1. Consider the isotropic 3-dimensional harmonic oscillator which is described by the potential $V(r) = m\omega^2 r^2/2$. Using the separation of variables, find the eigenvalues and the corresponding eigenfunctions.

⇒ i) Hamiltonian

$$H = \frac{\vec{P}^2}{2m} + V(\vec{x})$$

$$= \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2) + \frac{1}{2}m\omega^2(x^2+y^2+z^2)$$

$$= \left(\frac{P_x^2}{2m} + \frac{1}{2}m\omega^2 x^2\right) + \left(\frac{P_y^2}{2m} + \frac{1}{2}m\omega^2 y^2\right) + \left(\frac{P_z^2}{2m} + \frac{1}{2}m\omega^2 z^2\right)$$

이때. 1-dimensional hamiltonian $H(x)$ 를 다음과 같이 정의하자.

$$H(x) = \frac{P_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 \rightarrow \left(\text{1-dimensional harmonic oscillator}\right)$$

$$\therefore H = H(x) + H(y) + H(z)$$

iii) 이제.. H의 separable eigenfunction 을

$\psi(x,y,z) = X(x)\,Y(y)\,Z(z)$ 라 하고..

ψ의 eigenvalue 를 $E = E_x + E_y + E_z$ 라 하자.

$$H\psi(x,y,z) = E\psi(x,y,z)$$

$$\downarrow$$

$$\left(H(x) + H(y) + H(z)\right) X(x)\,Y(y)\,Z(z)$$

$$= (E_x + E_y + E_z)\, X(x)\,Y(y)\,Z(z)$$

$\therefore$ $X(x)$, $Y(y)$, $Z(z)$ 가 다음 세 eigenvalue problem 을 만족하면.. ψ는 H의 separable solution 이다.

$$\begin{cases} H(x)\,X(x) = E_x X(x) \\ H(y)\,Y(y) = E_y Y(y) \\ H(z)\,Z(z) = E_y Z(z) \end{cases}$$

이때 우리는 $H(x)$ (or y, z) 가 1-dimensional harmonic oscillator 인 것을 알고 있으므로..
그 eigenfunction $X(x)$ (or y, z) 를 이미 잘 알고 있고 그 eigenvalue E_x (or y, z) 역시 잘 알고 있다.

n으로 quantized.

$$X_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)\, e^{-\xi^2/2}$$

where $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$

and $H_n(\xi)$ is the Hermite polynomial of degree n in ξ.

(y, z 도 마찬가지!)

$$\therefore \left.\begin{aligned} E_{n_x} &= \hbar\omega\left(n+\tfrac{1}{2}\right) \\ E_{m_y} &= \hbar\omega\left(m+\tfrac{1}{2}\right) \\ E_{l_z} &= \hbar\omega\left(l+\tfrac{1}{2}\right) \end{aligned}\right\} \rightarrow \underline{E_{nml} = \hbar\omega\left(n+m+l+\tfrac{3}{2}\right)}$$

$$\psi_{nml}(x,y,z) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} \frac{e^{-\frac{1}{2}\cdot\frac{m\omega}{\hbar}(x^2+y^2+z^2)}}{\sqrt{2^{n+m+l}\, n!\, m!\, l!}}$$

$$\times H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right) \cdot H_m\left(\sqrt{\frac{m\omega}{\hbar}}\,y\right) \cdot H_l\left(\sqrt{\frac{m\omega}{\hbar}}\,z\right)$$

2. Consider an anisotropic harmonic oscillator described by the potential

$$V(x,y,z) = \frac{1}{2} m\omega_1^2 (x^2+y^2) + \frac{1}{2} m\omega_2^2 z^2 .$$

(a) Find the eigenstates using rectangular coordinates. What are the degeneracies of the states, assuming ω_1 and ω_2 are incommensurate?

(Incommensurate means that the ratio of the two numbers cannot be expressed as a ratio of integers.)

⇒ i) 문제 1의 결과를 약간만 수정하면 된다

Eigenstates.

$$\psi_{nml}(x,y,z) = \left(\frac{m\omega_1}{\pi\hbar}\right)^{1/2} \left(\frac{m\omega_2}{\pi\hbar}\right)^{1/4} \cdot \frac{e^{-\frac{1}{2}\frac{m\omega_1}{\hbar}(x^2+y^2)}}{\sqrt{2^{n+m+l}\, n!\, m!\, l!}} \times e^{-\frac{1}{2}\frac{m\omega_2}{\hbar} z^2}$$

(n, m, l are non-negative integers.)

$$\times H_n\left(\sqrt{\frac{m\omega_1}{\hbar}}\, x\right) H_m\left(\sqrt{\frac{m\omega_1}{\hbar}}\, y\right) \cdot H_l\left(\sqrt{\frac{m\omega_2}{\hbar}}\, z\right) .$$

Eigenvalues

$$E_{nml} = \hbar\omega_1 (n+m+1) + \hbar\omega_2 \left(l + \frac{1}{2}\right) .$$

ii)

$$E_{nml} = \hbar\omega_1(n+m+1) + \hbar\omega_3\left(l+\frac{1}{2}\right)$$

l이 동일하기만 하면.. $(n+m)$이 같은 값을 가지면

degenerate states.

