} \cdot 6! = 30 a_B^2;\end{aligned}$$

So we have got:

$$\boxed{\langle r^2 \rangle_{2s} = 42 a_B^2}$$

$$\boxed{\langle r^2 \rangle_{2p} = 30 a_B^2}$$

③ Find the probability that the 2s and 2p states are inside the rms radius for a 1s state with $Z=3$. Argue why your result means that the 2s state in lithium has less energy than 2p state.

- First let's find rms. for $Z=3$ atom:

$$\begin{aligned}\underline{\langle r^2 \rangle_{1s}} &\equiv \int_0^\infty dr \cdot r^4 |R_{10}(r)|^2 = [\text{using table 4.7 from Griffiths}] = \\ &= \int_0^\infty dr \cdot r^4 \cdot 4 \left(\frac{Z}{a}\right)^3 e^{-2r/Z/a_B} = [\text{making change of variable } t = \frac{2r/Z}{a_B}] = \\ &= \left(\frac{a_B}{2Z}\right)^2 \cdot \frac{1}{2^3} \cdot 4 \int_0^\infty dt \cdot t^4 \cdot e^{-t} = \frac{24}{2^3} \left(\frac{a_B}{Z}\right)^2 = 3 \left(\frac{a_B}{Z}\right)^2 = \frac{a_B^2}{3} \text{ for } Z=3,\end{aligned}$$

so $\boxed{r_{1s} = \sqrt{\langle r^2 \rangle_{1s}} = \frac{a_B}{\sqrt{3}}}$; is r.m.s. we need

⑥ Now we are ready to find probabilities:

① First of all one more time let's consider general state $\Psi_{nem}(\vec{r})$. Then probability density is given by $|\Psi_{nem}(\vec{r})|^2 = |R_{ne}(r)|^2 |\Psi_{em}|^2$ and probability to be found inside r_{1s} for the electron is given by:

$$P(n, l, m) = \int_0^{r_{1s}} d^3\vec{r} |\Psi_{nem}(\vec{r})|^2 = \int_0^{r_{1s}} dr \cdot r^2 |R_{ne}(r)|^2 \underbrace{\int dS |Y_{lm}(\theta, \phi)|^2}_{\text{due to normalisation}} = \\ = \int_0^{r_{1s}} dr \cdot r^2 |R_{ne}(r)|^2$$

② Now let's consider particularly $2s$ state:

$$P_{2s} = \int_0^{r_{1s}} dr \cdot r^2 |R_{2s}|^2 = \int_0^{r_{1s}} dr \cdot r^2 \cdot 4 \frac{1}{(2a_B)^3} \left(1 - \frac{r}{2a_B}\right)^2 e^{-r/a_B} =$$

$$= \left[\begin{array}{l} \text{changing variable } t = \frac{r}{a_B}, \text{ note} \\ \text{that integral up. limit is then } t_{\max} = \frac{r_{1s}}{a_B} = \frac{1}{\sqrt{3}} \end{array} \right] =$$

$$= \frac{1}{2} \int_0^{\frac{1}{\sqrt{3}}} dt \cdot t^2 \left(1 - \frac{1}{2}t\right)^2 e^{-t} = \frac{1}{2} \int_0^{\frac{1}{\sqrt{3}}} dt \left(t^2 - t^3 + \frac{1}{4}t^4\right) e^{-t} = \frac{1}{2}(A + B + \frac{1}{4}C)$$

Where:

$$\bullet A = \int_0^{\frac{1}{\sqrt{3}}} dt \cdot t^2 e^{-t} = \left[\begin{array}{l} \text{taking by parts} \\ \text{several times} \end{array} \right] = -t^2 e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} + \int_0^{\frac{1}{\sqrt{3}}} dt \cdot 2t e^{-t} = \\ = (-t^2 - 2t) e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} + 2 \int_0^{\frac{1}{\sqrt{3}}} dt e^{-t} = -(-t^2 - 2t + 2) e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} = \\ = 2 - \left(\frac{1}{3} + \frac{2}{\sqrt{3}} + 2\right) e^{-\frac{1}{\sqrt{3}}} = 4,1873 \cdot 10^{-2};$$

$$\bullet B = - \int_0^{\frac{1}{\sqrt{3}}} dt \cdot t^3 e^{-t} = t^3 e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} - \int_0^{\frac{1}{\sqrt{3}}} dt \cdot 3t^2 e^{-t} = (t^3 + 3t^2) e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} - \\ - \int_0^{\frac{1}{\sqrt{3}}} dt \cdot 6t e^{-t} = (t^3 + 3t^2 + 6t) e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} - 6 \int_0^{\frac{1}{\sqrt{3}}} dt e^{-t} = (t^3 + 3t^2 + 6t + 6) e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} = \\ = -6 + \left(\frac{1}{3\sqrt{3}} + 1 + \frac{6}{\sqrt{3}} + 6\right) e^{-\frac{1}{\sqrt{3}}} = -1,758 \cdot 10^{-2}$$

$$\bullet C = \int_0^{\frac{1}{\sqrt{3}}} dt \cdot t^4 e^{-t} = -t^4 e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} + \int_0^{\frac{1}{\sqrt{3}}} dt \cdot 4t^3 e^{-t} = -(t^4 + 4t^3) e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} + \\ + \int_0^{\frac{1}{\sqrt{3}}} dt \cdot 12t e^{-t} = -(t^4 + 4t^3 + 12t) e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} + 12 \int_0^{\frac{1}{\sqrt{3}}} dt e^{-t} = -(t^4 + 4t^3 + 12t + 12) e^{-t} \Big|_0^{\frac{1}{\sqrt{3}}} = \\ = 24 - \left(\frac{1}{3} + \frac{4}{3\sqrt{3}} + 4 + \frac{24}{\sqrt{3}} + 24\right) e^{-\frac{1}{\sqrt{3}}} = 7,957 \cdot 10^{-3}$$

