FISIKA KUANTIKOA:

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6. ariketa orria:

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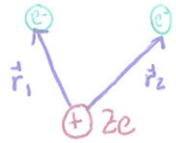
2)

He atomoaren hamiltondarra: $$H = \overbrace{-\frac{\hbar^2}{2m_e}\nabla^2_{\vec r_1} - \frac{Ze^2}{4\pi\varepsilon_0 r_1}}^{H_{01}} \overbrace{-\frac{\hbar^2}{2m_e}\nabla^2_{\vec r_2} - \frac{Ze^2}{4\pi\varepsilon_0 r_2}}^{H_{02}} + \overbrace{\frac{e^2}{4\pi\varepsilon_0 |\vec r_1 - \vec r_2|}}^{W}$$



- $\psi(\vec r_1, \vec r_2) = \psi_{n_1 l_1 m_{l_1}}(\vec r_1)\, \psi_{n_2 l_2 m_{l_2}}(\vec r_2)$ $W = 0$ balitz,

  $H_0 = H_{01} + H_{02}$-ren autofuntzioa.

"trial wave-function"

- $\psi_{\tilde Z}(r_1, r_2) = \frac{1}{\pi}\left(\frac{\tilde Z}{a_0}\right)^3 e^{-\tilde Z (r_1 + r_2)/a_0}$ (Metodo bariazionala aplikatzeko proba uhin-funtzioa)

$\psi_{\tilde Z}$-k ψ_{100}-ren itxura

- $\langle H \rangle_{\tilde Z} = \langle \psi_{\tilde Z} | H | \psi_{\tilde Z} \rangle = \langle H_0^1 \rangle_{\tilde Z} + \langle H_0^2 \rangle_{\tilde Z} + \left\langle \frac{e^2}{4\pi\varepsilon_0 |\vec r_1 - \vec r_2|} \right\rangle_{\tilde Z} =$

$\langle T \rangle$ Z-ren indep.

$|100\rangle, |100\rangle$

$$\langle 100 | H_0^1 | 100 \rangle_{\tilde Z} + \langle 100 | H_0^2 | 100 \rangle_{\tilde Z} + \left\langle \frac{e^2}{4\pi\varepsilon_0 |\vec r_1 - \vec r_2|} \right\rangle_{\tilde Z} = (\tilde Z^2 E_I - 2 Z \tilde Z E_I) \cdot 2 +$$

bikoitza, uniala

$$\left\langle \frac{e^2}{4\pi\varepsilon_0 |\vec r_1 - \vec r_2|} \right\rangle_{\tilde Z} = -\tilde Z E_I (2(2Z - \tilde Z) - 5/4) \quad *'$$

$$\hookrightarrow \frac{\partial \langle H \rangle_{\tilde Z}}{\partial \tilde Z} = 0 \rightarrow \tilde Z_0 = \frac{27}{16} = 1'69 < Z = 2 \rightarrow \langle H \rangle_m = -77'5 \text{ eV}$$

$$*' \quad \frac{e}{4\pi\varepsilon_0} \cdot \frac{1}{\pi^2} \left(\frac{\tilde Z}{a_0}\right)^6 \left(\frac{a_0}{\tilde Z}\right)^5 \frac{1}{2} \underbrace{\int d\vec r_1 \int d\vec r_2 \frac{e^{-(r_1 + r_2)}}{|\vec r_1 - \vec r_2|}}_{\text{Taulatan}} = \frac{e}{4\pi\varepsilon_0} \cdot \frac{1}{\pi^2} \left(\frac{\tilde Z}{a_0}\right)^6 \cancel{\left(\frac{a_0}{\tilde Z}\right)^5} \frac{1}{2}\, 5/4 \cdot (4\pi)^2$$

(Spinik gabe)

1)

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 x^2, \qquad \langle x | \psi_\alpha \rangle = \psi_\alpha(x) = e^{-\alpha x^2}$$

- Normalizatu ⇒ $\langle \psi_\alpha | \psi_\alpha \rangle = \int_{-\infty}^{\infty} dx\, |\psi_\alpha(x)|^2 = \int_{-\infty}^{\infty} e^{-2\alpha x^2} A^2\, dx = 1$ (1)

- $\langle H \rangle_\psi$ ⇒ $\langle \psi | H | \psi \rangle = \langle H \rangle_\psi = \int_{-\infty}^{\infty} A^2 dx\, \psi_\alpha^*(x)\, \hat H \psi_\alpha(x) = \int_{-\infty}^{\infty} A^2 dx\, \psi_\alpha^*(x) \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 x^2\right) \psi_\alpha(x)$

$$A^2 \int_{-\infty}^{\infty} dx\, \psi_\alpha^*(x) \left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_\alpha}{\partial x^2} + \frac{1}{2} m\omega^2 x^2 \psi_\alpha\right) = A^2 \int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} \left(-\frac{\hbar^2}{2m} e^{-\alpha x^2}\, 2\alpha(2\alpha x^2 - 1) + \frac{1}{2} m\omega^2 x^2 e^{-\alpha x^2}\right) =$$

*

$$A^2\int_{-\infty}^{\infty} e^{-2\alpha x^2} dx \left(\frac{\alpha\hbar^2}{2m}(1-2\alpha x^2)+\frac{1}{2}m\omega^2x^2\right) = A^2\int_{-\infty}^{\infty} e^{-2\alpha x^2}\left(\frac{\hbar^2}{2m}+x^2\left(\frac{1}{2}m\omega^2-\frac{\hbar^2\alpha}{m}\right)\right)dx \overset{*^2}{=} A^2\int_{-\infty}^{\infty} e^{-2\alpha x^2}\frac{\hbar^2\alpha}{m} +$$

$$A^2\left(\frac{1}{2}m\omega^2-\frac{2\hbar^2\alpha^2}{m}\right)\cdot\frac{1}{4\alpha}\int_{-\infty}^{\infty}e^{-2\alpha x^2}dx \underset{(1)}{=} \frac{\hbar^2\alpha}{m}+\frac{1}{4\alpha}\left(\frac{1}{2}m\omega^2-\frac{2\hbar^2\alpha^2}{m}\right) = \boxed{\frac{\hbar^2\alpha}{2m}+\frac{1}{8}m\omega^2\cdot\frac{1}{\alpha}}$$

$*^1$ $$\frac{\partial^2}{\partial x^2}(\psi_\alpha(x)) = \frac{\partial^2}{\partial x^2}\left(e^{-\alpha x^2}\right) = \frac{\partial}{\partial x}\left(-2\alpha x e^{-\alpha x^2}\right) = -2\alpha e^{-\alpha x^2}+4\alpha^2x^2e^{-\alpha x^2} = 2\alpha e^{-\alpha x^2}(2\alpha x^2-1)$$

$*^2$ $$\int_{-\infty}^{\infty} e^{-2\alpha x^2}x^2\,dx = \cancel{-\frac{x}{4\alpha}e^{-2\alpha x^2}\Big]_{-\infty}^{\infty}} + \frac{1}{4\alpha}\int_{-\infty}^{\infty}e^{-2\alpha x^2}dx$$

$$\begin{cases} u = x \to du = dx \\ dv = e^{-2\alpha x^2}x\,dx \to v = -\frac{1}{4\alpha}e^{-2\alpha x^2}\end{cases}$$

Metodo bariazionala $\psi_\alpha(x)$-rekin oplikatuz osziladore harmonikoaren oinarrizko egoera lortu:

$$\langle H\rangle_{\psi_\alpha} \geq E_0 \Rightarrow \frac{d\langle H\rangle}{d\alpha} = \frac{\hbar^2}{2m}-\frac{m\omega^2}{8\alpha^2} = 0 \to \frac{m\omega^2}{8\alpha^2} = \frac{\hbar^2}{2m} \to \alpha^2 = \frac{m^2\omega^2}{4\hbar^2} \to \alpha \geq 0 \to$$

$$\alpha = \frac{m\omega}{2\hbar} \Rightarrow \psi_0 = \left(\frac{m\omega}{2\hbar}\right)^{1/4}e^{-\frac{m\omega}{2\hbar}x^2} \quad ; \quad \langle H\rangle_{\psi_\alpha} = \frac{\hbar\omega}{2}$$

3)

$$E = m_e c^2\left\{1+(Z\alpha)^2\left[n-j-1/2+\sqrt{(j+1/2)^2-(Z\alpha)^2}\right]^{-2}\right\}^{-1/2}$$ garatu $(Z\alpha)$-rekiko $\left(\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c}\right)$

$$\sqrt{(j-1/2)^2-Z^2\alpha^2} = (j-1/2)\sqrt{1-\left(\frac{Z\alpha}{j-1/2}\right)^2} = (j-1/2)\left(1-\frac{1}{2}\left(\frac{Z\alpha}{j-1/2}\right)^2\right)+O((Z\alpha)^4)$$

Orduan: $$(Z\alpha)^2\left[n-j-1/2+\sqrt{(j-1/2)^2-(Z\alpha)^2}\right]^2 \simeq (Z\alpha)^2\left[n-j-1/2+(j-1/2)\left(1-\frac{1}{2}\left(\frac{Z\alpha}{j-1/2}\right)^2\right)\right]^2 =$$

$$(Z\alpha)^2\left[n-\cancel{j}-1/2+\cancel{j}-1/2-\frac{1}{2}j\left(\frac{Z\alpha}{j-1/2}\right)^2+\frac{1}{4}\left(\frac{Z\alpha}{j-1/2}\right)^2\right]^2 = (Z\alpha)^2\left[n-1-\frac{j}{2}\left(\frac{Z\alpha}{j-1/2}\right)^2+\frac{1}{4}\left(\frac{Z\alpha}{j-1/2}\right)^2\right]^2 =$$

$$(Z\alpha)^2\left[(n-1)+\left(\frac{Z\alpha}{j-1/2}\right)^2\left(\frac{1}{4}-\frac{j}{2}\right)\right]^2 \simeq (Z\alpha)^2\left[(n-1)^2+\left(\frac{Z\alpha}{j-1/2}\right)^4\left(\frac{1}{4}-\frac{j}{2}\right)^2+2(n-1)\left(\frac{Z\alpha}{j-1/2}\right)^2\left(\frac{1}{4}-\frac{j}{2}\right)\right] \simeq$$

$$(Z\alpha)^2\left[(n-1)^2+2(n-1)\left(\frac{Z\alpha}{j-1/2}\right)^2\left(\frac{1}{4}-\frac{j}{2}\right)\right]$$

$$E = m_e c^2\frac{1}{\sqrt{1+(Z\alpha)^2\left[n-j-1/2+\sqrt{(j+1/2)^2-(Z\alpha)^2}\right]^{-2}}} \Rightarrow \left(1+(Z\alpha)^2\left(n-j-1/2+\sqrt{(j+1/2)^2-(Z\alpha)^2}\right)^{-2}\right)^{-1/2} \simeq$$

$$1-\frac{1}{2}(Z\alpha)^2\left(n-j-1/2+\sqrt{(j+1/2)^2-(Z\alpha)^2}\right)^{-2} \quad (1)$$

$$\sqrt{(j+1/2)^2-(Z\alpha)^2} = (j+1/2)\sqrt{1-\left(\frac{Z\alpha}{j+1/2}\right)^2} \simeq (j+1/2)\left(1-\frac{1}{2}\left(\frac{Z\alpha}{j+1/2}\right)^2\right) = (j+1/2)-\frac{1}{2}\frac{(Z\alpha)^2}{(j+1/2)} \Rightarrow$$

$$\left(n-j-1/2+\sqrt{(j+1/2)^2-(Z\alpha)^2}\right)^{-1}(Z\alpha) \simeq \left(n-\cancel{j}-\cancel{1/2}+\cancel{j}+\cancel{1/2}-\frac{1}{2}\frac{(Z\alpha)^2}{j+1/2}\right)^{-1}(Z\alpha) = \left(n-\frac{1}{2}\frac{(Z\alpha)^2}{j+1/2}\right)^{-1}(Z\alpha)$$

$$\Rightarrow \left((Z\alpha)\left(n-j-1/2+\sqrt{(j+1/2)^2-(Z\alpha)^2}\right)^{-1}\right)^2 = (Z\alpha)^2\frac{1}{\left(n-\frac{1}{2}\frac{(Z\alpha)^2}{(j+1/2)}\right)^2} = \frac{(Z\alpha)^2}{\left(n-\frac{1}{2}\frac{(Z\alpha)^2}{(j+1/2)}\right)^2} =$$

$$(Z\alpha)^2\frac{1}{n^2\left(1-\frac{(Z\alpha)^2}{2(j+1/2)n}\right)^2} \simeq \frac{(Z\alpha)^2}{n}\left(1+\frac{Z(Z\alpha)^2}{Z(j+1/2)n}\right)+\dots$$

→ arbuiatu $O((Z\alpha)^4)$ terminoak

$$E = m_ec^2\left(1-\frac{1}{2}\frac{(Z\alpha)^2}{n^2}-\frac{1}{2}\frac{(Z\alpha)^4}{n^3}\left(\frac{1}{j+1/2}+\dots\right)\right) \simeq m_ec^2\left(1-\frac{1}{2}\frac{(Z\alpha)^2}{n^2}\right)$$

4)

H_0 hidrogeno-atomoaren hamiltoniarra ez-erlatibista.