$\therefore$ $(n+m+1)$개의 degeneracy 존재.

(b) Can the energy eigenstates be eigenstates of L^2? or L_z? Explain in each case.

⇒ i) energy eigenstate, 즉 H의 eigenstate가 동시에 L^2과 L_z의 eigenstate가 되려면..

$$[H, L^2] = 0. \qquad [H, L_z] = 0$$

이면 된다.

ii)

$$H = \frac{1}{2}m\omega_1^2(x^2+y^2) + \frac{1}{2}m\omega_3^2 z^2.$$

그리고

$$L^2 = L_x^2 + L_y^2 + L_z^2.$$

$$L_z = xP_y - yP_x$$ 이다.

ii) 등장할 commutator를 미리 계산해두자.

$$[x, L_x] = [x, yP_z - zP_y] = 0$$

$$[x, L_y] = [x, zP_x - xP_z]$$

$$= z[x, P_x] = i\hbar z$$

$$[x, L_z] = [x, xP_y - yP_x] = -i\hbar y$$

$$[y, L_x] = [y, yP_z - zP_y]$$

$$= -z[y, P_y] = -i\hbar z.$$

$$[y, L_y] = [y, zP_x - xP_z] = 0.$$

$$[y, L_z] = [y, xP_y - yP_z]$$

$$= x[y, P_y] = i\hbar x.$$

$$[z, L_x] = [z, yP_z - zP_y] = i\hbar y$$

$$[z, L_y] = [z, zP_x - xP_z] = -i\hbar x.$$

$$[z, L_z] = 0.$$

정리

$[x, L_x] = 0.$	$[y, L_x] = -i\hbar z$	$[z, L_x] = i\hbar y$
$[x, L_y] = i\hbar z.$	$[y, L_y] = 0.$	$[z, L_y] = -i\hbar x$
$[x, L_z] = -i\hbar y$	$[y, L_z] = i\hbar x.$	$[z, L_z] = 0.$

iii)

$$[H, L^2] = \left[\frac{1}{2}m\omega_1^2(x^2+y^2) + \frac{1}{2}m\omega_2^2 z^2,\ L^2\right]$$

$$= \frac{1}{2}m\omega_1^2\left[x^2+y^2,\ L_x^2+L_y^2+L_z^2\right]$$

$$+\frac{1}{2}m\omega_2^2\left[z^2,\ L_x^2+L_y^2+L_z^2\right].$$

$$= \frac{1}{2}m\omega_1^2\left\{[x^2, L_y^2] + [x^2, L_z^2] + [y^2, L_x^2] + [y^2, L_z^2]\right\}$$

$$+\frac{1}{2}m\omega_2^2\left\{[z^2, L_x^2] + [z^2, L_y^2]\right\}.$$

- $[x^2, L_y^2] = [x^2, L_y]L_y + L_y[x^2, L_y]$

$$= [x, L_y]xL_y + x[x, L_y]L_y + L_y x[x, L_y] + L_y[x, L_y]x.$$

$$= i\hbar z x L_y + x\cdot i\hbar z\cdot L_y + L_y x\cdot i\hbar z + L_y\cdot i\hbar z x$$

$$= 2i\hbar\, xzL_y + 2i\hbar\, L_y xz.$$

$$= (2i\hbar)\left[xzL_y + L_y xz\right]$$

• $[x^2, L_z^2] = x^2 L_z^2 - L_z^2 x^2$

$$x^2 L_z^2 = x x L_z L_z$$
$$= x \{ L_z x + [x, L_z] \} L_z$$
$$= x L_z x L_z - i\hbar\, xy L_z$$
$$= L_z x x L_z - 2i\hbar\, xy L_z$$
$$= L_z^2 x^2 - 2i\hbar\, xy L_z - 2i\hbar\, L_z xy$$

$\therefore [x^2, L_z^2] = -(2i\hbar)[xy L_z + L_z xy]$.

• $[y^2, L_x^2] = y^2 L_x^2 - L_x^2 y^2$

$$y^2 L_x^2 = yy L_x L_x$$
$$= y \{ L_x y + [y, L_x] \} L_x$$
$$= y L_x y L_x - i\hbar\, yz L_x$$
$$= L_x^2 y^2 - 2i\hbar [yz L_x + L_x yz]$$

$\therefore [y^2, L_x^2] = -(2i\hbar)[yz L_x + L_x yz]$

• $[y^2, L_z^2] = y^2 L_z^2 - L_z^2 y^2$

$$y^2 L_z^2 = yy L_z L_z = y \{ L_z y + [y, L_z] \} L_z$$
$$= y L_z y L_z + i\hbar xy L_z$$

$\therefore [y^2, L_z^2] = (2i\hbar) \cdot [xy L_z + L_z xy]$.

$\cdot\ [z^2, L_x^2] = z^2 L_x^2$

$= z\{L_x z + [z, L_x]\}L_x$

$\therefore [z^2, L_x^2] = (2i\hbar)[zxL_x + L_x zx]$

$\cdot\ [z^2, L_y^2] = z\{L_y z + [z, L_y]\}L_y$

$= -(2i\hbar)[zxL_y + L_y zx]$

iv) $\therefore [H, L^2] = \frac{1}{2}m\omega_1^2 \{(2i\hbar)[xzL_y + L_y xz]$

$\cancel{-(2i\hbar)[xyL_z + L_z xy]}$

$-(2i\hbar)[yzL_x + L_x yz]$

$\cancel{+(2i\hbar)[xyL_z + L_z xy]}\}$

$+\frac{1}{2}m\omega_2^2\{(2i\hbar)[zxL_x + L_x zx]$

$-(2i\hbar)[zxL_y + L_y zx]\}$

$\neq 0$.