⑦ Summing all together we get $P_{2s} \approx 1,3\%$

③ Finally we consider $2p$ state:

$$P_{2p} = \int_0^{a_B \sqrt{3}} dr \cdot r^2 \cdot |R_{2p}|^2 = \int_0^{r_{ls}} dr \cdot r^2 \cdot \frac{1}{3} \frac{1}{(2a_B)^3} \left(\frac{r}{a_B}\right)^2 e^{-\frac{r}{a_B}} = \left[t = \frac{r}{a_B}\right] = \\ = \frac{1}{24} \int_0^{\sqrt{3}} dt \cdot t^4 \cdot e^{-t} = \frac{1}{24} C = 0,33 \cdot 10^{-3}, \text{ i.e.}$$

$$P_{2p} \approx 0,03\%$$

Explanation about energies of $2s$ and $2p$ states

- Notice that $P_{2p} < P_{2s}$ thus $2s$ electron "spends" more time inside $1s$ orbit. When electron is inside $1s$ r.m.s., it "see" unscreened nucleus (i.e. $Z=3$).
- As we remember energy levels of the hydrogen-like atom is $E_n = -\frac{Z^2}{2n^2} \cdot \frac{e^2}{4\pi\epsilon_0 a_0}$; so the energy for $Z=3$ is lower then $Z=1$. Thus $E_{2s} < E_{2p}$ and

$2s$ level is filled before $2p$.

- Notice contradictory fact $\langle r^2 \rangle_{2s} > \langle r^2 \rangle_{2p}$ i.e. $2s$ electron in average is more distinct from the nucleus then $2p$ electron, but still probability to find $2s$ electron inside $1s$ r.m.s., i.e. close to nucleus, is higher then the same probability for $2p$ electron.

Problem III Consider 2 electrons in a p orbital:

- ① Ignoring their spins, write down all 9 states, using a basis where they are either symmetric or antisymmetric.

Let's build our states out of states with particular projections $\hat{L}_{z1,2}$ of 1st electron (m_1) and second electron (m_2). As total angular momentum has L_z projection given by the sum of m_1 and m_2 ($m=m_1+m_2$)

⑧ we can classify states according to momentum projection m :

① $m=2$ This is maximally possible value of m .

As both electrons are p-electrons they both have $l=1$, thus for both of them $-1 \leq m_{1,2} \leq 1$ and maximal value of m is then given by

$$m = m_1 + m_2 = 1 + 1 = 2;$$

The only possible state with $m=2$ is

$$|1,1\rangle \text{ (we use notations } |m_1, m_2\rangle \text{ for the states here)}$$

It is symmetric state. (we change order of particles and the state remains the same)

② $m=1$ Possible states are $|0,1\rangle$ and $|1,0\rangle$

They can be combined into symmetric state $\frac{1}{\sqrt{2}}(|0,1\rangle + |1,0\rangle)$

and antisymmetric state $\frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle)$

③ $m=0$ Possible states are $|1,-1\rangle, |-1,1\rangle, |0,0\rangle$

They can be combined into 2 symmetric states $\frac{1}{\sqrt{2}}(|1,-1\rangle + |-1,1\rangle)$,

$|0,0\rangle$ (+ all linear combinations of this 2 states) and

antisymmetric state $\frac{1}{\sqrt{2}}(|1,-1\rangle - |-1,1\rangle)$

④ $m=-1$ Possible states $|0,-1\rangle$ and $|-1,0\rangle$ are combined

into symmetric $\frac{1}{\sqrt{2}}(|0,-1\rangle + |-1,0\rangle)$ and antisymmetric

$\frac{1}{\sqrt{2}}(|1,0\rangle + |0,-1\rangle)$ states

⑤ $m=-2$ The only possible state $|-1,-1\rangle$ is symmetric.

Let's summarize in the table:

m	Symm. states	antisymm. state
2	$ 1,1\rangle$	—II—
1	$\frac{1}{\sqrt{2}}(1,0\rangle + 0,1\rangle)$	$\frac{1}{\sqrt{2}}(1,0\rangle - 0,1\rangle)$
0	$ 0,0\rangle; \frac{1}{\sqrt{2}}(1,-1\rangle + -1,1\rangle)$	$\frac{1}{\sqrt{2}}(1,-1\rangle - -1,1\rangle)$
-1	$\frac{1}{\sqrt{2}}(-1,0\rangle + 0,-1\rangle)$	$\frac{1}{\sqrt{2}}(-1,0\rangle - 0,-1\rangle)$
-2	$ -1,-1\rangle$	—II—

(g) Show that the antisymmetric states are part of an $L=1$ multiplet, where L is the total orbital angular momentum. What does this imply for L for the symmetric states?

To show that antisymmetric states are part of $L=1$; we act with lowering \hat{L}_- and raising operators \hat{L}_+

$$\hat{L}_{\pm} |j, m\rangle = \pm \sqrt{j(j+1) - m(m\pm 1)} |j, m\pm 1\rangle$$

$$\text{and } \hat{L}_{\pm} = \hat{L}_{\pm}^{(1)} + \hat{L}_{\pm}^{(2)}$$

- If we act with \hat{L}_+ on $\frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle)$ we get

$$\hat{L}_+ \frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle) = \frac{1}{\sqrt{2}} [(\hat{L}_+^{(1)} + \hat{L}_+^{(2)})|0,1\rangle - (\hat{L}_+^{(1)} + \hat{L}_+^{(2)})|1,0\rangle]$$