$\{H_0, L^2, S^2, L_z, S_z\}$ BTMB $\Rightarrow$ $\{|n, l, s, m_l, m_s\rangle\}$ oinarri komuna

W_{SO} spin-orbita elkarrekintzari dagokion matrizea diagonalizatu $n=2$.

$n=2$, $s=1/2$ (e^--a), $l=1,0$, $m_l=-1,0,1$, $m_s=\pm 1/2$ → 8×8-ko matrizea

- $l=1 \rightarrow m_l=-1,0,1$, $m_s=\pm 1/2$ (2p) → 6×6-ko matrizea → Diagonalizatu behar dugu!
- $l=0 \rightarrow m_l=0$, $m_s=\pm 1/2$ (2s) → 2×2-ko matrizea

W_{SO} $\{|n\ l\ s\ m_l\ m_s\rangle\}$ oinarrian <u>ez</u> da diagonala, baina bai $\{|n\ l\ s\ j\ m\rangle\}$ oinarrian:

↳ blokeka baliteke

* $s=1/2$, $l=1$, $m = m_s+m_l = \begin{cases}-3/2\\-1/2\\1/2\\3/2\end{cases} \rightarrow j=3/2,\ 1/2$ * $l=0 \rightarrow m=\pm 1/2 \rightarrow j=1/2$

$$\langle W_{SO}\rangle_{nlsjm} = \frac{(Z\alpha)^2 E_n^0}{n^2}\left(\frac{n}{j+1/2}-\frac{n}{l+1/2}+\delta_{l,0}\right) = -\frac{E_I}{4}\left(\frac{2}{j+1/2}-\frac{2}{l+1/2}+\delta_{l,0}\right)\frac{(\alpha)^2}{4}$$

↳ Diagonaleko elementuak.

$|n\ l\ s\ j\ m\rangle$ autobektoreak $\{|n\ l\ s\ m_l\ m_s\rangle\}$ autobektoreen oinarrian garatzeko

Clebsch-Gordon-en koefizienteak erabili.

5)

$n=3$ zenbaki kuantikoaren egitura mehea.

$$E_n = m_e c^2 + E_n^\circ \left[1 + \left(\frac{Z\alpha}{n}\right)^2 \left(\frac{n}{j+1/2} - 3/4\right) + O\left((Z\alpha)^4\right)\right]$$

$n=3 \rightarrow l = 2,1,0 \quad (s=1/2) \qquad$ (Endekapena $g = 2 \cdot 3^2 = 18$)

- $l = 2 \rightarrow m_l = -2,-1,0,1,2 \quad , \quad m_s = -1/2, 1/2$ $\qquad j_{min} = |l-s|$

  $m = m_l + m_s = -5/2, -3/2, -1/2, 1/2, 3/2, 5/2 \rightarrow j = 5/2, 3/2$

- $l = 1 \rightarrow m_l = -1,0,1 \quad , \quad m_s = -1/2, 1/2$

  $m = m_l + m_s = -3/2, -1/2, 1/2, 3/2 \rightarrow j = 3/2, 1/2$

- $l = 0 \rightarrow m_l = 0 \rightarrow m_s = -1/2, 1/2 \rightarrow m = \pm 1/2 \rightarrow j = 1/2$

j-ren 3 balio daude gutxira, beraz 3 energia maila egongo dira.

* $j = 1/2 \Rightarrow |j=1/2, l=0, m=1/2\rangle, |j=1/2, l=0, m=-1/2\rangle,$

$|j=1/2, l=1, m=-1/2\rangle, |j=1/2, l=1, m=+1/2\rangle, \qquad g=4$

$$E_1 = m_e c^2 + E_3^\circ \left[1 + \left(\frac{Z\alpha}{3}\right)^2 \left(3 - 3/4\right)\right]$$

* $j = 3/2 \Rightarrow |j=3/2, l=1, m=-3/2\rangle, |j=3/2, l=1, m=-1/2\rangle,$

$|j=3/2, l=1, m=1/2\rangle, |j=3/2, l=1, m=3/2\rangle, |j=3/2, l=2, m=-3/2\rangle,$

$|j=3/2, l=2, m=-1/2\rangle, |j=3/2, l=2, m=1/2\rangle, |j=3/2, l=2, m=3/2\rangle$

$$g = 8 \quad , \quad E_2 = m_e c^2 + E_3^\circ \left(1 + \left(\frac{Z\alpha}{3}\right)^2 \left(\frac{3}{2} - \frac{3}{4}\right)\right)$$

* $j = 5/2 \Rightarrow |j=5/2, l=2, m=-5/2\rangle, |j=5/2, l=2, m=-3/2\rangle,$

$|j=5/2, l=2, m=-1/2\rangle, |j=5/2, l=2, m=1/2\rangle, |j=5/2, l=2, m=3/2\rangle,$

$|j=5/2, l=2, m=5/2\rangle \Rightarrow g = 6 \qquad$ Endekapena partzialki apurtu.

$$E_3 = m_e c^2 + E_3^\circ \left(1 + \left(\frac{Z\alpha}{3}\right)^2 (1 - 3/4)\right)$$

6) Bi partikulaz osatutako sistema

$$H = A J_1 \cdot J_2 = \frac{A}{2}(J^2 - J_1^2 - J_2^2) \qquad (\vec{J} = \vec{J}_1 + \vec{J}_2)$$

H-ren autobalioak $\{|j_1, j_2, j, m\rangle\}$ dira eta autobektoreak:

$$H|j_1\, j_2\, j\, m\rangle = \underbrace{\frac{A}{2}[j(j+1) - j_1(j_1+1) - j_2(j_2+1)]}_{E_{j,j_1,j_2}} \hbar^2\, |j_1\, j_2\, j\, m\rangle$$

$$|\psi(0)\rangle = |j_1, m_1; j_2, m_2\rangle = |j_1, m_1\rangle \otimes |j_2, m_2\rangle = |1, 0; 1/2, 1/2\rangle$$

Garatu egingo dugu $\{|j_1\, j_2\, j\, m\rangle\}$ oinarrian: (Argi dago $j_1 = 1$ eta $j_2 = 1/2$ izango direla eta $m = m_1 + m_2 = 1/2$)

- $j_1 = 1,\ j_2 = 1/2 \Rightarrow j_{max} = j_1 + j_2 = 3/2$ eta $j_{min} = |j_1 - j_2| = 1/2$ (j-k bi balio posible izango ditu)

- $|m_1 = 0, m_2 = 1/2\rangle = \alpha|j = 3/2, m = 1/2\rangle + \beta|j = 1/2, m = 1/2\rangle$ izango da.

* $|j = 3/2, m = 3/2\rangle = |m_1 = 1, m_2 = 1/2\rangle$

* $|j = 3/2, m = 1/2\rangle = \frac{1}{\hbar\sqrt{3}} J_- |j = 3/2, m = 3/2\rangle = \frac{1}{\hbar\sqrt{3}}(J_{1-}|m_1 = 1, m_2 = 1/2\rangle + J_{2-}|m_1 = 1, m_2 = 1/2\rangle) = \frac{1}{\cancel{\hbar}\sqrt{3}}(\cancel{\hbar}\sqrt{2}|m_1 = 0, m_2 = 1/2\rangle + \cancel{\hbar}|m_1 = 1, m_2 = -1/2\rangle) = \sqrt{\frac{2}{3}}|m_1 = 0, m_2 = 1/2\rangle + \frac{1}{\sqrt{3}}|m_1 = 1, m_2 = -1/2\rangle$

* $|j = 1/2, m = 1/2\rangle = a|m_1 = 0, m_2 = 1/2\rangle + b|m_1 = 1, m_2 = -1/2\rangle$

Ortogonaltasuna $\Rightarrow \langle j = 1/2, m = 1/2 | j = 3/2, m = 1/2\rangle = a\sqrt{\frac{2}{3}} + \frac{b}{\sqrt{3}} = 0 \rightarrow b = -\sqrt{2}a$

$$|j = 1/2, m = 1/2\rangle = \frac{1}{\sqrt{3}}|m_1 = 0, m_2 = 1/2\rangle - \sqrt{\frac{2}{3}}|m_1 = 1, m_2 = -1/2\rangle$$

Orduan $\Rightarrow |m_1 = 0, m_2 = 1/2\rangle = \frac{1}{\sqrt{3}}(\sqrt{2}|j = 3/2, m = 1/2\rangle + |j = 1/2, m = 1/2\rangle)$

a) $\langle H \rangle$? $\quad \langle H \rangle = \langle \psi | H | \psi \rangle = \left(\sqrt{\frac{2}{3}}\right)^2 \frac{A}{2} \left[\frac{3}{2}\left(\frac{3}{2}+1\right) - 2 - \frac{3}{4} \right] \hbar^2 +$

$$\frac{A}{(\sqrt{3})^2} \frac{\hbar^2}{2} \left[\cancel{\frac{3}{4}} - 2 - \cancel{\frac{3}{4}} \right] = \frac{\cancel{2}}{3} \frac{A}{\cancel{2}} \left[\frac{15}{4} - \frac{3}{4} - 2 \right] \hbar^2 + \frac{1}{3} \frac{A}{\cancel{2}} \left[-\cancel{2} \right] \hbar^2 =$$

$$\frac{A}{3} \hbar^2 [1 - 1] = 0$$

b) J^2-ren neurketa posibleak $\rightarrow$ $j = 3/2$, $j = 1/2 \Rightarrow \hbar^2 \frac{15}{4}$ eta $\hbar^2 \frac{3}{4}$

$$P(j=3/2) = \sum_{m=-j}^{j} |\langle 3/2, m | \psi \rangle|^2 = \frac{2}{3}$$

$$P(j=1/2) = \sum_{m=-j}^{j} |\langle 1/2, m | \psi \rangle|^2 = \frac{1}{3}$$

c) $|\psi(0)\rangle = |1, 0 ; 1/2, 1/2\rangle = \sqrt{\frac{2}{3}} |j=3/2, m=1/2\rangle + \frac{1}{\sqrt{3}} |j=1/2, m=1/2\rangle$

$j = 3/2 \rightarrow E_{j j_1 j_2} = \frac{A\hbar^2}{2}$, $j = 1/2 \rightarrow E_{j j_1 j_2} = -A\hbar^2$

$$\Rightarrow |\psi(t)\rangle = \sqrt{\frac{2}{3}} e^{-\frac{A\hbar}{2} t i} |j=3/2, m=1/2\rangle + \frac{1}{\sqrt{3}} e^{A\hbar t i} |j=1/2, m=1/2\rangle$$

d) $(J_1)_z$ behagarriaren itxarotako balioa $t>0$.