$\therefore$ energy eigenstate는 L^2의 eigenstate X.

($\omega_1 = \omega_2$ 일때는.. $[H, L^2] = 0$)

c) $[H, L_z] = \frac{1}{2} m\omega_1^2 [x^2+y^2, L_z]$

$$+ \cancel{\frac{1}{2} m\omega_2^2 [z^2, L_z]} \to 0$$

$$= \frac{1}{2} m\omega_1^2 \{ x[x, L_z] + [x, L_z]x + y[y, L_z] + [y, L_z]y \}.$$

$$= \frac{1}{2} m\omega_1^2 \{ x\cdot(-i\hbar y) + (-i\hbar y)\cdot x + y\cdot(i\hbar x) + (i\hbar x)\cdot y \} = 0.$$

$\therefore$ energy eigenstate는 L_z의 eigenstate 가능

($\omega_2 \neq \omega_1$ 일때도)

3. A particle in a spherically symmetric potential is described by the wave function

$$\psi(x, y, z) = C\,(xy + yz + zx)\,e^{-\alpha r^2}.$$

(a) Express ψ in terms of the spherical harmonics.

$\Rightarrow$ i) spherical coordinate 에서.

$x = r\sin\theta\cos\phi.$

$y = r\sin\theta\sin\phi.$

$z = r\cos\theta.$

$$\therefore \psi(r, \theta, \phi) = C r^2 \underbrace{\Big(\sin^2\theta\cos\phi\sin\phi + \sin\theta\cos\theta\sin\phi + \sin\theta\cos\theta\cos\phi \Big)}_{:= \text{A}} e^{-\alpha r^2}$$

- $\sin^2\theta \cdot \dfrac{e^{i\phi} + e^{-i\phi}}{2} \quad \dfrac{e^{i\phi} - e^{-i\phi}}{2i}$

$$= \frac{1}{4i} \cdot \sin^2\theta \cdot \left(e^{i2\phi} - e^{-i2\phi}\right)$$

- $\sin\theta\cos\theta \cdot \dfrac{e^{i\phi} - e^{-i\phi}}{2i}$

$$= \frac{1}{2i} \sin\theta\cos\theta \left(e^{i\phi} - e^{-i\phi}\right)$$

$$\cdot \ \sin\theta\cos\theta \ \frac{e^{i\phi}+e^{-i\phi}}{2}$$

$$= \frac{1}{2}\sin\theta\cos\theta\left(e^{i\phi}+e^{-i\phi}\right)$$

$$A = -\frac{i}{4}\sin^2\theta\left(e^{i2\phi}-e^{-i2\phi}\right)$$

$$-\frac{i}{2}\sin\theta\cos\theta\left(e^{i\phi}-e^{-i\phi}\right)$$

$$+\frac{1}{2}\sin\theta\cos\theta\left(e^{i\phi}+e^{-i\phi}\right)$$

$$= -\frac{i}{4}\sin^2\theta\, e^{i2\phi} - \frac{i}{4}\sin^2\theta\, e^{-i2\phi}$$

$$+\frac{1-i}{2}\cdot\sin\theta\cos\theta\, e^{i\phi}$$

$$+\frac{1+i}{2}\sin\theta\cos\theta\, e^{-i\phi}$$

٢٩)

$$Y_{22}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{i2\phi}$$

$$Y_{21}(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_{2-1}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\, e^{-i\phi}$$

$$Y_{2-2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{-i2\phi}$$

iii)

$$\therefore A = -\frac{i}{4}\cdot 4\cdot\sqrt{\frac{2\pi}{15}}\cdot Y_{22}(\theta,\phi)$$

$$-\frac{i}{4}\cdot 4\cdot\sqrt{\frac{2\pi}{15}}\ Y_{2-2}(\theta,\phi)$$

$$+\frac{1-i}{2}\cdot(-2)\cdot\sqrt{\frac{2\pi}{15}}\ Y_{21}(\theta,\phi)$$

$$+\frac{1+i}{2}\cdot 2\sqrt{\frac{2\pi}{15}}\ Y_{2-1}(\theta,\phi)$$

$$=\sqrt{\frac{2\pi}{15}}\Big[-i\,Y_{22}(\theta,\phi)-i\,Y_{2-2}(\theta,\phi)$$

$$-(1-i)\,Y_{21}(\theta,\phi)+(1+i)\,Y_{2-1}(\theta,\phi)\Big].$$

iv) $$\psi(r,\theta,\phi)=C\cdot r^2 e^{-\alpha r^2}\cdot\sqrt{\frac{2\pi}{15}}$$

$$\times\Big[-i\,Y_{22}(\theta,\phi)-i\,Y_{2-2}(\theta,\phi)$$

$$-(1-i)\,Y_{21}(\theta,\phi)+(1+i)\,Y_{2-1}(\theta,\phi)\Big].$$

(b) Find the probabilities to have $l = 0, 1, 2$, respectively.