First let's find following actions of \hat{L}_{\pm} :

$$\hat{L}_+^{(1)} |0,1\rangle = \pm \sqrt{1 \cdot 2 - 0} |1,1\rangle = \sqrt{2} \pm |1,1\rangle;$$

$$\hat{L}_+^{(1)} |1,0\rangle = \hat{L}_+^{(2)} |0,1\rangle = 0; \quad \hat{L}_+^{(2)} |1,0\rangle = \sqrt{2} \pm |1,1\rangle; \text{ so that:}$$

$$\hat{L}_+ \frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle) = \pm (\pm |1,1\rangle - |1,1\rangle) = 0, \text{ i.e.}$$

the state we have written angular momentum l is equal to

$$m = m_1 + m_2 = 1, \text{ i.e. } l=1:$$

$$|\pm, 1\rangle = \frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle) \text{ i.e. this is indeed } l=1 \text{ state, q.e.d.}$$

$$|l, m\rangle$$

state

- Now we start acting with lowering operators $\hat{L}_- = \hat{L}_-^{(1)} + \hat{L}_-^{(2)}$

$$\hat{L}_- |1,1\rangle = \frac{1}{\sqrt{2}} ((\hat{L}_-^{(1)} + \hat{L}_-^{(2)}) |0,1\rangle - (\hat{L}_-^{(1)} + \hat{L}_-^{(2)}) |1,0\rangle)$$

Now we use:

$$\hat{L}_-^{(1)} |0,1\rangle = \pm \sqrt{1 \cdot 2 - 0} |1,-1\rangle = \sqrt{2} \pm |1,-1\rangle;$$

$$\hat{L}_-^{(1)} |1,0\rangle = \sqrt{2} \pm |0,0\rangle; \quad \hat{L}_-^{(2)} |0,1\rangle = \sqrt{2} \pm |0,0\rangle; \quad \hat{L}_-^{(2)} |1,0\rangle = \sqrt{2} \pm |1,-1\rangle$$

So that we get

$$\hat{L}_- |1,1\rangle \equiv \sqrt{2} \pm |1,0\rangle = \frac{\sqrt{2} \pm}{\sqrt{2}} (|1,-1\rangle + |0,0\rangle - |0,0\rangle - |1,-1\rangle) \text{ we}$$

see that we has got second antisymmetric state

$$\frac{1}{\sqrt{2}}(|1,1\rangle - |1,-1\rangle) \text{ i.e. it has } l=1 \text{ too, q.e.d.}$$

- Acting one more time we get:

$$\frac{1}{\sqrt{2}}((\hat{L}_-^{(1)} + \hat{L}_-^{(2)}) |1,-1\rangle - (\hat{L}_-^{(1)} + \hat{L}_-^{(2)}) |1,-1\rangle)$$

(10) Using:

$$\hat{L}_-^{(1)} | -1, 1 \rangle = 0; \quad \hat{L}_-^{(1)} | 1, -1 \rangle = \hbar \sqrt{2 \cdot 1 - 0} | 0, -1 \rangle = \sqrt{2} \hbar | 0, -1 \rangle;$$

$$\hat{L}_-^{(2)} | 1, -1 \rangle = 0; \quad \hat{L}_-^{(2)} | -1, 1 \rangle = \sqrt{2} \hbar | -1, 0 \rangle;$$

So that

$$\hat{L}_- \frac{1}{\sqrt{2}} (| 1, -1 \rangle - | -1, 1 \rangle) = \hbar (| 0, -1 \rangle - | -1, 0 \rangle) \text{ is}$$

proportional to the last antisymmetric state, i.e. state

$$\frac{1}{\sqrt{2}} (| -1, 0 \rangle - | 0, -1 \rangle) \text{ has } l=1 \text{ too, q.e.d.}$$

- Thus we see that all antisymmetric states has $l=1$.

As we sum 2 $l=1$ momentum possible values for total angular momentum is $l=0, 1, 2$. In general symmetry of w.f. is given by $(-1)^l$ i.e. if

- l is odd state is antisymmetric. } valid for summing
- l is even state is symmetric. } momentum of 2 particles
- Note that we can act with $\hat{L}^2 = (\hat{L}_1 + \hat{L}_2)^2 = \hat{L}_1^{(1)} \hat{L}_2^{(1)} + (\hat{L}_1^{(2)} + \hat{L}_2^{(2)}) (\hat{L}_1^{(2)} + \hat{L}_2^{(2)})$ and find \hat{L}^2 for all 3 antisymmetric states directly.

- (c) Now consider 3 electrons in p state. Write down the state that is completely antisymmetric. What is the total value of l ?

Antisymmetric state can be constructed with Slater determinant (see lecture notes)

$$|\Psi\rangle_{AS} = \frac{1}{\sqrt{6}} \begin{vmatrix} |1\rangle_1 & |0\rangle_1 & |-1\rangle_1 \\ |1\rangle_2 & |0\rangle_2 & |-1\rangle_2 \\ |1\rangle_3 & |0\rangle_3 & |-1\rangle_3 \end{vmatrix} = \frac{1}{\sqrt{6}} (|10-1\rangle + |1-10\rangle + |0-11\rangle - |1-10\rangle - |01-1\rangle - |11-10\rangle)$$

Total projection of angular momentum for this state is $m = m_1 + m_2 + m_3 = 0$; ($m=0$)

Easiest way to find l is to act with raising operator

$$\hat{L}_+ = \hat{L}_1^{(1)} + \hat{L}_1^{(2)} + \hat{L}_1^{(3)}$$

$$\begin{aligned}
 \hat{L}_+ |\psi\rangle_{\text{as}} &= \frac{1}{\sqrt{6}} \left(\hat{L}_+^{(0)} |110-1\rangle + \hat{L}_+^{(1)} |-110\rangle + \hat{L}_+^{(2)} |10-11\rangle - \right. \\
 &\quad - \hat{L}_+^{(4)} |-101\rangle - \hat{L}_+^{(5)} |01-1\rangle - \hat{L}_+^{(6)} |1-10\rangle + \hat{L}_+^{(7)} |10-1\rangle + \hat{L}_+^{(8)} |-110\rangle + \\
 &\quad + \hat{L}_+^{(9)} |10-11\rangle - \hat{L}_+^{(10)} |-101\rangle - \hat{L}_+^{(11)} |01-1\rangle - \hat{L}_+^{(12)} |1-10\rangle + \\
 &\quad + \hat{L}_+^{(13)} |10-1\rangle + \hat{L}_+^{(14)} |-110\rangle + \hat{L}_+^{(15)} |0-11\rangle - \hat{L}_+^{(16)} |-101\rangle - \\
 &\quad \left. - \hat{L}_+^{(17)} |101-1\rangle - \hat{L}_+^{(18)} |11-10\rangle \right) = \frac{\hbar\sqrt{2}}{\sqrt{6}} (0 + |1010\rangle + |1111\rangle - \\
 &\quad - |1001\rangle - |111-1\rangle + 0 + |111-1\rangle + 0 + |1001\rangle - |1111\rangle - 0 - \\
 &\quad - |1100\rangle + |1100\rangle + |1111\rangle + 0 - 0 - |1000\rangle - |1111\rangle) = 0,
 \end{aligned}$$