Orain $|\psi(t)\rangle$ garatu egingo dugu $\{|j_1, j_2, m_1, m_2\rangle\}$ oinarrian:

* $|j=3/2, m=1/2\rangle = \sqrt{\frac{2}{3}} |j_1=1, m_1=0 ; j_2=1/2, m_2=+1/2\rangle$

$\frac{1}{\sqrt{3}} |j_1=1, m_1=1 ; j_2=1/2, m_2=-1/2\rangle$

* $|j=1/2, m=1/2\rangle = \frac{1}{\sqrt{3}} |j_1=1, m_1=0 ; j_2=1/2, m_2=1/2\rangle - \sqrt{\frac{2}{3}} |j_1=1, m_1=1 ; j_2=1/2, m_2=-1/2\rangle$

$$|\psi(t)\rangle = \frac{2}{3} e^{-\frac{A\hbar}{2} t i} |m_1=0, m_2=1/2\rangle + \frac{\sqrt{2}}{3} e^{-\frac{A\hbar}{2} t i} |m_1=1, m_2=-1/2\rangle + \frac{1}{\sqrt{3}} e^{A\hbar t i} |m_1=0, m_2=1/2\rangle +$$

$$-\sqrt{\frac{2}{3}} e^{+A\hbar t i} |m_1=1, m_2=-1/2\rangle = \frac{1}{3} \left[\left(e^{-A\hbar t i/2} \, 2 + e^{A\hbar t i} \right) |m_1=0, m_2=1/2\rangle + \right.$$

$\sqrt{2}(e^{-A\hbar t i/2} - e^{A\hbar t i}) |m_1=1, m_2=-1/2\rangle]$

J_{1z} neurtu $\Rightarrow$ $\langle J_{1z}\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |\langle m_1, m_2|\Psi(t)\rangle|^2 \hbar m_1 = \frac{2\hbar}{9}\left|e^{-A\hbar t i/2} - e^{A\hbar t i}\right|^2 =$

$\frac{2\hbar}{9}(e^{-A\hbar t i/2} - e^{A\hbar t i})(e^{A\hbar t i/2} - e^{-A\hbar t i}) = \frac{2\hbar}{9}(2 - e^{-3A\hbar t i/2} - e^{3A\hbar t i/2}) =$

$\frac{2\hbar}{9}(2 - (e^{-3A\hbar t i/2} + e^{3A\hbar t i/2})) = \frac{2\hbar}{9}(2 - 2\cos(\frac{3\hbar t A}{2})) =$

$\frac{4\hbar}{9}(1-\cos(\frac{3\hbar t A}{2})) = \frac{4\hbar}{9}\cdot 2\sin^2(\frac{3\hbar t A}{4}) = \frac{8\hbar}{9}\sin^2(\frac{3\hbar A}{4}t)$

e) J^2 behagarrian hasierako aldiuneko neurketa $\to$ $J^2 = \frac{15\hbar}{4}$ $\to$ $j=3/2$ $\to$

$|\Psi'(0)\rangle = \frac{\hat{P}_j|\Psi\rangle}{\sqrt{\langle\Psi|\hat{P}_j|\Psi\rangle}} = \frac{1}{\sqrt{\langle\Psi|\hat{P}_j|\Psi\rangle}} \sum_{m=-j}^{j} |j, m\rangle\langle j, m|\Psi\rangle = |j=3/2, m=1/2\rangle$

$|\Psi'(t)\rangle = |j=3/2, m=1/2\rangle e^{-A\hbar t i/2}$ $(j_1, j_2$ finkoak dira$)$

- $\langle H\rangle = \langle\Psi'|H|\Psi'\rangle = \frac{A\hbar^2}{2}$ (egoera geldikorra da $|\Psi(t)\rangle$)

- $|j=3/2, m=1/2\rangle e^{-A\hbar t i/2} = |\Psi'(t)\rangle = \left[\sqrt{\frac{2}{3}}|m_1=0, m_2=1/2\rangle + \frac{1}{\sqrt{3}}|m_1=1, m_2=-1/2\rangle\right]\cdot$

$e^{-A\hbar t i/2}$

$\langle (J_2)_z\rangle = \sum_{m_2=-j_2}^{j_2}\sum_{m_1=-j_1}^{j_1} |\langle m_1, m_2|\Psi'(t)\rangle|^2 \hbar m_2 = \frac{2}{3}\frac{\hbar}{2} + \frac{1}{3}\left(-\frac{\hbar}{2}\right) = \frac{\hbar}{6}$

7.) $H = A S_1\cdot S_2 = \frac{A}{2}(S^2 - S_1^2 - S_2^2)$ $\Rightarrow$ 6. ariketaren berdina; $J_1 = S_1$ eta $J_2 = S_2$

Autobektoreak eta autobalioak: $|s_1, s_2, s, m_s\rangle$ eta $E_{s_1,s_2,s} = \frac{A\hbar^2}{2}[s(s+1) - s_1(s_1+1) - s_2(s_2+1)]$

a) Singletea eta tripletea $\Rightarrow$ $s_1 = 1/2$, $s_2 = 1/2$

$\downarrow$ $S=0$ (singletea), $\downarrow$ $S=1$ (tripletea)

Singletea $\Rightarrow$ $s=0$, $s_1=s_2=1/2$ $\Rightarrow$ $E_{singlete} = -\frac{A\hbar^2}{2}\,\frac{3}{2} = -\frac{3A\hbar^2}{4}$

Tripletea $\Rightarrow$ $s=1$, $s_1=s_2=1/2$ $\Rightarrow$ $E_{triplete} = \frac{A\hbar^2}{4}$

b) $B = B_0\hat{k}$ $\rightarrow$ $H = H_0 - (\vec{M}_1+\vec{M}_2)\cdot\vec{B} = H_0 + \frac{2\mu_B}{\hbar}(\vec{S}_1+\vec{S}_2)\cdot\vec{B} = H_0 + \frac{2\mu_B}{\hbar}(S_{1z}+S_{2z})B =$

$H_0 + \frac{2\mu_B}{\hbar}B\underbrace{(S_{1z}+S_{2z})}_{S_z} = AS_1\cdot S_2 + W$ ($W \Rightarrow$ perturbazioa)

H_0-ren autobektoreak $|s_1\ s_2\ s\ m_s\rangle$ eta autobalioak $E^0_{s_1s_2s} = \frac{A\hbar^2}{2}[s(s+1) +$

$-s_1(s_1+1) - s_2(s_2+1)] = \frac{A\hbar^2}{2}[s(s+1) - \frac{3}{2}]$

$s_1=s_2=1/2$ (finkoak)

$s=1,0$ $\rightarrow$ endakapena $s=1 \rightarrow m_s=-1,0,1$ izan daitezkeelako.

- Singletearen energia $\rightarrow$ $E_{singlet} = \varepsilon_0 + \varepsilon_1\lambda + O(\lambda^2)$

$\varepsilon_0 = E^0_{s=0} = -\frac{3A\hbar^2}{4}$, $|0\rangle = |\overset{s_1}{1/2}\ \overset{s_2}{1/2}\ \overset{s}{0}\ \overset{m_s}{0}\rangle$

$\lambda\varepsilon_1 = \langle 0|W|0\rangle \overset{*'}{=} \frac{2\mu_B B}{\hbar}\left[\frac{1}{2}\frac{\hbar}{2} - \frac{1}{2}\frac{\hbar}{2} - \frac{\hbar}{4} + \frac{\hbar}{4}\right] = 0$

$*'$ $|s=0, m_s=0\rangle$ garatu behar dugu $\{|s_1, m_{s_1}; s_2, m_{s_2}\rangle\}$ oinarrian

$|s=0, m_s=0\rangle = \frac{1}{\sqrt{2}}[|m_1=1/2, m_2=-1/2\rangle - |m_1=-1/2, m_2=1/2\rangle]$

$E_{singlet}(\lambda) = \varepsilon_0 + O(\lambda^2) = -\frac{3A\hbar^2}{4} + O(\lambda^2)$

- Tripletearen energia $\rightarrow$ $E_{triplete}(\lambda) = \varepsilon_0 + \varepsilon_1\lambda + O(\lambda^2)$ $\varepsilon_0 = E^0_{trip} = \frac{A\hbar^2}{4}$

ε_1 lortzeko W diagonalizatu $E(s=1)$ azpiespazioan.

$s=1 \rightarrow m_s=-1,0,1$ (3x3-ko matrizea) $\rightarrow$ $W^{(1)}$ kalkulatuko dugu

$W^{(1)} \Rightarrow \circ\, |s=1, m_s=1\rangle = |m_1=1/2, m_z=1/2\rangle = |+,+\rangle$

$\circ\, |s=1, m_s=0\rangle = \frac{1}{\sqrt{2}}\left[|m_1=1/2, m_2=-1/2\rangle + |m_1=-1/2, m_2=1/2\rangle\right] = \frac{1}{\sqrt{2}}\left[|+,-\rangle + |-,+\rangle\right]$

$\circ\, |s=1, m_s=-1\rangle = \left[|m_1=-1/2, m_2=-1/2\rangle\right] = |-,-\rangle$

$$\langle 1\,1|W|1\,1\rangle = \frac{2\mu_B B}{\hbar}\left(\frac{\hbar}{2}+\frac{\hbar}{2}\right) = \frac{2\hbar\mu_B B}{\hbar} = 2\mu_B B$$

$$\langle 1\,1|W|1\,0\rangle = \frac{2\mu_B B}{\hbar}(0) = 0$$

$$\langle 1\,1|W|1\,-1\rangle = \frac{2\mu_B B}{\hbar}(0) = 0$$

$$\langle 1\,0|W|1\,0\rangle = \frac{2\mu_B B}{\hbar}\left(\frac{1}{\sqrt{2}}\frac{\hbar}{2}+\frac{1}{\sqrt{2}}\frac{\hbar}{2}\right) = \sqrt{2}\mu_B B$$

$$\langle 1\,0|W|1\,1\rangle = 0$$

$$\langle 1\,0|W|1\,-1\rangle = 0$$

$$\langle 1\,-1|W|1\,-1\rangle = \frac{2\mu_B B}{\hbar}\left(-\frac{\hbar}{2}-\frac{\hbar}{2}\right) = -2\mu_B B$$

$$\langle 1\,-1|W|1\,1\rangle = 0$$

$$\langle 1\,-1|W|1\,0\rangle = 0$$

$$\Rightarrow W^{(1)} = \begin{pmatrix} 2\mu_B B & 0 & 0 \\ 0 & \sqrt{2}\mu_B B & 0 \\ 0 & 0 & -2\mu_B B \end{pmatrix} \rightarrow \text{Diagonala da}$$

$$\lambda\varepsilon_1^1 = 2\mu_B B \Rightarrow E^1_{\text{mpiule}} = A\frac{\hbar^2}{4} + 2\mu_B B + O(B^2)$$

$$\lambda\varepsilon_1^2 = \sqrt{2}\mu_B B \Rightarrow E^2_{\text{mpiule}} = A\frac{\hbar^2}{4} + \sqrt{2}\mu_B B + O(B^2)$$

$$\lambda\varepsilon_1^3 = -2\mu_B B \Rightarrow E^3_{\text{mpiule}} = A\frac{\hbar^2}{4} - 2\mu_B B + O(B^2)$$

Endekapena apurtzen da

* Baita soluzio zehatza dago, $|s_1\, s_2\, s\, m_s\rangle$ H-ren autobektoreak direlako.