⇒ i) (a) 에서 구한 $\psi(r, \theta, \phi)$ 를 보면..

$l = 2$ 인 spherical harmonics 밖에 없다.

∴ $\underline{l = 2 \text{ 일 확률 } 1.}$ // (나머지는 0).

(c) If l is found to be $l = 2$, find the probabilities with $m = \pm 2, \pm 1, 0$.

⇒. i) $Y_{lm}(\theta, \phi)$는 다음과 같이 normalize 되어 있다.

$$\int d\Omega \, Y_{l'm'}^{*}(\theta, \phi) \, Y_{lm}(\theta, \phi)$$

$$= \frac{4\pi}{(2l+1)} \delta_{ll'} \delta_{mm'}.$$

이때 $\psi(r, \theta, \phi)$는 $l = 2$ 인 state 들로 이루어져 있으므로.. normalization 이 모두 동일하다.

ii)

m=2 인 확률 $= \dfrac{|-i|^2}{|-i|^2 + |-i|^2 + |1-i|^2 + |1+i|^2}$

$= \dfrac{1}{1+1+2+2} = \dfrac{1}{6}.$

m=1 인 확률 $= \dfrac{|1-i|^2}{|-i|^2 + |-i|^2 + |1-i|^2 + |1+i|^2}$

$= \dfrac{2}{6} = \dfrac{1}{3}.$

m=0 인 확률 $= 0.$

m=-1 인 확률 $= \dfrac{2}{6} = \dfrac{1}{3}.$

m=-2 인 확률 $= \dfrac{1}{6}$

4. Consider a three-dimensional problem in which the potential has the very specific form

$$V(\vec{r}) = V_1(x) + V_2(y) + V_3(z).$$

(a) Write down the time-independent Schrödinger equation in one-dimensional form using separation of variables.

⇒ i) 1번 문제에서 한 것처럼.. H의 eigenfunction 을

$\psi(x, y, z) \equiv X(x)\, Y(y)\, Z(z)$ 라고 하면.. (그리고 그 eigenvalue $E = E_1 + E_2 + E_3$)

X, Y, Z 는 다음의 1-dimensional Schrödinger equation을 각각 만족한다.

$$\left[\frac{P_x^2}{2m} + V_1(x)\right] X(x) = E_1\, X(x)$$

$$\left[\frac{P_y^2}{2m} + V_2(y)\right] Y(y) = E_2\, Y(y)$$

$$\left[\frac{P_z^2}{2m} + V_3(z)\right] Z(z) = E_3\, Z(z)$$

이때.. ψ 의 eigenvalue $E = E_1 + E_2 + E_3$

(b) Consider the states in a rectangular box of sides L_1, L_2, and L_3 respectively. The origin is at one corner of the box. The wave function ψ_E should vanish at each of the walls. Obtain the energy eigenvalues and the corresponding eigenfunctions.

⇒. i) (a) 에서 봤듯이... X, Y, Z 는 각각 1-dimensional Schrödinger equation을 만족하고.. 각각이 particle in the box 문제이다. $(a, b, c = 1, 2, 3, \cdots)$

$$\therefore X_a(x) = \sqrt{\frac{2}{L_1}} \sin\left(\frac{a\pi}{L_1} x\right) \rightarrow E_1 = \frac{\pi^2 \hbar^2}{2mL_1^2} a^2$$

$$Y_b(y) = \sqrt{\frac{2}{L_2}} \sin\left(\frac{b\pi}{L_2} y\right) \rightarrow E_2 = \frac{\pi^2 \hbar^2}{2mL_2^2} b^2$$

$$Z_c(z) = \sqrt{\frac{2}{L_3}} \sin\left(\frac{c\pi}{L_3} z\right) \rightarrow E_3 = \frac{\pi^2 \hbar^2}{2mL_3^2} c^2$$

ii)

$$\therefore \psi_{abc}(x, y, z) = \sqrt{\frac{8}{L_1 L_2 L_3}} \sin\left(\frac{a\pi}{L_1} x\right) \sin\left(\frac{b\pi}{L_2} y\right) \sin\left(\frac{c\pi}{L_3} z\right)$$

where $E_{abc} = \frac{\pi^2 \hbar^2}{2m}\left(\frac{a^2}{L_1^2} + \frac{b^2}{L_2^2} + \frac{c^2}{L_3^2}\right)$.

$(a, b, c = 1, 2, 3, \cdots)$

(c) For the same problem as in (b), take the periodic boundary conditions. That is, ψ_E assumes the same value on any pair of opposite walls of the box. Obtain the energy eigenvalues and the corresponding eigenfunctions.