So we see that

$$\hat{L}_+ |\psi\rangle_{\text{as}} = 0 \quad \text{and thus for this state } \underline{\ell=0};$$

①

Seminar 18 (Exam 2012)

Problem II Consider the following w.r.t. for a particle in 1d box

$$\psi(x) = C [4\psi_1(x) - 3\psi_2(x) - \psi_3(x) - 3\psi_4(x) + i\psi_5(x)]$$

where $\psi_n(x)$ are normalized eigenstates with energies $E_n = E_1 n^2$ (E_1 is the energy of the ground state)

ⓐ Find C so that $\psi(x)$ is properly normalised

Normalisation condition reads:

$$1 \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} dx |\psi(x)|^2 = |C|^2 \left(\int_{-\infty}^{\infty} dx |\psi_1|^2 + 9 \int_{-\infty}^{\infty} dx |\psi_2|^2 + 8 \int_{-\infty}^{\infty} dx |\psi_3|^2 + 9 \int_{-\infty}^{\infty} dx |\psi_4|^2 + \right. \\ \left. + \int_{-\infty}^{\infty} dx |\psi_5|^2 - 12 \int_{-\infty}^{\infty} dx \psi_1^* \psi_2 - 12 \int_{-\infty}^{\infty} dx \psi_2^* \psi_1 + \text{other cross terms} \right)$$

as ψ_1, \dots, ψ_5 form orthonormal basis

$$\int |\psi_1|^2 = \int |\psi_2|^2 = \dots = \int |\psi_5|^2 = 1;$$

$$\int \psi_1^* \psi_2 = \int \psi_1^* \psi_3 = \dots = [\text{all other cross terms}] = 0;$$

Then we get finally $|C|^2 (16 + 9 + 1 + 9 + 1) = 36 |C|^2 \Rightarrow$

$$\Rightarrow C = \frac{1}{6} \text{ up to phase.}$$

ⓑ Find the probability that a measurement of the particle's energy will be $9E_1$.

Probability of measuring eigenvalue E_n is

given by the inner product $P_n = |\langle \psi_n | \psi \rangle|^2$ where

$|\psi_n\rangle$ is eigenstate corresponding to eigenvalue E_n .

In our particular case this inner product is

$$P_3 = |\langle \psi_3 | \psi \rangle|^2 = |C \underbrace{\int_0^\infty 4\psi_3^* \psi_1}_{0} - 3C \underbrace{\int_0^\infty \psi_3^* \psi_2}_{0} - C \underbrace{\int_0^\infty \psi_3^* \psi_3}_{1} - \\ - 3C \underbrace{\int_0^\infty \psi_3^* \psi_4}_{0} + iC \underbrace{\int_0^\infty \psi_3^* \psi_5}_{0}|^2$$

$$\text{So that } P_3 = |C|^2 = \frac{1}{36} ; \quad \boxed{P_3 = \frac{1}{36}}$$

ⓒ Find expectation value of the energy in terms of the ground state energy E_1 .

② First we find $\hat{H}\Psi$:

$$\hat{H}\Psi = C \left[4 \underbrace{\hat{H}\Psi_1}_{E_1\Psi_1} - 3 \underbrace{\hat{H}\Psi_2}_{(E_2=4E_1)\Psi_2} - \underbrace{\hat{H}\Psi_3}_{(E_3=9E_1)\Psi_3} - 3 \underbrace{\hat{H}\Psi_4}_{(E_4=16E_1)\Psi_4} + i \underbrace{\hat{H}\Psi_5}_{(E_5=25E_1)\Psi_5} \right]$$

Now if we write down expectation value for the energy we get:

$$\langle E \rangle \equiv \int dx \Psi^* H \Psi = |C|^2 \left[16E_1 \int \Psi_1^* \Psi_1 + 9 \cdot 4E_1 \int \Psi_2^* \Psi_2 + 9E_1 \int \Psi_3^* \Psi_3 + \right. \\ \left. + 3 \cdot 3 \cdot 16E_1 \int \Psi_4^* \Psi_4 + 25E_1 \int \Psi_5^* \Psi_5 + \text{cross terms like } -12 \cdot 4 \int \Psi_1^* \Psi_2 E_2 \text{ which all go to "0" due to orthonormality of the basis} \right]$$

Then we finally get:

$$\langle E \rangle = \frac{1}{36} \cdot E_1 (16 + 36 + 9 + 144 + 25) = \frac{230}{36} E_1 = \frac{115}{18} E_1;$$

$$\boxed{\langle E \rangle = \frac{115}{18} E_1;}$$

③ Assuming that $\Psi(x,0) = \Psi(x)$, find $\Psi(x,t)$ in terms of E_1 and $\Psi_n(x)$