FISIKA KVANTIKOA:

- $|\vec{r}, \varepsilon\rangle_u = \sum_{\varepsilon'} \int d\vec{r}\,' \underbrace{\langle \vec{r}\,'\varepsilon' | \vec{r}\,\varepsilon\rangle_u}_{\delta(\vec{r}-\vec{r}\,')\langle \varepsilon' | \varepsilon\rangle_u} |\vec{r}\,'\varepsilon'\rangle = \sum_{\varepsilon'} \langle \varepsilon' | \varepsilon\rangle_u |\vec{r}\,\varepsilon\rangle$

- $\hat{A}$ bikoizmoa eta S_z neurtzen baditugu aldiberean:
  ↳ a_n-n: $P_n^{\varepsilon} = |\langle n\,\varepsilon | \psi\rangle|^2$ $\quad \langle \vec{r}\,\varepsilon | \psi\rangle = \psi_\varepsilon(\vec{r})$

  $|n\,\varepsilon\rangle = \sum_{\varepsilon'} \int d\vec{r}\, \underbrace{\langle \vec{r}\,\varepsilon' | n\,\varepsilon\rangle}_{\langle \vec{r} | n\rangle \langle \varepsilon' | \varepsilon\rangle = \delta_{\varepsilon\varepsilon'}} |\vec{r}\,\varepsilon'\rangle = \int \langle \vec{r} | n\rangle |\vec{r}, \varepsilon\rangle d\vec{r} \qquad P_n^{\varepsilon} = |\langle n | \psi_\varepsilon\rangle|^2$

4. ariketa orria

17-03-01

1) $|\psi\rangle$ e^--ren egoerari dagokion autobektorea, $|\psi\rangle \in \mathcal{H}$

$\{p_x, p_y, p_z, S_z, S^2\}$ BTMB

a) Elektroi bat momentuaren p balioarekin eta S_z-ren $\hbar/2$ balioarekin aurkitzeko probabilitate-dentsitatea.

$$[\bar{\psi}](\vec{p}) = \begin{pmatrix} \bar{\psi}_+(\vec{p}) \\ \bar{\psi}_-(\vec{p}) \end{pmatrix} \qquad \{|\vec{p}, \varepsilon\rangle\}\text{-n}$$

↳ Fourier-en transformatuak

$$P = |\langle \vec{p}, + | \psi\rangle|^2 = |\bar{\psi}_+(\vec{p})|^2$$

b) Elektroi bat posizioan r balioarekin eta S_x-ren $\hbar/2$ balioarekin aurkitzeko probabilitate-dentsitatea.

$$[\psi](\vec{r}) = \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} \qquad \{|\vec{r}, \varepsilon\rangle\}\text{-n}$$

↳ Bi uhin funtzio

$$P = |{}_x\langle \vec{r}, + | \psi\rangle|^2 \overset{*}{=} \frac{1}{2} |\psi_+(\vec{r}) + \psi_-(\vec{r})|^2$$

$|\vec{r}, +\rangle_x = \frac{1}{\sqrt{2}}[|\vec{r}, +\rangle + |\vec{r}, -\rangle] \Rightarrow *\ {}_x\langle \vec{r}, + | \psi\rangle = \int d^3r' \left[\psi_+(\vec{r}\,')\frac{1}{\sqrt{2}} \underbrace{\langle \vec{r}, + | \vec{r}\,', +\rangle}_{\delta(\vec{r}-\vec{r}\,')} + \frac{\psi_-(\vec{r}\,')}{\sqrt{2}} \underbrace{\langle \vec{r}, - | \vec{r}\,', -\rangle}_{\delta(\vec{r}-\vec{r}\,')}\right.$

2)

a) $S \cdot p$ eragilearen adierazpen matriziala. $\quad S = 1/2$ harturz:

$$S \cdot p = S_x p_x + S_y p_y + S_z p_z$$

$\{|p, \varepsilon\rangle\}$ oinarrian: (p zehaztuta)

$$(S \cdot p) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} p_x & 0 \\ 0 & p_x \end{pmatrix} + \frac{\hbar i}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} p_y & 0 \\ 0 & p_y \end{pmatrix} + \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} p_z & 0 \\ 0 & p_z \end{pmatrix} =$$

$$\frac{\hbar}{2}\left[\begin{pmatrix} 0 & p_x \\ p_x & 0 \end{pmatrix} + i\begin{pmatrix} 0 & -p_y \\ p_y & 0 \end{pmatrix} + \begin{pmatrix} p_z & 0 \\ 0 & -p_z \end{pmatrix}\right] = \frac{\hbar}{2}\left[\begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & -p_z \end{pmatrix}\right]$$

b) $S \cdot p$ eragilearen autobalioak lortu. Lor bitez, halaber, eragile horren eta p_x, p_y eta p_z eragileen aldiberako autobektoreak.

$$\frac{\hbar}{2}\begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & -p_z \end{pmatrix} \Rightarrow \begin{vmatrix} \hbar/2\, p_z - \lambda & \frac{\hbar}{2}(p_x - ip_y) \\ \frac{\hbar}{2}(p_x+ip_y) & -\frac{\hbar}{2}p_z - \lambda \end{vmatrix} = -\left(\frac{\hbar}{2}p_z - \lambda\right)\left(\frac{\hbar}{2}p_z + \lambda\right) - \frac{\hbar^2}{4}\left(p_x^2 + p_y^2\right) =$$

$$-\frac{\hbar^2}{4}p_z^2 + \lambda^2 - \frac{\hbar^2}{4}(p_x^2 + p_y^2) = -\frac{\hbar^2}{4}p^2 + \lambda^2 = 0 \to \lambda = \pm\frac{\hbar}{2}p$$

- $\lambda_1 = \frac{\hbar}{2}p \Rightarrow \frac{\hbar}{2}\begin{pmatrix} p_z - p & p_x - ip_y \\ p_x+ip_y & -p_z - p \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} a(p_z - p) + b(p_x - ip_y) \\ a(p_x+ip_y) - b(p_z+p) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow$

$$a(p_z - p) = b(ip_y - p_x) \to b = \frac{p_z - p}{ip_y - p_x}a = \frac{p - p_z}{p_x - ip_y}a$$

Normalizatu $\Rightarrow$ $A^2\left(1 + \left|\frac{p-p_z}{p_x - ip_y}\right|^2\right) = A^2\left(1 + \frac{(p-p_z)^2}{p_x^2+p_y^2}\right) = A^2\left(\frac{p_x^2+p_y^2 + p^2 + p_z^2 - 2pp_z}{p_x^2+p_y^2}\right) =$

$$A^2\left(\frac{2p^2 - 2pp_z}{p_x^2+p_y^2}\right) = 1 \to A = \sqrt{\frac{p_x^2+p_y^2}{2p^2 - 2pp_z}} = \sqrt{\frac{p_x^2+p_y^2}{2(p^2-p_z)}}$$

$$|\Psi_1\rangle = \sqrt{\frac{p_x^2+p_y^2}{2(p^2 - pp_z)}}\left(|p,+\rangle + \frac{(p-p_z)}{(p_x - ip_y)}|p,-\rangle\right)$$

- $\lambda_2 = -\frac{\hbar}{2}p \Rightarrow \frac{\hbar}{2}\begin{pmatrix} p_z + p & p_x - ip_y \\ p_x+ip_y & -p_z + p \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} a(p_z+p) + b(p_x - ip_y) \\ a(p_x+ip_y) + b(p - p_z) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow$

$$a(p_z + p) = b(ip_y - p_x), \quad b = a\frac{(p_z+p)}{ip_y - p_x} = -a\frac{(p_z+p)}{p_x - ip_y}$$

Normalizatu $\Rightarrow$ $A^2\left(1 + \frac{(p_z+p)^2}{p_x^2+p_y^2}\right) = A^2\left(\frac{p_x^2+p_y^2+p_z^2+p^2+2p_zp}{p_x^2+p_y^2}\right) = A^2\left(\frac{2p^2+2p_zp}{p_x^2+p_y^2}\right) = 1$

$$A = \sqrt{\frac{p_x^2+p_y^2}{2p(p+p_z)}}$$

$$|\Psi_2\rangle = \sqrt{\frac{p_x^2+p_y^2}{2p(p+p_z)}}\left(|p,+\rangle - \frac{(p_z+p)}{p_x - ip_y}|p,-\rangle\right)$$

$\hat{p}_x$, $\hat{p}_y$ eta $\hat{p}_z$ eragileen aldibereko autobektoreak $\Rightarrow$ $|\Psi_1\rangle$, $|\Psi_2\rangle$

3) Elektroi baten egoera adierazten duen spinorea:

$$[\Psi](r) = R(r) \begin{pmatrix} \frac{1}{\sqrt{3}} Y_1^0(\theta,\phi) \\ \sqrt{\frac{2}{3}} Y_1^1(\theta,\phi) \end{pmatrix} = \begin{pmatrix} \Psi_+(r) \\ \Psi_-(r) \end{pmatrix}$$

$$|\Psi\rangle = \int d\vec{r}^3 \left[\Psi_+ |r, +\rangle + \Psi_- |r, -\rangle \right]$$

a) Normalizatuta egoteko: $\langle \Psi | \Psi \rangle = 1 \Rightarrow \langle \Psi | \Psi \rangle = \int d^3r \, [\Psi_+^*(r) \Psi_+(r) +$

$\Psi_-^*(r)\Psi_-(r)] = \int d^3r \, [|\Psi_+|^2 + |\Psi_-|^2] = \int d^3r \, |R(r)|^2 \left(\frac{1}{3}|Y_1^0|^2 + \frac{2}{3}|Y_1^1|^2 \right) =$

normalizatuta $Y_l^m(\theta,\phi)$

$\frac{1}{3}\int d^3r \, |R(r)|^2 |Y_1^0|^2 + \frac{2}{3}\int d^3r \, |R(r)|^2 |Y_1^1|^2 = \frac{1}{3}\int dr \cdot r^2 |R(r)|^2 + \frac{2}{3}\int dr \cdot r^2 |R(r)|^2 =$

$\int dr \cdot r^2 |R(r)|^2 = 1 \qquad (1)$

b) S_z behagarriaren itxarotako balioa eta behagarri horren neurketaren emaitza posibleei dagozkien probabilitateak.