⇒ i) (b)에서와 같은 방법을 사용하면.. (a.b.c are integers.)

$$X_a(x) = \sqrt{\frac{1}{L_1}} \cdot \exp\left(i \cdot \frac{2\pi a}{L_1} x\right) \rightarrow E_1 = \frac{\hbar^2}{2m}\left(\frac{2\pi a}{L_1}\right)^2$$

$$Y_b(y) = \sqrt{\frac{1}{L_2}} \exp\left(i \frac{2\pi b}{L_2} y\right) \rightarrow E_2 = \frac{\hbar^2}{2m}\left(\frac{2\pi b}{L_2}\right)^2$$

$$Z_c(z) = \sqrt{\frac{1}{L_3}} \exp\left(i \frac{2\pi c}{L_3} z\right) \rightarrow E_3 = \frac{\hbar^2}{2m}\left(\frac{2\pi c}{L_3}\right)^2$$

ii)

$$\therefore \psi_{abc}(x,y,z) = \sqrt{\frac{1}{L_1 L_2 L_3}} \exp\left[i 2\pi \left(\frac{ax}{L_1} + \frac{by}{L_2} + \frac{cz}{L_3}\right)\right]$$

where $E_{abc} = \frac{4\pi^2\hbar^2}{2m}\left(\frac{a^2}{L_1^2} + \frac{b^2}{L_2^2} + \frac{c^2}{L_3^2}\right)$.

(a.b.c = integers.)

(d) For the problem in (c), compute the total number of states $N(E)$ of energy less than or equal to E. And obtain the density of states $\rho(E)$ defined as $\rho(E) = dN/dE$.

→ i)

$$E = E_1 + E_2 + E_3$$

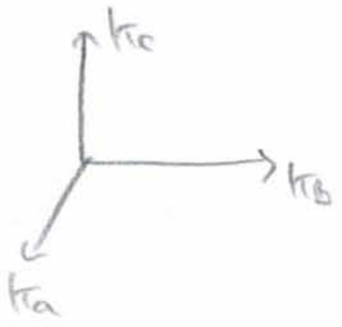
$$= \frac{\hbar^2}{2m}\left(\frac{2\pi a}{L_1}\right)^2 + \frac{\hbar^2}{2m}\left(\frac{2\pi b}{L_2}\right)^2 + \frac{\hbar^2}{2m}\left(\frac{2\pi c}{L_3}\right)^2.$$

↓

$$\frac{2mE}{\hbar^2} = k_a^2 + k_b^2 + k_c^2.$$

where $k_a = \frac{2\pi a}{L_1}$, $k_b = \frac{2\pi b}{L_2}$, $k_c = \frac{2\pi c}{L_3}$.

일단 a, b, c 가 정수이므로.. 다음 k-space 상에서..



부피 $\left(\frac{2\pi}{L_1}\right)\cdot\left(\frac{2\pi}{L_2}\right)\cdot\left(\frac{2\pi}{L_3}\right)$ 당 하나의 state 존재.

$\therefore \frac{(2\pi)^3}{L_1 L_2 L_3}$ 당 1개의 state

m

ii) 그런데 에너지가 E 보다 작은 state를 span 하는 k-space 상 부피는 .. $\frac{4\pi}{3}\cdot\left(\frac{2mE}{\hbar^2}\right)^{3/2}$ 이다.

$$= \frac{4\pi}{3\hbar^3}\cdot\left(\sqrt{2mE}\right)^3.$$

$$\therefore N(E) = \frac{\frac{4\pi}{3\hbar^3}\cdot\left(\sqrt{2mE}\right)^3}{\frac{(2\pi)^3}{L_1L_2L_3}} = \frac{L_1L_2L_3(2m)^{3/2}\cdot E^{3/2}}{6\pi^2\hbar^3}$$

$$= \frac{L_1L_2L_3}{6\pi^2}\cdot\left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

iii) $\therefore \rho(E) = \frac{dN}{dE} = \frac{L_1L_2L_3}{6\pi^2}\cdot\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{3}{2}\cdot E^{1/2}.$

$$= \frac{L_1L_2L_3}{4\pi^2}\cdot\left(\frac{2m}{\hbar^2}\right)^{3/2}\cdot\sqrt{E}.$$

5. An electron in the Coulomb field of a proton is in the following state of coherent superposition of hydrogenic states:

$$\frac{1}{3}\left[\psi_{100} + \sqrt{3}\,\psi_{210} - \sqrt{5}\,\psi_{320}\right].$$

Calculate the expectation values of energy, $\vec{L}^2$, and L_z for this state.

⇒ i) 우리에게 주어진 state를 $|\alpha\rangle$ 라고 하고..

$\psi_{100} \rightarrow |100\rangle$

$\psi_{210} \rightarrow |210\rangle$

$\psi_{320} \rightarrow |320\rangle$ 이라 하자.

$$\therefore |\alpha\rangle = \frac{1}{3}\left[|100\rangle + \sqrt{3}\,|210\rangle - \sqrt{5}\,|320\rangle\right]$$

이때.. $|100\rangle$, $|210\rangle$, $|320\rangle$ 은 L^2 과 L_z 의 eigenstate 들이다.

$$\begin{cases} \vec{L}^2|n\,l\,m\rangle = \hbar^2 l(l+1)\,|n\,l\,m\rangle \\ L_z|n\,l\,m\rangle = \hbar m\,|n\,l\,m\rangle \end{cases}$$

ii) $\langle \vec{L}^2 \rangle = \langle \alpha | \vec{L}^2 | \alpha \rangle$

$$= \frac{1}{9}\Big[\hbar^2 0(0+1) \langle 100|100 \rangle$$

$$+ \hbar^2 1.(1+1).3 \langle 210|210 \rangle$$

$$+ \hbar^2 2.(2+1).5 \langle 320|320 \rangle \Big]$$

$$= \frac{1}{9}.\left[6\hbar^2 + 30\hbar^2 \right]$$

$$= 4\hbar^2$$

$\langle L_z \rangle = \langle \alpha | L_z | \alpha \rangle$

$$= \frac{1}{9}\Big[\hbar.0 \langle 100|100 \rangle$$

$$+ \hbar.0.3 \langle 210|210 \rangle$$

$$+ \hbar.0.5 \langle 320|320 \rangle \Big] = 0.$$

v

iii) 여기 energy expectation value 를 구하자.