To find time evolved w.r.t. we should act with time evolution operator $e^{-i\hat{H}t/\hbar}$ on initial state:

$$\Psi(x,t) = e^{-i\hat{H}t/\hbar} \Psi(x,0) \text{ (usually we expand initial state)}$$

$$\Psi(x) = \sum_n c_n \Psi_n(x) \text{ in series of } \hat{H} \text{ eigenstates } \Psi_n. \text{ Here}$$

$$c_n = \langle \Psi_n | \Psi \rangle = \int dx \Psi_n^* \Psi, \text{ and then use equation}$$

$$e^{-i\hat{H}t/\hbar} |\Psi_n\rangle = e^{-iE_n t/\hbar} |\Psi_n\rangle \text{ where } E_n \text{ is } \hat{H} \text{ eigenvalue}$$

corresponding to $|\Psi_n\rangle$. But here expansion is already done for us and we just write:

$$e^{-i\hat{H}t/\hbar} \Psi(x) = \frac{1}{6} \left[4 e^{iE_1 t/\hbar} \Psi_1 - 3 e^{-iE_2 t/\hbar} \Psi_2 - e^{-iE_3 t/\hbar} \Psi_3 - 3 e^{-iE_4 t/\hbar} \Psi_4 + i e^{-iE_5 t/\hbar} \Psi_5 \right]$$

so that:

$$\boxed{\Psi(x,t) = \frac{2}{3} e^{-iE_1 t/\hbar} \Psi_1 - \frac{1}{2} e^{-iE_2 t/\hbar} \Psi_2 - \frac{1}{6} e^{-iE_3 t/\hbar} \Psi_3 - \frac{1}{2} e^{-iE_4 t/\hbar} \Psi_4 + i e^{-iE_5 t/\hbar} \Psi_5;}$$

(3)

Problem III Consider 2-state system of a spin $\frac{1}{2}$ particle, where the eigenstates of \hat{S}_z are given by

$$|\uparrow\rangle \equiv \begin{bmatrix} 1 \\ 0 \end{bmatrix}; \quad |\downarrow\rangle \equiv \begin{bmatrix} 0 \\ 1 \end{bmatrix};$$

Suppose there is a magnetic field \vec{B} pointing in z -direction $\vec{B} = (0, 0, B)$ and a corresponding Hamiltonian is given by

$$H = -\vec{B} \cdot \vec{\mu}, \text{ where } \vec{\mu} = -\frac{e}{mc} \vec{S}, \quad \vec{S} = \frac{\hbar}{2} \vec{\sigma};$$

First of all let's write down matrix representation of \hat{H} explicitly:

$$\begin{aligned} \hat{H} &= -\vec{B} \cdot \vec{\mu} = -B_z \cdot \mu_z = \frac{e}{mc} B_z \cdot S_z = \frac{e\hbar}{2mc} B S_3 \Rightarrow \\ \Rightarrow \hat{H} &= \frac{eB\hbar}{2mc} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}; \end{aligned}$$

- ① Find the normalised energy eigenstates and eigenvalues.
- Matrix is already diagonalized and we don't need to find anything:

• $E_- = -\frac{eB\hbar}{2mc}$; $|\Psi_-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |\downarrow\rangle$;

• $E_+ = \frac{eB\hbar}{2mc}$; $|\Psi_+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |\uparrow\rangle$;

- Here we have just written terms standing on the diagonal of matrix and corresponding basis vectors, which are eigenvectors if matrix is already diagonal.
- Physically we have found that energy is minimal when spin is pointing against the magnetic field and vice versa.

- ② Find the normalized eigenstates and eigenvalues of \hat{S}_x in terms of eigenstates of \hat{S}_z ;

First of all \hat{S}_x operator is given by the following

Pauli matrix: $\hat{S}_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ in the basis of eigenstates

④ of \hat{S}_z : $| \uparrow \rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$; $| \downarrow \rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$;

Now we can find eigensystem of \hat{S}_x :

- Secular equation

$$0 = \det(S_x - \lambda \mathbb{I}) = \begin{vmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{vmatrix} = \lambda^2 - \frac{\hbar^2}{4} = 0 \Rightarrow \lambda = \pm \frac{\hbar}{2} \text{ are 2 eigenvalues.}$$

- Now let's find eigenstates of the general form $|\Psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$;

① $\lambda_- = -\frac{\hbar}{2}$, eq. for eigenstate is: $\frac{\hbar}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \end{bmatrix} = 0 \Rightarrow a = -b$;

$$|\Psi_-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}} (| \uparrow \rangle - | \downarrow \rangle);$$

② $\lambda_+ = \frac{\hbar}{2}$, eq. for eigenstate is: $\frac{\hbar}{2} \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \end{bmatrix} = 0 \Rightarrow a = b$;

so that $|\Psi_+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} (| \uparrow \rangle + | \downarrow \rangle)$

- (c) Assume that at $t=0$ the spin state is the negative eigenstate of \hat{S}_x . Find the state as a function of time, t .

$$|\Psi, t=0\rangle = |\Psi_-\rangle = \frac{1}{\sqrt{2}} (| \uparrow \rangle - | \downarrow \rangle)$$

Now acting with time evolution operator $e^{-i\hat{H}t/\hbar}$

$$|\Psi, t\rangle = e^{-i\hat{H}t/\hbar} |\Psi, t=0\rangle = \frac{1}{\sqrt{2}} (e^{-i\hat{H}t/\hbar} | \uparrow \rangle - e^{-i\hat{H}t/\hbar} | \downarrow \rangle)$$

Now as $| \uparrow \rangle$ and $| \downarrow \rangle$ are eigenstates of hamiltonian \hat{H} we get:

$$\exp(-i\frac{\hat{H}t}{\hbar}) | \uparrow \rangle = \exp(-i\frac{E_{\uparrow}t}{\hbar}) | \uparrow \rangle = \exp(-i\frac{eB}{2mc}t) | \uparrow \rangle;$$

$$\exp(-i\frac{\hat{H}t}{\hbar}) | \downarrow \rangle = \exp(-i\frac{E_{\downarrow}t}{\hbar}) | \downarrow \rangle = \exp(i\frac{eB}{2mc}t) | \downarrow \rangle;$$