- Balio posibleak $+\frac{\hbar}{2}$ eta $-\frac{\hbar}{2}$.
- $\langle S_z \rangle = \langle \Psi | S_z | \Psi \rangle = \int dr^3 \, (\Psi_+^*(r) \quad \Psi_-^*(r)) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} \Psi_+(r) \\ \Psi_-(r) \end{pmatrix} =$

$\frac{\hbar}{2}\int dr^3 \, (\Psi_+^*(r) \quad -\Psi_-^*(r)) \begin{pmatrix} \Psi_+(r) \\ \Psi_-(r) \end{pmatrix} = \frac{\hbar}{2}\int dr^3 \, [|\Psi_+(r)|^2 - |\Psi_-(r)|^2] =$

$\frac{\hbar}{2}\int dr^3 \, |R(r)|^2 \left(\frac{1}{3}|Y_1^0|^2 - \frac{2}{3}|Y_1^1|^2 \right) = \frac{\hbar}{2}\left(\frac{1}{3}\int dr \cdot r^2 |R(r)|^2 - \frac{2}{3}\int dr \cdot r^2 |R(r)|^2 \right) \overset{(1)}{=}$

$-\frac{\hbar}{2} \cdot \frac{1}{3} = -\frac{\hbar}{6}$

- $dP(\hbar/2) = |\langle r, + | \Psi \rangle|^2 d^3r = |\Psi_+(r)|^2 dr^3 \Rightarrow P(\hbar/2)$ lortzeko espazio osoan integratu beharko dugu.

$$P(\hbar/2) = \int |\psi_+(r)|^2 d^3r = \int dP(\hbar/2)\, d^3r = \frac{1}{3}\int |Y_1^0(\theta,\phi)|^2 |R(r)|^2 d^3r =$$

$Y_1^0(\theta,\phi)$ normalizatuta dago

$$\frac{1}{3}\int |R(r)|^2 d^3r\, r^2 \overset{(1)}{=} \frac{1}{3}$$

- $dp(-\hbar/2) = |\langle r, -|\psi\rangle|^2 d^3r = |\psi_-(r)|^2 d^3r \Rightarrow P(-\hbar/2)$ lortzeko espazio osoan integratu beharko dugu

$Y_1^1(\theta,\phi)$ normalizatuta dago

$$P(-\hbar/2) = \int dP(-\hbar/2)\, d^3r = \frac{2}{3}\int |Y_1^1(\theta,\phi)|^2 |R(r)|^2 d^3r = \frac{2}{3}\int |R(r)|^2 \overset{(1)}{=} \frac{2}{3}$$

- Gainera $\langle S_z\rangle = \frac{\hbar}{2} P(\hbar/2) - \frac{\hbar}{2} P(-\hbar/2) = \frac{\hbar}{2}\left(\frac{1}{3} - \frac{2}{3}\right) = -\frac{\hbar}{6}$

c) Lor bitez L_z behagarriaren itxarotako balioa eta behagarri horren neurketaren emaitza posibleei dagozkien probabilitateak.

- L_z neurtzean $\to m$ lortu. $\{L^2, L_z, S^2, S_z\}$-ren autobektoreak

$$|K, l, m, \varepsilon\rangle \Rightarrow \langle r|K, l, m_l\rangle = R_{Kl}(\vec{r})\, Y_l^m(\theta,\phi)$$

$$\sum_K \langle K\, l\, m\, \varepsilon|\psi\rangle = \int r^2 dr\, a_{lm}^{\varepsilon}(r)$$

- $$P_m = \sum_\varepsilon \sum_K \sum_l |\langle K\, l\, m, \varepsilon|\psi\rangle|^2 = \sum_\varepsilon \sum_l \int dr\, r^2 |a_{lm}^{\varepsilon}(r)|^2$$

$$* |K\, l\, m, \varepsilon\rangle = \sum_{\varepsilon'} \int d^3r \underbrace{\langle \vec{r},\varepsilon'|K,l,m,\varepsilon\rangle}_{\langle \vec{r}|K,l,m\rangle\langle\varepsilon',\varepsilon\rangle} |\vec{r},\varepsilon'\rangle = \int d^3r\, R_{Kl}(r) Y_l^m(\theta,\phi)|\vec{r},\varepsilon\rangle$$

$$\langle\varepsilon',\varepsilon\rangle = \delta_{\varepsilon'\varepsilon}$$

K ordez r nahiz erradiala har genezake

$$\psi^\varepsilon(\vec{r}) = \sum_l \sum_m a_{lm}^{\varepsilon}(r) Y_l^m(\theta,\phi)$$ erradiala

$$|\psi^\varepsilon\rangle = \sum_l \sum_m \int r^2 dr\, a_{lm}^{\varepsilon}(r)|r\, l\, m\, \varepsilon\rangle$$ erradiala

$m = 0, 1$ dira balio posibleak.

- $$P_0 = \sum_K \sum_\varepsilon \sum_l |\langle K\, l\, 0.\, \varepsilon|\psi\rangle|^2 = \sum_\varepsilon \sum_l \int dr\, r^2 |a_{l0}^{\varepsilon}(r)|^2 = \sum_l \int dr\, r^2 |a_{l0}^{+}(r)|^2 +$$

$$\sum_l \int dr\, r^2 |a_{l0}^{-}(r)|^2 = \frac{1}{3}\int dr\, r^2 |R(r)|^2 \overset{(1)}{=} \frac{1}{3}$$

$$P_{\hbar} = \sum_{K}\sum_{\varepsilon}\sum_{\lambda} |\langle \lambda, 1, 1, \varepsilon | \psi \rangle|^2 = \sum_{\varepsilon}\sum_{\lambda} \int r^2 dr \, |a_{\lambda 1}^{\varepsilon}(r)|^2 = \int dr\, r^2 \sum_{\lambda} |a_{\lambda 1}^{+}(r)|^2 +$$

$$\int dr\, r^2 \sum_{\lambda} |a_{\lambda 1}^{-}(r)|^2 = \frac{2}{3} \underbrace{\int dr\, r^2 |R(r)|^2}_{1} = \frac{2}{3}$$

$$\psi^{\varepsilon}(\vec{r}) = \sum_{\lambda}\sum_{m} a_{\lambda m}^{\varepsilon}(r)\, Y_{\lambda}^{m}(\theta,\varphi) \rightarrow |\psi\rangle = \sum_{\varepsilon}\sum_{\lambda}\sum_{m} \int dr\, r^2 a_{\lambda m}^{\varepsilon}(r)\, |\underset{\downarrow}{r}\, \lambda\, m\, \varepsilon\rangle$$

erradiala ondoko soilik

$$|r\, \lambda\, m\, \varepsilon\rangle = \int d\Omega\, Y_{\lambda}^{m}(\Omega)\, |\Omega\rangle \otimes \underset{\downarrow \text{ erradiala}}{|r, \varepsilon\rangle}$$

d) Froga bedi elektroi r posizioan eta spin-aren edozein orientazio rekin aurkitzeko dagoen probabilitate dentsitatea isotropoa dela, hots, probabilitate-dentsitate honek posizioaren aldagai angeluarrekiko menpekotasunik ez duela.

$$P(r) = \sum_{\varepsilon} P^{\varepsilon}(r) = P^{+}(r) + P^{-}(r) = |\psi_{+}(r)|^2 + |\psi_{-}(r)|^2 = \frac{1}{3} |Y_1^0(\theta,\varphi)|^2 |R(r)|^2 +$$

$$\frac{2}{3} |Y_1^1(\theta,\varphi)|^2 |R(r)|^2 = \frac{|R(r)|^2}{3} \left(|Y_1^0(\theta,\varphi)|^2 + 2|Y_1^1(\theta,\varphi)|^2 \right) = \frac{|R(r)|^2}{\cancel{3}} \left(\frac{1}{4}\frac{\cancel{3}}{\pi} \cos^2\theta + \frac{\cancel{3}}{4\pi} \sin^2\theta \right) =$$

$$\frac{|R(r)|^2}{4\pi} (\sin^2\theta + \cos^2\theta) = \frac{|R(r)|^2}{4\pi}$$

→ Egin c) atala bezala

e) L_z behagarriaren neurketaren emaitza $\hbar$ dela emanik, aurki bedi neurketa honen ondoren elektroiak izango duen egoerari dagokion spinorea.

Neurketa egin ondoren $m=1$ izango da ⇒ proiekzioa. $|\psi'\rangle = \frac{\hat{P}_n |\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}}$

$$|\psi'\rangle = \sum_{\lambda}\sum_{\varepsilon}\sum_{K} |K, \lambda, 1, \varepsilon\rangle \langle K, \lambda, 1, \varepsilon | \psi\rangle = \sum_{\lambda}\sum_{\varepsilon}\sum_{K} |K\, \lambda, 1, \varepsilon\rangle \langle K, \lambda, 1, \varepsilon | \psi\rangle =$$

$$\sum_{K}\sum_{\lambda}\sum_{\varepsilon} |K, \lambda, 1, \varepsilon\rangle \langle K, \lambda, 1 | \psi_{\varepsilon}\rangle \Rightarrow [\psi'](r) = \begin{pmatrix} \psi'_{+}(r) \\ \psi'_{-}(r) \end{pmatrix}$$

$$\psi'_{+} = \langle r, + | \psi' \rangle = \sum_{K}\sum_{\lambda} \langle r, + | K, \lambda, 1, + \rangle \langle K, \lambda, 1 | \psi_{+} \rangle = 0$$

$$\psi'_{-} = \langle r, - | \psi' \rangle = \sum_{K}\sum_{\lambda} \langle r, - | K, \lambda, 1, - \rangle \langle K, \lambda, 1 | \psi_{-} \rangle = \sqrt{\frac{2}{3}}\, Y_1^1(\theta,\varphi)\, R(r)$$

Normalizatuz $\Rightarrow$ $[\Psi'](r) = R(r) \begin{pmatrix} 0 \\ Y_1^1(\theta,\phi) \end{pmatrix}$ $R(r) = \sum_K R_{Kl}(r) \underbrace{\int dr' r'^2 R^*_{Kl}(r') R(r')}_{\| (R_{Kl}(r), R(r)) \|}$

Garapena $R_{Kl}(r)$-n

4.)

$$[\Psi](r) = R(r) \begin{pmatrix} Y_0^0(\theta,\phi) + \frac{1}{\sqrt{3}} Y_1^0(\theta,\phi) \\ \frac{1}{\sqrt{3}} Y_1^1(\theta,\phi) - \frac{1}{\sqrt{3}} Y_1^0(\theta,\phi) \end{pmatrix} = \begin{pmatrix} \Psi_+(r) \\ \Psi_-(r) \end{pmatrix}$$

a) Lor bedi $R(r)$ funtzioak betetzen duen normalizazio-baldintza.