ψ_{100}, ψ_{210}, ψ_{320} 은 역시 H의 eigenstate

이고 그 quantum number 는 각각 1, 2, 3 이다.

energy quantum number 가 n인 경우.. 그 에너지는

$$E_n = -\frac{1}{2}\mu c^2 \frac{(Z\alpha)^2}{n^2}$$ 이다.

$$\therefore \langle E \rangle = \langle \alpha | H | \alpha \rangle$$

$$= \frac{1}{9}\Big[-\frac{1}{2}\mu c^2 \cdot \frac{(Z\alpha)^2}{1^2} \cdot 1$$

$$-\frac{1}{2}\mu c^2 \cdot \frac{(Z\alpha)^2}{2^2} \cdot 3$$

$$-\frac{1}{2}\mu c^2 \cdot \frac{(Z\alpha)^2}{3^2} \cdot 5 \Big]$$

$$= -\frac{1}{2}\mu c^2 (Z\alpha)^2 \left[\frac{1}{9} + \frac{1}{9}\cdot\frac{3}{4} + \frac{1}{9}\cdot\frac{5}{9} \right]$$

$$= -\frac{1}{2}\mu c^2 (Z\alpha)^2 \, \frac{36+27+20}{324}$$

$$= -\frac{1}{2}\mu c^2 (Z\alpha)^2 \cdot \frac{83}{324}$$

6. (a) Find the momentum-space wave function for an electron in the hydrogenic ground state.

⇒ i) the hydrogenic ground state.

$$\psi_{nlm}(\vec{r}) \rightarrow \psi_{100}(\vec{r}) = R_{10}(r)\, Y_{00}(\theta, \phi)$$

$$= 2 \cdot \left(\frac{Z}{a_0}\right)^{3/2} \cdot e^{-Zr/a_0} \cdot \frac{1}{\sqrt{4\pi}}.$$

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

where $$H = \frac{\vec{p}^2}{2\mu} - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

(where μ is the reduced mass.

and Ze is the charge of the nucleus.)

and.. $$a_0 = \frac{\hbar}{\mu c \alpha}$$ (and α = fine structure constant.) $\simeq \frac{1}{137}$.

ii) $$\psi_{100}(\vec{x}) = \langle \vec{x} | \psi_{100} \rangle.$$

Note that..

$$|\psi_{100}\rangle = \int d^3x \; |\vec{x}\rangle\langle\vec{x}|\psi_{100}\rangle$$

∴ The momentum space wave function

$$\rightarrow \langle \vec{p} | \psi_{100} \rangle = \int d^3x \; \langle \vec{p} | \vec{x} \rangle \langle \vec{x} | \psi_{100} \rangle.$$

iii) If we adopt the following normalization conditions for $|\vec{x}\rangle$ and $|\vec{p}\rangle$:

$$\langle \vec{x}' | \vec{x} \rangle = \delta^3 (\vec{x} - \vec{x}')$$
$$\langle \vec{p}' | \vec{p} \rangle = \delta^3 (\vec{p} - \vec{p}'),$$

then..

$$\langle \vec{p}' | \vec{p} \rangle = \int d^3x \, \langle \vec{p}' | \vec{x} \rangle \langle \vec{x} | \vec{p} \rangle$$
$$= \int d^3x \, \langle \vec{x} | \vec{p}' \rangle^* \langle \vec{x} | \vec{p} \rangle$$
$$= \delta^3 (\vec{p} - \vec{p}')$$
$$= \frac{1}{(2\pi\hbar)^3} \int d^3x \, \exp\left[i \frac{(\vec{p} - \vec{p}')}{\hbar} \cdot \vec{x} \right]$$
$$= \int d^3x \, \frac{1}{(2\pi\hbar)^{3/2}} \exp\left[-i \frac{\vec{p}' \cdot \vec{x}}{\hbar} \right]$$
$$\times \frac{1}{(2\pi\hbar)^{3/2}} \exp\left[+i \frac{\vec{p} \cdot \vec{x}}{\hbar} \right]$$

$$\therefore \langle \vec{x} | \vec{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} \exp\left[+i \frac{\vec{p} \cdot \vec{x}}{\hbar} \right]$$

iv)

$$\langle \vec{p} | \psi_{100} \rangle = \int d^3x \cdot \langle \vec{p} | \vec{x} \rangle \langle \vec{x} | \psi_{100} \rangle$$

$$= \int d^3x \; \langle \vec{x} | \vec{p} \rangle^* \; \langle \vec{x} | \psi_{100} \rangle$$

$$= \int d^3x \cdot \frac{1}{(2\pi\hbar)^{3/2}} \cdot \exp\left[i \frac{\vec{p} \cdot \vec{x}}{\hbar} \right] \cdot \frac{1}{\sqrt{\pi}} \cdot \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}$$

$$= \frac{1}{\sqrt{\pi}} \cdot \left(\frac{Z}{2\pi\hbar a_0} \right)^{3/2} \cdot \underbrace{\int d^3x \cdot \exp\left[i \frac{pr\cos\theta}{\hbar} \right] e^{-Zr/a_0}}_{A}$$

where $p = |\vec{p}|$ and $r = |\vec{x}|$ and..