So that

$$|\Psi, t\rangle = \frac{1}{\sqrt{2}} \left(e^{-i\frac{eB}{2mc}t} | \uparrow \rangle - e^{i\frac{eB}{2mc}t} | \downarrow \rangle \right);$$

- (d) Find the expectation value $\langle \hat{S}_z \rangle$ as a function of t for the state in (c)

• By the definition:

$$\textcircled{5} \quad \langle \hat{S}_z \rangle = \langle \psi_+ | \hat{S}_z | \psi_+ \rangle = \frac{1}{\sqrt{2}} [e^{i \frac{eB}{2mc} t}, -e^{-i \frac{eB}{2mc} t}] \cdot \begin{bmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{bmatrix} \cdot \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i \frac{eB}{2mc} t} \\ -e^{i \frac{eB}{2mc} t} \end{bmatrix} =$$

$$= \frac{\hbar}{4} [e^{i \frac{eB}{2mc} t}, -e^{-i \frac{eB}{2mc} t}] \cdot \begin{bmatrix} e^{-i \frac{eB}{2mc} t} \\ e^{i \frac{eB}{2mc} t} \end{bmatrix} = 0;$$

• The other way to derive time dependent expectation value, is to notice that

$[\hat{H}, \hat{S}_z] \sim [\hat{S}_x, \hat{S}_z] = 0$ and thus $\langle \hat{S}_z \rangle$ is conserved in time : $\frac{d}{dt} \langle \hat{S}_z \rangle = 0$;

Thus it is enough to find expectation value in the initial moment of time $t=0$:

$$\langle \hat{S}_z \rangle = \langle \psi_- | \hat{S}_z | \psi_- \rangle = \frac{\hbar}{4} [1 \ -1] \cdot \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -1 \end{bmatrix} = 0 \text{ which coincides with previous result.}$$

② Find the expectation value $\langle \hat{S}_x \rangle$ as a function of t for the state in ①

By definition expectation value is given by:

$$\langle \hat{S}_x \rangle \equiv \langle \psi_+ | \hat{S}_x | \psi_+ \rangle = \frac{\hbar}{4} [e^{i \frac{eB}{2mc} t}, -e^{-i \frac{eB}{2mc} t}] \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} e^{-i \frac{eB}{2mc} t} \\ -e^{i \frac{eB}{2mc} t} \end{bmatrix} =$$

$$= \frac{\hbar}{4} [e^{i \frac{eB}{2mc} t}, -e^{-i \frac{eB}{2mc} t}] \cdot \begin{bmatrix} -e^{i \frac{eB}{2mc} t} \\ e^{-i \frac{eB}{2mc} t} \end{bmatrix} = -\frac{\hbar}{4} (e^{i \frac{eB}{mc} t} + e^{-i \frac{eB}{mc} t}) =$$

$$= -\frac{\hbar}{2} \cos\left(\frac{eB}{mc} t\right); \text{ so that we get:}$$

$$\boxed{\langle \hat{S}_x \rangle = -\frac{\hbar}{2} \cos\left(\frac{eB}{mc} t\right);}$$

This basically shows spin precession in external magnetic field.

Problem II Suppose we have 5 noninteracting identical particles with mass m in 1d h.o. with potential, $V(x) = \frac{1}{2} m\omega^2 x^2$;

① Assuming that the particles are bosons, find the ground-state energy of this system.

⑥ Spectrum of 1d h.o. is given by the energies:

$$E_n = \hbar\omega(n + \frac{1}{2})$$

If the particles are bosons they can occupy the same state. So ground state energy for five bosons is given by:

$$E = 5 \cdot E_0 = \frac{5}{2} \hbar\omega$$

$$E = \frac{5}{2} \hbar\omega$$

⑦ Assuming that the particles are fermions without spin, find the ground-state energy of this system.

Due to Pauli exclusion principle we can put only one spinless fermion on each level. Then the ground state energy:

$$E = \sum_{n=0}^4 E_n = \frac{1}{2} \hbar\omega + \frac{3}{2} \hbar\omega + \frac{5}{2} \hbar\omega + \frac{7}{2} \hbar\omega + \frac{9}{2} \hbar\omega = \frac{25}{2} \hbar\omega, \text{ so we}$$

get $E = \frac{25}{2} \hbar\omega$

⑧ Assuming that the particles are spin- $\frac{1}{2}$ fermions find the ground-state energy of this system.

Due to Pauli exclusion principle we can put only two spin- $\frac{1}{2}$ fermions on each level. Then the ground state is

$$E = 2E_0 + 2E_1 + E_2 = \hbar\omega + 3\hbar\omega + \frac{5}{2}\hbar\omega = \frac{13}{2}\hbar\omega,$$

So $E = \frac{13}{2}\hbar\omega$

⑨ Assuming that the particles are spin- $\frac{1}{2}$ fermions find the degeneracy of the ground-state.

Filling $n=0$ and $n=1$ levels is unique (i.e. there is no degeneracy) but on the last level we have only one electron which can be putted with either spin up or spin down, i.e. it has the degeneracy

$$D = 2;$$

(7)

② Assuming that the particles are spin- $\frac{1}{2}$ fermions find the first 2 excited energy levels and their degeneracy.

• To find excited energy level let's introduce notation

$n_1 n_2 n_3 n_4 n_5 n_6 \dots$ for the level with n_1 fermi on the first level E_0 , n_2 on E_1 -level and so on.