$\langle \Psi | \Psi \rangle = 1$

$$\langle \Psi | \Psi \rangle = \int d^3r \left[|\Psi_+(r)|^2 + |\Psi_-(r)|^2 \right] \overset{*}{=} \int d^3r |R(r)|^2 \Big(|Y_0^0|^2 + \frac{2}{3} |Y_1^1|^2 +$$

Y_l^m orton.

$$\frac{1}{3} |Y_1^0|^2 + Y_0^0 Y_1^{1*} + Y_1^1 Y_0^{0*} - Y_1^{1*} Y_1^0 \frac{1}{3} - Y_1^1 Y_1^{0*} \cdot \frac{1}{3} \Big) = \int dr\, r^2 |R(r)|^2$$

$$\left(1 + \frac{2}{3} + \frac{1}{3} \right) = 2 \int dr\, r^2 |R(r)|^2 = 1 \Rightarrow \int d^3r |R(r)|^2 = \frac{1}{2} \quad (1)$$

$$* \quad |\Psi_+(r)|^2 = \left(Y_0^0 + \frac{1}{\sqrt{3}} Y_1 \right)^* \left(Y_0^0 + \frac{1}{\sqrt{3}} Y_1 \right) |R(r)|^2 = \Big(|Y_0^0|^2 + \frac{1}{3} |Y_1^1|^2 + Y_0^0 Y_1^{1*} +$$

$$Y_0^{0*} Y_1^1 \Big) |R(r)|^2$$

$$|\Psi_-(r)|^2 = \left(\frac{Y_1^1}{\sqrt{3}} - \frac{Y_1^0}{\sqrt{3}} \right)^* \left(\frac{Y_1^1}{\sqrt{3}} - \frac{Y_1^0}{\sqrt{3}} \right) |R(r)|^2 = \frac{1}{3} |R(r)|^2 \Big(|Y_1^1|^2 + |Y_1^0|^2 - Y_1^{1*} Y_1^0 +$$

$$- Y_1^1 Y_1^{0*} \Big)$$

b) Lor bitez S_z behagarriaren neurketen emaitza posibleei dagozkien probabilitateak. $\pm \hbar/2$ neur daitezke.

$$dP(\hbar/2) = |\langle r, + | \Psi \rangle|^2 d^3r = |\Psi_+(r)|^2 d^3r \Rightarrow P(\hbar/2) \text{ lortzeko}$$

bolumen osoan integratu behar da.

$$P(\hbar/2) = \int dP(\hbar/2) = \int |\Psi_+(r)|^2 d^3r = \int |R(r)|^2 \Big(|Y_0^0|^2 + \frac{1}{3} |Y_1^1|^2 + Y_0^0 Y_1^{1*} +$$

$Y_0^{0*} Y_1^1) = \int |R(r)|^2 r^2 dr \left(1 + \frac{1}{3}\right) = \frac{4}{3} \int r^2 |R(r)|^2 dr = \frac{4}{3} \cdot \frac{1}{2} = \frac{2}{3}$

$\hookrightarrow Y_l^m(\theta, \phi)$ ortonormalak (1)

$P(-\hbar/2) = 1 - P(\hbar/2) = \frac{1}{3}$

$\rightarrow$ esm 3) berdo

c) $\{L_z, S_x\}$ behagarrien neurketan emaitza posibleei dagozkien probabilitateak.

$S_x \to \frac{\hbar}{2}$ eta $-\frac{\hbar}{2}$ eta $L_z \to m = 0, 1$ $(l_z = m\hbar)$

$|k\, l\, m\, \pm\rangle_x = \frac{1}{\sqrt{2}}[|k\, l\, m\, +\rangle \pm |k\, l\, m\, -\rangle]$

- $P_m^{\varepsilon, x} = \sum_K \sum_l |{}_x\langle k\, l\, m, \varepsilon | \psi\rangle|^2 = \sum_l \int dr\, r^2 |a_{lm}^{\varepsilon, x}(r)|^2$

$* |k, l, m, \varepsilon\rangle_x = \sum_{\varepsilon'} \int d^3r \underset{\langle \vec{r} | k, l, m\rangle \langle \varepsilon' | \varepsilon\rangle_x}{\underset{\parallel}{\langle \vec{r}, \varepsilon' | k\, l\, m, \varepsilon\rangle_x}} |\vec{r}, \varepsilon'\rangle = \int d^3r\, R_{kl}\, Y_l^m(\theta\, \phi) |r, \varepsilon\rangle$

$\Rightarrow \begin{cases} \langle + | +\rangle_x = \frac{1}{\sqrt{2}} = \langle +, -\rangle_x \\ \langle - | x\rangle_x = \frac{1}{\sqrt{2}} = -\langle - | -\rangle_x \end{cases}$

- $P_0^{+,x} = \sum_K \sum_l |{}_x\langle k, l, 0, + | \psi\rangle|^2 = \sum_K \sum_l \left| \left(\frac{1}{\sqrt{2}} \cdot \langle k, l, 0, + | \psi\rangle + \frac{1}{\sqrt{2}} \langle k, l, 0, - | \psi\rangle \right) \right|^2 =$

$\frac{1}{2} \sum_K \sum_l \left| \left(\int d^3r\, R_{kl}^*(r) Y_l^{*0} (\psi_+) + \int d^3r\, R_{kl}^*(r) Y_l^{*0} \psi_- \right) \right|^2 = \frac{1}{2} \left(\underbrace{\cancel{2} \left| \int d^3r |R(r)|^2 \right|^2}_{\text{Gauzki, aurreko bezala}} + \right.$

$\left. 2 \left| \int d^3r |R(r)|^2 \cancel{\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)} \right|^2 \right) = 2 \cdot \frac{1}{2} \cdot \left(\frac{1}{2}\right)^2 = \frac{1}{2^2} = \frac{1}{4}$ $\quad * \underset{\underset{1}{\parallel}}{\sum_K \left| \int r^2 dr R^*_{kl} |R(r)| \right|}$

- $P_1^{+,x} = \sum_K \sum_l \left| \left(\frac{1}{\sqrt{2}} \langle k, l, 1, + | \psi\rangle + \frac{1}{\sqrt{2}} \langle k, l, 1, - | \psi\rangle \right) \right|^2 = \frac{1}{2} \left(\cancel{2} \left| \int d^3r |R(r)|^2 \right|^2 \cdot \frac{1}{3} \right) =$

$\cancel{2} \cdot \frac{1}{2} \left| \int d^3r |R(r)|^2 \right|^2 \cdot \frac{1}{3} = \cancel{2} \cdot \frac{1}{\cancel{2}} \cdot \frac{1}{3} \left(\frac{1}{2}\right)^2 = \frac{1}{12}$?

- $P_0^{-,x} = \sum_K \sum_l |{}_x\langle k, l, 0, - | \psi\rangle|^2 = \sum_K \sum_l \left| \left(\frac{1}{\sqrt{2}} \langle l, 0, + | \psi\rangle - \frac{1}{\sqrt{2}} \langle l, 0, - | \psi\rangle \right) \right|^2 =$

$\frac{1}{2} \left(\left| \sqrt{2} \int d^3r |R(r)|^2 \right|^2 + \left| \sqrt{2} \int d^3r |R(r)|^2 \left(\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{3}} \right) \right|^2 \right) = \frac{2}{2} \cdot \left(\frac{1}{4} + \frac{1}{4} \cdot \frac{4}{3} \right) = \frac{7}{12}$

(1)

• $P_1^{-x} = \sum_l |{}_x\langle l,1,-|\psi\rangle|^2 = \sum_l \left| \frac{1}{\sqrt{2}} \langle l,1,+|\psi\rangle - \frac{1}{\sqrt{2}} \langle l,1,-|\psi\rangle \right|^2 =$

$\frac{1}{2} \sum_l |\langle l,1,+|\psi\rangle + \langle l,1,-|\psi\rangle|^2 = \frac{1}{2} \left| \frac{\sqrt{2}}{\sqrt{3}} \int d^3r \, |R(r)|^2 \right|^2 \underset{(1)}{=} \frac{\cancel{2}}{\cancel{2}} \left| \frac{1}{\sqrt{3}} \cdot \frac{1}{2} \right|^2 = \frac{1}{12}$

d) L^2 behagarriaren neurketaren emaitza 0 dela emanik, aurki bedi neurketa horren ondoren elektroiak izango duen egoerari dagokion spinorea. Aurki bedi neurketaren ondoren elektroiak izango duen egoerari dagokion spinorea, L^2 behagarriaren neurketaren emaitza $2\hbar^2$ dela jakinik.

• $L^2 \to 0 \to l=0$

$|\psi'\rangle = \sum_{m=-l}^{l} \sum_{\varepsilon} |0,m,\varepsilon\rangle\langle 0,m,\varepsilon|\psi\rangle = \sum_{\varepsilon} |0,0,\varepsilon\rangle\langle 0,0,\varepsilon|\psi\rangle = |0,0,+\rangle\langle 0,0,+|\psi\rangle +$

$|0,0,-\rangle\langle 0,0,-|\psi\rangle \Rightarrow [\psi'](r) = \begin{pmatrix} \psi'_+(r) \\ \psi'_-(r) \end{pmatrix}$ Normalizatu gabe!

* $\psi'_+ = \langle r,+|\psi'\rangle = \langle r,+|0,0,+\rangle\langle 0,0,+|\psi\rangle + \cancel{\langle r,+|0,0,-\rangle} \langle 0,0,-|\psi\rangle =$

$Y_0^0(\theta,\varphi) R(r) \langle 0,0|\psi_+\rangle = Y_0^0(\theta,\varphi) R(r)$

* $\psi'_- = \langle r,-|\psi'\rangle = \langle r,-|\cancel{0,0,+}\rangle \langle 0,0,+|\psi\rangle + \langle r,-|0,0,-\rangle\langle 0,0,-|\psi\rangle =$

$Y_0^0(\theta,\varphi) R(r) \langle 0,0|\psi_-\rangle = 0 \Rightarrow [\psi'](r) = \begin{pmatrix} \sqrt{2}\, Y_0^0(\theta,\varphi) \\ 0 \end{pmatrix} R(r)$

• $L^2 \to 2\hbar^2 \to l=1$

$|\psi'\rangle = \sum_{m=-1}^{1} \sum_{\varepsilon} |1,m,\varepsilon\rangle\langle 1,m,\varepsilon|\psi\rangle = \sum_{m=-1}^{1} \left(|1,m,+\rangle\langle 1,m,+|\psi\rangle + |1,m,-\rangle\langle 1,m,-|\psi\rangle \right)$

$[\psi'](r) = \begin{pmatrix} \psi'_+(r) \\ \psi'_-(r) \end{pmatrix}$ Normalizatu gabe!

$* \ \psi_+^{\,1} = \langle r, + | \psi' \rangle = \sum_{m=-1}^{1} \left(\langle r, + | 1, m, + \rangle \langle 1, m, + | \psi \rangle + \langle r, + \cancel{| 1, m, - \rangle} \langle 1 m, + | \psi \rangle \right) =$

$$\sum_{m=-1}^{1} \left(Y_1^m(\theta, \varphi) R(r) \langle 1, m | \psi_+ \rangle \right) = \frac{1}{\sqrt{3}} Y_1^0(\theta, \varphi) R(r)$$

$* \ \psi_-^{\,1} = \langle r, - | \psi' \rangle = \sum_{m=-1}^{1} \left(\langle r, - \cancel{| 1, m, + \rangle} \langle 1, m, + | \psi \rangle + \langle r, - | 1, 1, m, - \rangle \langle 1, m, - | \psi \rangle \right)$

$$\sum_{m=-1}^{1} \left(Y_1^m(\theta, \varphi) R(r) \langle 1, m | \psi_- \rangle \right) = \frac{1}{\sqrt{3}} Y_1^1(\theta, \phi) R(r) - \frac{1}{\sqrt{3}} Y_1^0(\theta, \phi) R(r)$$

$$A^2\left(\frac{1}{3} + \frac{1}{3} + \frac{1}{3}\right) \cdot \frac{1}{2} = 1 = \frac{A^2}{2} \rightarrow A^2 = 2 \rightarrow A = \sqrt{2}$$ Normalizatuz

$$[\psi'](r) = \sqrt{\frac{2}{3}} R(r) \begin{pmatrix} Y_1^0(\theta, \varphi) \\ Y_1^1(\theta, \varphi) - Y_1^0(\theta, \varphi) \end{pmatrix}$$

5) Kontsidera bedi $s = 1/2$ spin-a duen osziladore harmoniko unidimentsionala. Osziladore harmoniko horren egoera adierazten duen spinorea honako hau da:

$$[\psi](x) = \frac{1}{\sqrt{5}} \begin{pmatrix} \psi_0(x) \\ 2\psi_1(x) \end{pmatrix} \Rightarrow \quad \psi_n(x) \text{ hamiltondarraren autofuntzioak.}$$

$\hookrightarrow$ Normalizatzeko

a) Energiaren itxarotako balioa eta energiaren neurketen emaitza posibleei dagozkien probabilitateak.