θ is the angle between $\vec{p}$ and $\vec{x}$.

v)

$$A = \int \underbrace{d^3x}_{\left(\begin{array}{l} dr \cdot r d\theta \cdot r\sin\theta \, d\phi \\ = r^2 \, dr \, d(\cos\theta) \, d\phi \end{array} \right)} \exp\left[i \frac{pr\cos\theta}{\hbar} \right] e^{-Zr/a_0}$$

$$= \underbrace{2\pi}_{d\phi \text{ integration}} \cdot \int dr \cdot r^2 e^{-Zr/a_0} \cdot \int_{-1}^{1} d(\cos\theta) \cdot \exp\left[i \frac{pr}{\hbar} \cos\theta \right]$$

(P)
$$\int_{-1}^{1} d(\cos\theta)\ \exp\left[i\frac{pr}{\hbar}\cos\theta\right]$$

$$= \frac{1}{i\frac{pr}{\hbar}}\cdot\left(\exp\left[i\frac{pr}{\hbar}\right] - \exp\left[-i\frac{pr}{\hbar}\right]\right)$$

$$\therefore \text{Ⓐ} = 2\pi\cdot\int_0^\infty dr\cdot r^2 e^{-Zr/a_0}\cdot\frac{1}{i\frac{pr}{\hbar}}\left(\exp\left[i\frac{pr}{\hbar}\right] - \exp\left[-\frac{ipr}{\hbar}\right]\right)$$

$$= -\frac{2\pi i\hbar}{p}\cdot\int_0^\infty dr\cdot\left\{r\ \exp\left[-\left(\frac{Z}{a_0} - i\frac{p}{\hbar}\right)r\right] - r\ \exp\left[-\left(\frac{Z}{a_0} + i\frac{p}{\hbar}\right)r\right]\right\}.$$

$$\int_0^\infty dr\ e^{-\alpha r} = \frac{1}{\alpha}$$

$$\int_0^\infty dr\cdot r e^{-\alpha r} = \frac{\partial}{\partial(-\alpha)}\left(\frac{1}{\alpha}\right) = \frac{1}{\alpha^2}$$

$$= -\frac{2\pi i\hbar}{p}\cdot\left[\frac{1}{\left(\frac{Z}{a_0} - i\frac{p}{\hbar}\right)^2} - \frac{1}{\left(\frac{Z}{a_0} + i\frac{p}{\hbar}\right)^2}\right]$$

$$\therefore \text{Ⓐ} = -\frac{2\pi i\hbar}{p}\cdot\frac{\left(\frac{Z}{a_0}+i\frac{p}{\hbar}\right)^2-\left(\frac{Z}{a_0}-i\frac{p}{\hbar}\right)^2}{\left[\left(\frac{Z}{a_0}-i\frac{p}{\hbar}\right)\left(\frac{Z}{a_0}+i\frac{p}{\hbar}\right)\right]^2}$$

$$= -\frac{2\pi i\hbar}{p}\cdot\frac{4i\cdot\frac{Z}{a_0}\cdot\frac{p}{\hbar}}{\left[\left(\frac{Z}{a_0}\right)^2+\left(\frac{p}{\hbar}\right)^2\right]^2}$$

$$= +\frac{8\pi\cancel{\hbar}}{\cancel{p}}\cdot\frac{Z}{a_0}\cdot\frac{\cancel{p}}{\cancel{\hbar}}\cdot\frac{1}{\left[\left(\frac{Z}{a_0}\right)^2+\left(\frac{p}{\hbar}\right)^2\right]^2}$$

$$= +\frac{8\pi Z}{a_0}\cdot\frac{1}{\left[\left(\frac{Z}{a_0}\right)^2+\left(\frac{p}{\hbar}\right)^2\right]^2}$$

(UPP)

$$\langle\vec{p}|\psi_{100}\rangle = \frac{1}{\sqrt{\pi}}\cdot\left(\frac{Z}{2\pi\hbar a_0}\right)^{3/2}\frac{8\pi Z}{a_0}\cdot\frac{1}{\left[\left(\frac{Z}{a_0}\right)^2+\left(\frac{p}{\hbar}\right)^2\right]^2}$$

$$= \frac{Z^{5/2}\cdot 8\pi}{\pi^2\; 2^{3/2}\cdot\hbar^{3/2}\; a_0^{5/2}}\cdot\frac{1}{\left[\left(\frac{Z}{a_0}\right)^2+\left(\frac{p}{\hbar}\right)^2\right]^2}$$

$$= \frac{2\sqrt{2}}{\pi}\cdot\frac{Z^{5/2}}{\hbar^{3/2}\; a_0^{5/2}}\;\frac{1}{\left[\left(\frac{Z}{a_0}\right)^2+\left(\frac{p}{\hbar}\right)^2\right]^2}$$

$$= \frac{2\sqrt{2}}{\pi}\left(\frac{Z}{\hbar a_0}\right)^{3/2}\frac{\frac{Z}{a_0}}{\left[\left(\frac{Z}{a_0}\right)^2+\left(\frac{p}{\hbar}\right)^2\right]^2}$$

(b) Using this wave function, calculate $\langle p^2 \rangle$ in the ground state of hydrogen.