In this notations ground state level is given by:

2 2 1 0 0 0

• Now to obtain first excited level we throw one fermion from one level to the nearest neighbour. As all levels are equidistant it really doesn't matter what electron we choose to throw. So we get 2 possibilities with the

2 1 2 0 0

energy

$$E^1 = E_0 + \hbar\omega = \frac{15}{2}\hbar\omega$$

2 2 0 1 0

$$E^1 = \frac{15}{2}\hbar\omega;$$

All cases have 2 filled

levels and 1 level with 1

electron which gives 2-fold degeneracy giving $D=2+2=4$ in total

• Finally we look for the second excited level. To obtain it we made one more throw of fermion:

1 2 2 0 0

$$D=2$$

with the energy

$$E^2 = E^1 + \hbar\omega \Rightarrow$$

2 1 1 1 0 1

$$D=2 \cdot 2 \cdot 2 = 8$$

$$\Rightarrow E^2 = \frac{17}{2}\hbar\omega;$$

2 2 0 0 1

$$D=2$$

Each level with one fermion gives degeneracy 2 and in total we get $D=2+8+2 \Rightarrow D^2=12$

Problem II Assume that the Hamiltonian $H=H_0+H'$ where

H_0 is the Hamiltonian for the 1d h.o.

$H_0 = \hbar\omega(\hat{a}^\dagger \hat{a} + \frac{1}{2})$ and H' is small perturbation given by $H' = 2((\hat{a}^\dagger)^3 + 3(\hat{a}^\dagger)^2 \hat{a} + 3\hat{a}^\dagger \hat{a}^2 + \hat{a}^3)$

⑧ ① Find the first order correction to the energy of the first excited and ground state energy

- Ground state of unperturbed h.o. is $|0\rangle$ such that $\hat{a}|0\rangle = 0$
- Let's find $\hat{H}'|0\rangle$:

Note that \hat{H}' is already normal ordered so this quite easy task:

$$\begin{aligned}\hat{H}'|0\rangle &= \lambda ((\hat{a}^+)^3 + 3(\hat{a}^+)^2\hat{a} + 3\hat{a}^+\hat{a}^2 + \hat{a}^3)|0\rangle = \lambda (\hat{a}^+)^3|0\rangle = \\ &= \lambda \cdot \sqrt{3!}|3\rangle = \sqrt{6}\lambda|3\rangle, \text{ where we have used the definition } |n\rangle \equiv \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle \text{ of } n^{\text{th}} \text{ excited level of h.o.}\end{aligned}$$

So $\hat{H}'|0\rangle = \sqrt{6}\lambda|3\rangle$

- Now we are able to find first order correction to the ground state energy:

$$\delta E_0^{(1)} \equiv \langle 0 | \hat{H}' | 0 \rangle = \sqrt{6}\lambda \langle 0 | 3 \rangle = 0, \Rightarrow \boxed{\delta E_0^{(1)} = 0};$$

② Find the first-order correction to the energy of the first excited state.

- Let's find $\hat{H}'|1\rangle$
- $$\hat{H}'|1\rangle = \lambda ((\hat{a}^+)^3 + 3(\hat{a}^+)^2\hat{a} + 3\hat{a}^+\hat{a}^2 + \hat{a}^3)|1\rangle$$
- Using formulas $\hat{a}^+|n\rangle = \sqrt{n+1}|n\rangle$; $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$; we get
- $$\begin{aligned}\hat{a}^3|1\rangle &\sim \hat{a}^2|0\rangle = 0; \quad 3\hat{a}^+\hat{a}^2|1\rangle \sim 3\hat{a}^+\hat{a}|0\rangle = 0; \\ 3(\hat{a}^+)^2\hat{a}|1\rangle &= 3(\hat{a}^+)^2|0\rangle = 3\sqrt{2}|2\rangle; \\ (\hat{a}^+)^3|1\rangle &= (\hat{a}^+)^4|0\rangle = \sqrt{4!}|4\rangle = 2\sqrt{6}|4\rangle;\end{aligned}$$
- So we get: $\boxed{\hat{H}'|1\rangle = \lambda (2\sqrt{6}|4\rangle + 3\sqrt{2}|2\rangle)}$
 - So first order correction to the first excited state energy:

$$\delta E_1^{(1)} \equiv \langle 1 | \hat{H}' | 1 \rangle = \lambda 2\sqrt{6} \langle 1 | 4 \rangle + \lambda 3\sqrt{2} \langle 1 | 2 \rangle = 0,$$

$$\boxed{\delta E_1^{(1)} = 0};$$

(9)

- (c) Find the second-order correction to the ground-state energy.

Second order correction to the energy is given by:

$$\delta E_0^{(2)} = \sum_{n=0}^{\infty} \frac{|\langle 0 | \hat{H}' | n \rangle|^2}{E_0 - E_n} = \sum_{n=0}^{\infty} \frac{1}{\hbar \omega n} \cdot |\langle n | \hat{H}' | 0 \rangle|^2$$

in our case we know that $\hat{H}'|0\rangle = \sqrt{6}\lambda|3\rangle$ so the only nonzero matrix element is

$$|\langle 3 | \hat{H}' | 0 \rangle|^2 = (\sqrt{6}\lambda)^2 = 6\lambda^2 \text{ and the correction is given by:}$$

$$\delta E_0^{(2)} = \frac{6\lambda^2}{3\hbar\omega} \Rightarrow$$

$$\boxed{\delta E_0^{(2)} = \frac{2\lambda^2}{\hbar\omega};}$$

Problem VII The potential energy of an electron around a spherically symmetric charge density is

$$U(r) = -\frac{e}{4\pi\epsilon_0 r} \cdot Q(r) \text{ where } Q(r) \text{ is the total charge inside the radius } r.$$

charge inside the radius r . Now consider an electron in the ground state of a hydrogenic potential:

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r};$$

Normalized radial w.t. are:

$$R_{10}(r) = 2 \left(\frac{Z}{a_0}\right)^{3/2} \exp\left(-\frac{Zr}{a_0}\right);$$

$$R_{20}(r) = 2 \left(\frac{Z}{2a_0}\right)^{3/2} \left(1 - \frac{Zr}{2a_0}\right) \exp\left(-\frac{Zr}{2a_0}\right);$$

$$R_{21}(r) = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right) \exp\left(-\frac{Zr}{2a_0}\right);$$

- (a) Find the probability that an electron in the ground state is within a distance r from the nucleus.