$$\langle H \rangle = \langle \psi | H | \psi \rangle = \int d^3r \, (\psi_+^*(r) \quad \psi_-^*(r)) \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix} \frac{\hbar\omega}{2} \begin{pmatrix} \psi_+(r) \\ \psi_-(r) \end{pmatrix} =$$

$$\frac{\hbar\omega}{2} \int dx \left(\frac{\psi_0^*(x)}{\sqrt{5}} \quad \frac{3 \cdot 2}{\sqrt{5}} \psi_1^*(x) \right) \begin{pmatrix} \frac{\psi_0(x)}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} \psi_1(x) \end{pmatrix} = \frac{\hbar\omega}{2} \int d^3r \left[\frac{1}{5} |\psi_0(x)|^2 + \frac{12}{5} |\psi_1(x)|^2 \right]$$

$\psi_n(x)$ normalizatuak

$$\frac{\hbar\omega}{2} \left(\frac{1}{5} + \frac{12}{5} \right) = \frac{13}{10} \hbar\omega$$

Neur daitezkeen balioak: $n = 0, 1 \Rightarrow E_0 = \frac{\hbar\omega}{2}$, $E_1 = \frac{3\hbar\omega}{2}$

$$P_0 = \sum_{\varepsilon} |\langle 0, \varepsilon | \psi \rangle|^2 = |\langle 0, + | \psi \rangle|^2 + |\langle 0, - | \psi \rangle|^2 = |\langle 0 | \psi_+ \rangle|^2 +$$

$$|\langle 0 | \psi_- \rangle|^2 = \frac{1}{5}$$

$$P_1 = \sum_{\varepsilon} |\langle 1, \varepsilon | \psi \rangle|^2 = |\langle 1, + | \psi \rangle|^2 + |\langle 1, - | \psi \rangle|^2 = |\langle 1 | \psi_+ \rangle|^2 +$$

$$|\langle 1 | \psi_- \rangle|^2 = \frac{4}{5}$$

b) x^2 behagarriaren itxarotako balioa. $\hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+) =$

$$\frac{\hbar}{2m\omega}\left[\hat{a}^2 + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a} + \hat{a}^{+2}\right] \Rightarrow [[\hat{x}^2]] \text{ matrizea}$$

$$\bullet \; \hat{x}^2|\psi\rangle = \frac{\hbar}{2m\omega}\hat{x}^2 \int \frac{dx}{\sqrt{5}} \left[\psi_0(x)|x,+\rangle + 2\psi_1(x)|x,-\rangle\right] =$$

$$\frac{\hbar}{2\sqrt{5}m\omega}\int dx \Big((\psi_0(x) + \sqrt{2}\psi_2(x))|x,+\rangle + (4\psi_1(x) + \sqrt{6}\psi_3(x))|x,-\rangle \Big)$$

$$\bullet \; \langle\psi|\hat{x}^2|\psi\rangle = \frac{\hbar}{2\sqrt{5}m\omega}\int dx \left[\psi_0^*(x)(\psi_0(x) + \sqrt{2}\psi_2(x)) + 2\psi_1^*(x)(4\psi_1(x) + \sqrt{6}\psi_3(x))\right] =$$

$$\frac{\hbar}{2\sqrt{5}m\omega}\int \frac{dx}{\sqrt{5}}\left[|\psi_0(x)|^2 + \sqrt{2}\psi_0^*(x)\psi_2(x) + 8|\psi_1(x)|^2 + 2\sqrt{6}\psi_1^*(x)\psi_3(x)\right] =$$

ψ_n normalizatuak

$$\frac{\hbar}{10m\omega}(1+8) = \frac{9\hbar}{10m\omega}$$

c) pS_x behagarriaren itxarotako balioa. $\hat{p} = -i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a} - \hat{a}^+)$

$$\hat{p}\hat{S}_x|\psi\rangle = -i\sqrt{\frac{\hbar m\omega}{2}}\int\frac{dx}{\sqrt{5}}(\hat{a} - \hat{a}^+)\hat{S}_x\left[\psi_0(x)|x,+\rangle + 2\psi_1(x)|x,-\rangle\right] =$$

$$-i\sqrt{\frac{\hbar m\omega}{10}}\int dx\ (\hat{a}-\hat{a}^{+})\hat{S}_x\left[\Psi_0(x)\ \frac{1}{\sqrt{2}}\left(|+\rangle_x+|-\rangle_x\right)+\frac{2\Psi_1(x)}{\sqrt{2}}\left(|+\rangle_x-|-\rangle_x\right)\right]=$$

$$-i\sqrt{\frac{\hbar m\omega}{20}}\int dx\ (\hat{a}-\hat{a}^{+})\ \hbar\left[\Psi_0(x)\ \left(|+\rangle_x-|-\rangle_x\right)+2\Psi_1(x)\left(|+\rangle_x+|-\rangle_x\right)\right]=$$

$$-i\sqrt{\frac{\hbar m\omega}{20}}\int dx\ \hbar\left[-\Psi_1(x)\ \underbrace{\left(|+\rangle_x-|-\rangle_x\right)}_{=\sqrt{2}|-\rangle}+2\left(\Psi_0(x)-\sqrt{2}\Psi_2(x)\right)\underbrace{\left(|+\rangle_x+|-\rangle_x\right)}_{=\sqrt{2}|+\rangle}\right]$$

$$\langle pS_x\rangle=\langle\Psi|\hat{p}\hat{S}_x|\Psi\rangle=-i\sqrt{\frac{\hbar m\omega}{10}}\ \hbar\int\frac{dx}{\sqrt{5}}\left[-\Psi_1^*(x)\ 2\Psi_1(x)+2\Psi_0^*(x)\left(\Psi_0(x)-\sqrt{2}\Psi_2(x)\right)\right]$$

$$-i\sqrt{\frac{\hbar m\omega}{20}}\ \hbar\cdot\frac{1}{\sqrt{5}}\int dx\left[-2|\Psi_1(x)|^2+2|\Psi_0(x)|^2-2\sqrt{2}\ \Psi_0^*(x)\Psi_2(x)\right]=$$

$\Psi_n(x)$ normal.

$$-i\sqrt{\frac{\hbar m\omega}{20}}\ \frac{\hbar}{\sqrt{5}}\ (-2+2)=0$$

6) $\mathcal{E}(j_1=2, j_2=1)$ azpiespazioaren baitan lor bedi $j=3$ zenbaki kuantikoari dagokion multipletea, $|j_1, j_2, m_1, m_2\rangle$ bektoreen konbinazio lineal bezala. Lor bitez, halaber, $\mathcal{E}(j_1=1, j_2=1/2)$ azpiespazioaren baitango Clebsch-Gordan-en koefiziente guztiak.

$$|j, m\rangle = \sum_{m_1, m_2} \langle m_1, m_2 | j, m\rangle |m_1, m_2\rangle \qquad m = m_1 + m_2 = \begin{cases} 3 \\ 2 \\ 1 \\ 0 \\ -1 \\ -2 \\ -3 \end{cases} \qquad (|m_1| \le j_1, \ |m_2| \le j_1)$$

$|m| \le j$ denez $j = 3, 2, 1, \cancel{0}$

$\{|m_1, m_2\rangle\} = \{ \underset{u_1}{|2,1\rangle}, \underset{u_2}{|2,0\rangle}, \underset{u_3}{|2,-1\rangle}, \underset{u_4}{|1,1\rangle}, \underset{u_5}{|1,0\rangle}, \underset{u_6}{|1,-1\rangle}, \underset{u_7}{|0,1\rangle}, \underset{u_8}{|0,0\rangle}, \underset{u_9}{|0,-1\rangle},$
$\underset{u_{10}}{|-1,1\rangle}, \underset{u_{11}}{|-1,0\rangle}, \underset{u_{12}}{|-1,-1\rangle}, \underset{u_{13}}{|-2,1\rangle}, \underset{u_{14}}{|-2,0\rangle}, \underset{u_{15}}{|-2,-1\rangle} \}$

- $j=3$ multipletea: $|3,3\rangle = |u_1\rangle$ (Modu bakarrean lor daiteke)

$$|3,2\rangle = \frac{1}{\hbar\sqrt{6}} J_- |3,3\rangle = \frac{1}{\hbar\sqrt{6}} (J_{1-} + J_{2-})|u_1\rangle = \frac{1}{\cancel{\hbar}\sqrt{6}} (\cancel{\hbar} 2 |1,1\rangle + \cancel{\hbar}\sqrt{2}|2,0\rangle) = \frac{1}{\sqrt{3}}(\sqrt{2}|u_4\rangle + |u_2\rangle)$$

$$|3,1\rangle = \frac{1}{\hbar\sqrt{10}} J_- |3,2\rangle = \frac{1}{\hbar\sqrt{10}} (J_{1-} + J_{2-})\left(\frac{\sqrt{2}}{\sqrt{3}}|u_4\rangle + \frac{1}{\sqrt{3}}|u_2\rangle\right) = \frac{1}{\hbar\sqrt{30}} (J_{1-} + J_{2-}) (\sqrt{2}|u_4\rangle + |u_2\rangle) =$$

$$\frac{1}{\sqrt{30}\cancel{\hbar}} [\sqrt{2}\cancel{\hbar}\sqrt{6}|0,1\rangle + 2\cancel{\hbar}|1,0\rangle + \cancel{\hbar}\, 2|1,0\rangle + \sqrt{2}\cancel{\hbar}|2,-1\rangle) = \sqrt{\frac{2}{5}}|0,1\rangle + \frac{4}{\sqrt{30}}|1,0\rangle +$$

$$\frac{1}{\sqrt{15}}|2,-1\rangle = \sqrt{\frac{2}{5}}|u_7\rangle + \frac{4}{\sqrt{30}}|u_5\rangle + \frac{1}{\sqrt{15}}|u_3\rangle$$

$$|3,0\rangle = \frac{1}{\hbar\sqrt{12}} J_- |3,1\rangle = \frac{1}{\hbar\sqrt{12}} (J_{1-} + J_{2-})\left(\sqrt{\frac{2}{5}}|0,1\rangle + \frac{4}{\sqrt{30}}|1,0\rangle + \frac{1}{\sqrt{15}}|2,-1\rangle\right) = \frac{1}{\hbar\sqrt{12}}\left(\sqrt{\frac{2}{5}}\cancel{\hbar}\sqrt{6}|-1,1\rangle + \right.$$

$$\frac{4}{\sqrt{30}}\cancel{\hbar}\sqrt{6}|0,0\rangle + \frac{1}{\sqrt{15}}\cancel{\hbar}2|1,-1\rangle + \sqrt{\frac{2}{5}}\cancel{\hbar}\sqrt{2}|0,0\rangle + \frac{4}{\sqrt{30}}\cancel{\hbar}\sqrt{2}|1,-1\rangle\Big) =$$

$$\frac{1}{\sqrt{5}}|-1,1\rangle + \frac{3}{\sqrt{15}}|0,0\rangle + \frac{1}{\sqrt{5}}|1,-1\rangle$$

$|3,-3\rangle = |u_{15}\rangle$ (Modu bakarrean lor daiteke)

$$|3,-2\rangle = \frac{1}{\hbar\sqrt{6}} J_+ |3,-3\rangle = \frac{1}{\hbar\sqrt{6}} (J_{1+} + J_{2+})|u_{15}\rangle = \frac{1}{\hbar\sqrt{6}} (\hbar 2|-1,-1\rangle + \sqrt{2}|-2,0\rangle) = \frac{1}{\sqrt{3}}(\sqrt{2}|u_{12}\rangle + |u_{14}\rangle)$$