$\Rightarrow$ i) $\langle p^2 \rangle = \langle \psi_{100} | p^2 | \psi_{100} \rangle$

$$= \int d^3p \, \langle \psi_{100} | \vec{p} \rangle \, p^2 \, \langle \vec{p} | \psi_{100} \rangle$$

$$= \int d^3p \, p^2 \, \underbrace{|\langle \vec{p} | \psi_{100} \rangle|^2}_{\text{no angle dependence.}}$$

$$= 4\pi \cdot \int_0^\infty dp \cdot p^2 \cdot p^2 \, \frac{8}{\pi^2} \left(\frac{Z}{\hbar a_0} \right)^3 \frac{\left(\frac{Z}{a_0}\right)^2}{\left[\left(\frac{Z}{a_0}\right)^2 + \left(\frac{p}{\hbar}\right)^2 \right]^4}$$

$$= 4\pi \cdot \frac{8}{\pi^2} \left(\frac{Z}{a_0} \right)^5 \cdot \frac{1}{\hbar^3}$$

$$\times \underbrace{\int_0^\infty dp \, p^4 \cdot \frac{1}{\left[\left(\frac{Z}{a_0}\right)^2 + \left(\frac{p}{\hbar}\right)^2 \right]^4}}_{B}$$

ii) $$Ⓑ = \hbar^5 \cdot \int_0^\infty d\left(\frac{p}{\hbar}\right) \left(\frac{p}{\hbar}\right)^4 \cdot \frac{1}{\left[\left(\frac{Z}{a_0}\right)^2 + \left(\frac{p}{\hbar}\right)^2\right]^4}$$

$$= \hbar^5 \cdot \int_0^\infty dx \; x^4 \cdot \frac{1}{\left[\left(\frac{Z}{a_0}\right)^2 + x^2\right]^4}$$

$$= \hbar^5 \cdot \int_0^\infty dx \; x^4 \cdot \frac{1}{\left(\frac{Z}{a_0}\right)^8 \left[1 + \left(\frac{a_0 x}{Z}\right)^2\right]^4}$$

$$= \hbar^5 \cdot \frac{\left(\frac{Z}{a_0}\right)^5}{\left(\frac{Z}{a_0}\right)^8} \int_0^\infty dy \; y^4 \cdot \frac{1}{(y^2+1)^4}$$

$$= \frac{\hbar^5 \cdot a_0^3}{Z^3} \int_0^\infty dy \; y^4 \cdot \frac{1}{(y^2+1)^4}$$

$$\left(\begin{array}{ll} y = \tan\theta & 0 < \theta < \pi/2. \\ dy = \sec^2\theta \, d\theta & \\ 1 + y^2 = \sec^2\theta. & \end{array}\right)$$

$$= \frac{\hbar^5 a_0^3}{Z^3} \cdot \int_0^{\pi/2} d\theta \; \sec^2\theta \cdot \tan^4\theta \cdot \frac{1}{\sec^8\theta}$$

$$= \frac{\hbar^5 a_0^3}{Z^3} \cdot \underbrace{\int_0^{\pi/2} d\theta \cdot \cos^6\theta \cdot \frac{\sin^4\theta}{\cos^4\theta}}_{Ⓒ}$$

iii) $\textcircled{C} = \int_0^{\pi/2} d\theta \cdot \cos^2\theta \overbrace{\sin^4\theta}^{(1-\cos^2\theta)^2}$

$$= \int_0^{\pi/2} d\theta \; \cos^2\theta \sin^4\theta$$

$$= \int_0^{\pi/2} d\theta \; \cos^2\theta \, (1-\cos^2\theta)^2$$

$$= \int_0^{\pi/2} d\theta \left(\cos^2\theta - 2\cos^4\theta + \cos^6\theta \right)$$

$$\left(\begin{aligned} &\int_0^{\pi/2} d\theta \cos^2\theta = \frac{\pi}{4} \\ &\int_0^{\pi/2} d\theta \cos^4\theta = \frac{3\pi}{16} \\ &\int_0^{\pi/2} d\theta \cos^6\theta = \frac{5\pi}{32} \end{aligned} \right.$$

$$= \left[\frac{\pi}{4} - \frac{3\pi}{8} + \frac{5\pi}{32} \right]$$

$$= \pi \frac{8-12+5}{32} = \frac{\pi}{32}$$

$$\therefore \textcircled{B} = \frac{\hbar^5 a_0^3}{Z^3} \cdot \frac{\pi}{32}$$

iv) $\therefore \langle p^2 \rangle = \frac{32}{\pi} \cdot \frac{Z^5}{a_0^5} \cdot \frac{1}{\hbar^3} \, \frac{\hbar^5 a_0^3}{Z^3} \, \frac{\pi}{32} = \left(\frac{Z\hbar}{a_0} \right)^2$