- The probability for the electron in the state Ψ_{nem} to be inside the sphere with the radius r is

$$P_{nem} = \int dr \cdot r^2 |R_{nem}(r)|^2 \cdot \underbrace{\int d\Omega Y_{lm}^m}_{\text{due to normalisation of spherical polynomials.}}$$

(10) So we are left with $P(nlm) = \frac{1}{\pi} \int_0^r dr \cdot r^2 |R_{nlm}|^2$

- In particular for the ground state we get:

$$P = \int_0^r dr \cdot r^2 |R_{101}|^2 = \int_0^r dr \cdot r^2 \cdot 4 \left(\frac{Z_1}{a_n} \right)^3 \exp \left(-\frac{2Z_1 r}{a_n} \right) = \left[\begin{array}{l} \text{changing } t = \frac{2Z_1 r}{a_n} \\ \text{variable} \end{array} \right] =$$

$$= \frac{1}{2} \int_0^{r \cdot \frac{2Z_1}{a_n}} dt \cdot t^2 e^{-t} = \frac{1}{2} \left(-t^2 - 2t - 2 \right) e^{-t} \Big|_0^{r \cdot \frac{2Z_1}{a_n}} = 1 - \frac{1}{2} \left(\left(\frac{2rZ_1}{a_n} \right)^2 + \frac{4rZ_1}{a_n} + 2 \right) e^{-\frac{2rZ_1}{a_n}}$$

So we have got the following probability:

$$P = 1 - \left(2 \left(\frac{rZ_1}{a_n} \right)^2 + 2 \frac{rZ_1}{a_n} + 1 \right) e^{-\frac{2rZ_1}{a_n}}$$

(B) Now suppose that a second electron is added. It sees the potential from the nucleus as well as a repulsive potential due to its interaction with the first electron in the ground state.

Assume that the second electron sees the first electron as a charged cloud, where the charge density of the cloud is proportional to the probability density. Using eq(1) find the effective potential that the second electron sees due to the first electron.

If charge density is proportional to probability density $g(r) \sim |R_{101}|^2$ then total charge inside the ball of radius

r is $Q(r) \sim P(r)$. Proportionality coefficient is

then e . Indeed in this case

$$Q(r) = e \left(1 - \left(2 \left(\frac{rZ_1}{a_n} \right)^2 + 2 \frac{rZ_1}{a_n} + 1 \right) e^{-\frac{2rZ_1}{a_n}} \right)$$

so that if $r \rightarrow \infty$ $Q(\infty) = -e$, i.e. total charge in space is e (one electron).

Then using formula 1 we get effective potential that the second electron sees due to first one:

$$U(r) = + \frac{e^2}{4\pi\epsilon_0 r} \left(1 - \left(2 \left(\frac{rZ_1}{a_n} \right)^2 + 2 \frac{rZ_1}{a_n} + 1 \right) e^{-\frac{2rZ_1}{a_n}} \right)$$

- (L1) (c) Treating your result from (b) as a first order perturbation find the correction to the energy for the 2-electron hydrogenic atom if one electron is in the ground state and the second is in the 2p ($l=1$ state)

If we treat $U(r)$ as correction we get first

order correction to the energy given by:

$$\begin{aligned}\delta E_{2p}^{(1)} &\equiv \langle 21m | U(r) | 21m \rangle = \int_0^\infty dr \cdot r^2 |R_{21}|^2 \cdot U(r) \cdot \underbrace{\int d\Omega |Y_{1m}|^2}_{\text{due to normalisation.}} = \\ &= \int_0^\infty dr \cdot r^2 U(r) \cdot |R_{21}|^2 = \\ &= \frac{e^2}{4\pi\epsilon_0} \cdot \frac{1}{3} \cdot \left(\frac{Z}{2a_p}\right)^3 \int_0^\infty dr \cdot r^2 \left(\frac{Zr}{a_p}\right)^2 \left[1 - \left(2\left(\frac{rZ}{a_p}\right)^2 + 2\frac{rZ}{a_p} + 1 \right) e^{-\frac{2rZ}{a_p}} \right] e^{-\frac{Zr}{a_p}} = \\ &= \frac{e^2}{12\pi\epsilon_0} \left[\left(\frac{Z}{2a_p}\right)^3 \int_0^\infty dr \cdot r \left(\frac{Zr}{a_p}\right)^2 e^{-\frac{Zr}{a_p}} - \left(\frac{Z}{2a_p}\right)^3 \int_0^\infty dr \cdot r \left(\frac{Zr}{a_p}\right)^2 \left(2\left(\frac{Zr}{a_p}\right)^2 + 2\frac{Zr}{a_p} + 1\right) e^{-\frac{3Zr}{a_p}} \right] \\ &= \left[\text{changing variable} \right] = \frac{e^2 Z}{12\pi\epsilon_0 a_p} \left[\frac{1}{8} \int_0^\infty dt \cdot t^3 e^{-t} - \frac{1}{8} \cdot \frac{1}{3^4} \int_0^\infty dy \cdot y^3 \left(\frac{2}{9}y^2 + \frac{2}{3}y + 1\right) e^{-y} \right]\end{aligned}$$

as $\int_0^\infty dt \cdot t^n e^{-t} = n!$ so that:

$$\begin{aligned}\delta E_{2p}^{(1)} &= \frac{e^2 Z}{96\pi\epsilon_0 a_p} \left[3! - \frac{1}{3^4} \left(\frac{2}{9} 5! + \frac{2}{3} 4! + 3! \right) \right] = \frac{e^2 Z}{96\pi\epsilon_0 a_p} \cdot \left(6 - \frac{1}{81} \left(\frac{2}{3} 40 + 16 + 6 \right) \right) = \\ &= \frac{41}{72} \frac{e^2 Z}{\pi\epsilon_0 a_p} \Rightarrow \boxed{\delta E_{2p}^{(1)} = \frac{41}{72} \frac{e^2 Z}{\pi\epsilon_0 a_p}}\end{aligned}$$