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$$|3,-1\rangle = \frac{1}{\hbar\sqrt{10}} J_+ |3,-2\rangle = \frac{1}{\hbar\sqrt{10}} (J_{1+}+J_{2+})\left(\sqrt{\frac{2}{3}}\,|u_{12}\rangle + \frac{1}{\sqrt{3}}|u_{14}\rangle\right) = \frac{1}{\cancel{\hbar}\sqrt{30}}\left(\sqrt{2}\,\cancel{\hbar}\sqrt{6}\,|0,-1\rangle + \right.$$

$$\left.\cancel{\hbar}\,2\,|-1,0\rangle + \cancel{\hbar}\sqrt{2}\sqrt{2}\,|-1,0\rangle + \cancel{\hbar}\sqrt{2}\,|-2,1\rangle\right) = \sqrt{\frac{2}{5}}\,|0,-1\rangle + \frac{4}{\sqrt{30}}|-1,0\rangle + \frac{1}{\sqrt{15}}|-2,1\rangle$$

- $\mathcal{E}(j_1=1, j_2=1/2)$ azpiespazioan baitongo Clebsch-Gordan-en koefizienteak:

$$|j,m\rangle = \sum_{m_1,m_2} \langle m_1,m_2|j,m\rangle |m_1,m_2\rangle \qquad m = m_1+m_2 = \begin{cases} 3/2 \\ 1/2 \\ -1/2 \\ -3/2 \end{cases} \rightarrow |m|\le j \rightarrow j = 3/2,\ 1/2$$

$$\{|m_1,m_2\rangle\} = \{\underset{u_1}{|1,1/2\rangle}, \underset{u_2}{|1,-1/2\rangle}, \underset{u_3}{|0,1/2\rangle}, \underset{u_4}{|0,-1/2\rangle}, \underset{u_5}{|-1,1/2\rangle}, \underset{u_6}{|-1,-1/2\rangle}\}$$

- $j=3/2 \Rightarrow |3/2,3/2\rangle = |u_1\rangle$ (modu bakarrean lor daiteke)

$|3/2,-3/2\rangle = |u_6\rangle$ (modu bakarrean lor daiteke)

$$|3/2,1/2\rangle = \frac{1}{\hbar\sqrt{3}} J_- |3/2,3/2\rangle = \frac{1}{\hbar\sqrt{3}}(J_{1-}+J_{2-})(|1,1/2\rangle) = \frac{1}{\cancel{\hbar}\sqrt{3}}\left(\sqrt{2}\,\cancel{\hbar}\,|0,1/2\rangle + 1\cdot\cancel{\hbar}\right.$$

$$\left.|1,-1/2\rangle\right) = \sqrt{\frac{2}{3}}\,|0,1/2\rangle + \frac{1}{\sqrt{3}}|1,-1/2\rangle$$

$$|3/2,-1/2\rangle = \frac{1}{\hbar\sqrt{3}} J_+ |3/2,-3/2\rangle = \frac{1}{\hbar\sqrt{3}}(J_{1+}+J_{2+})|-1,-1/2\rangle = \frac{1}{\cancel{\hbar}\sqrt{3}}\left(\sqrt{2}\,\cancel{\hbar}\,|0,-1/2\rangle + \right.$$

$$\left.\cancel{\hbar}\,|-1,1/2\rangle\right) = \sqrt{\frac{2}{3}}\,|0,-1/2\rangle + \frac{1}{\sqrt{3}}|-1,1/2\rangle$$

- $j=1/2 \Rightarrow |1/2,1/2\rangle = \alpha\,|0,1/2\rangle + \beta\,|1,-1/2\rangle \rightarrow$ ortogonaltasuna opliketu:

$$\langle 3/2,1/2|1/2,1/2\rangle = \sqrt{\frac{2}{3}}\,\alpha + \frac{\beta}{\sqrt{3}} = 0 \rightarrow \alpha = -\frac{\beta}{\sqrt{2}} \rightarrow \beta = -\sqrt{2}\,\alpha$$

$$|1/2,1/2\rangle = \frac{1}{\sqrt{3}}\left(|0,1/2\rangle - \sqrt{2}\,|1,-1/2\rangle\right) = \frac{1}{\sqrt{3}}|0,1/2\rangle - \sqrt{\frac{2}{3}}\,|1,-1/2\rangle$$

$|1/2,-1/2\rangle = \alpha\,|-1,1/2\rangle + \beta\,|0,-1/2\rangle \rightarrow$ ortogonaltasuna opliketu:

$$\langle 3/2,-1/2|1/2,-1/2\rangle = \alpha\sqrt{\frac{1}{3}} + \beta\sqrt{\frac{2}{3}} = 0 \rightarrow \beta = -\frac{\alpha}{\sqrt{2}} \rightarrow \alpha = -\sqrt{2}\,\beta$$

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

Clebsch-Gordan-en koefizienteak:

$\langle 1,1/2\,|\,3/2,3/2\rangle = 1$; $\langle 1,1/2\,|\,3/2,1/2\rangle = 0$, $\langle 1,1/2\,|\,3/2,-1/2\rangle = 0$,

$\langle 1,1/2\,|\,3/2,-3/2\rangle = 0$, $\langle 1,-1/2\,|\,3/2,3/2\rangle = 0$, $\langle 1,-1/2\,|\,3/2,1/2\rangle = \frac{1}{\sqrt3}$,

$\langle 1,-1/2\,|\,3/2,-1/2\rangle = 0$, $\langle 1,-1/2\,|\,3/2,-3/2\rangle = 0$, $\langle 0,1/2\,|\,3/2,3/2\rangle = 0$,

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

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

$\langle 0,-1/2\,|\,3/2,-3/2\rangle = 0$, $\langle -1,1/2\,|\,3/2,3/2\rangle = 0$, $\langle -1,1/2\,|\,3/2,1/2\rangle = 0$,

$\langle -1,1/2\,|\,3/2,-1/2\rangle = \frac{1}{\sqrt3}$; $\langle -1,1/2\,|\,3/2,-3/2\rangle = 0$, $\langle -1,-1/2\,|\,3/2,3/2\rangle = 0$,

$\langle -1,-1/2\,|\,3/2,1/2\rangle = 0$, $\langle -1,-1/2\,|\,3/2,-1/2\rangle = 0$, $\langle -1,-1/2\,|\,3/2,-3/2\rangle = 1$

7.) $j_1 = j_2 = 1 \rightarrow m_1, m_2 = 1,0,-1 \rightarrow m = m_1 + m_2 = \left\{\begin{array}{c} 2 \\ 1 \\ 0 \\ -1 \\ -2 \end{array}\right. \rightarrow j = 0,1,2$

a) $m_1 = 1$ eta $m_2 = -1$ direla emanik, izan litezke j delakoak har ditzakeen balioak eta dagozkien probabilitateak:

$m = m_1 + m_2 \Rightarrow m = 0 \rightarrow j = 0,1,2$ izan daiteke ; $|\overset{m_1}{1},\overset{m_2}{-1}\rangle$ egoera

• $j = 2 \Rightarrow |\overset{j}{2},\overset{m}{2}\rangle = |1,1\rangle$; $|2,1\rangle = \frac{1}{\hbar 2} J_- |2,2\rangle = \frac{1}{2\hbar}(J_{1-} + J_{2-})|1,1\rangle =$

$\frac{1}{2\cancel{\hbar}}(\sqrt2\cancel{\hbar}\,|0,1\rangle + \sqrt2\cancel{\hbar}\,|1,0\rangle) = \frac{1}{\sqrt2}(|0,1\rangle + |1,0\rangle)$

$|\overset{j}{2},\overset{m}{0}\rangle = \frac{1}{\hbar\sqrt6} J_- |2,1\rangle = \frac{1}{\hbar\sqrt6}(J_{1-} + J_{2-})\frac{1}{\sqrt2}(|\overset{m_1}{0},\overset{m_2}{1}\rangle + |\overset{m_1}{1},\overset{m_2}{0}\rangle) = \frac{1}{2\sqrt3\cancel{\hbar}}(\sqrt2\cancel{\hbar}\,|-1,1\rangle +$

$\sqrt2\cancel{\hbar}\,|0,0\rangle + \sqrt2\cancel{\hbar}\,|0,0\rangle + \sqrt2\cancel{\hbar}\,|1,-1\rangle) = \frac{1}{\sqrt6}(|-1,1\rangle + |1,-1\rangle + 2|0,0\rangle)$

$P_{j=2} = |\langle 2,0\,|\,1,-1\rangle|^2 = \frac{1}{6}$

• $j=1 \Rightarrow |1,1\rangle = \alpha|0,1\rangle + \beta|1,0\rangle \Rightarrow$ ortogonaltasuna aplikatu:

$$\langle 2,1|1,1\rangle = \frac{\alpha}{\sqrt{2}} + \frac{\beta}{\sqrt{2}} = 0 \rightarrow \alpha = -\beta \Rightarrow |1,1\rangle = \frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle)$$

$$|1,0\rangle = \frac{1}{\sqrt{2}\hbar} J_- |1,1\rangle = \frac{1}{\sqrt{2}\hbar}(J_{1-} + J_{2-})\frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle) = \frac{1}{2\cancel{\hbar}}\left(\sqrt{2}\cancel{\hbar}|-1,1\rangle + \right.$$

$$\left. - \cancel{\sqrt{2}\hbar|0,0\rangle} + \cancel{\sqrt{2}\hbar|0,0\rangle} - \sqrt{2}\cancel{\hbar}|1,-1\rangle\right) = \frac{1}{\sqrt{2}}(|-1,1\rangle - |1,-1\rangle)$$

$$P_{j=1} = |\langle 1,0|1,-1\rangle|^2 = \frac{1}{2}$$

• $j=0 \Rightarrow |0,0\rangle = \alpha|1,-1\rangle + \beta|-1,1\rangle + \gamma|0,0\rangle \Rightarrow$ ortogonaltasuna:

$$\langle 0,0|1,0\rangle = \frac{\beta}{\sqrt{2}} - \frac{\alpha}{\sqrt{2}} = 0 \rightarrow \alpha = \beta$$

$$\langle 0,0|2,0\rangle = \frac{\alpha}{\sqrt{6}} + \frac{\beta}{\sqrt{6}} + \frac{2\gamma}{\sqrt{6}} = 0 \rightarrow \alpha + \beta = -2\gamma = 2\alpha \rightarrow \gamma = -\alpha$$

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

$$P_{j=0} = |\langle 0,0|1,-1\rangle|^2 = \frac{1}{3}$$

* Oharra: $P_{j=0} + P_{j=1} + P_{j=2} = 1$ dela.

b) $j=2$ eta $m=1$ direla emanik, lor bitez $(J_1)_z$ delakoak har ditzaken balioak eta dagozkien probabilitateak.

$|2,1\rangle = \frac{1}{\sqrt{2}}(|0,1\rangle + |1,0\rangle) \rightarrow J_{1z}$ $\hbar$ eta 0 balioak hartu ahal izango ditu $\Rightarrow$

$$\left.\begin{aligned} P_\hbar &= \sum_{i=-1}^{1} |\langle 1,i|2,1\rangle|^2 = \frac{1}{2} \\ P_0 &= \sum_{i=-1}^{1} |\langle 0,i|2,1\rangle|^2 = \frac{1}{2} \end{aligned}\right\} P_\hbar + P_0 = 1$$

$\sigma_y = i\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

FISIKA KUANTIKOA

Kontrola — *2017.eko Martxoak 24*

1. Kontsidera dezagun bi dimentsioko bektore-espazio baten $\{|1>, |2>\}$ oinarri ortonormala. Kontsidera dezagun, halaber, bi dimentsioko bektore-espazio horretako Pauli-ren σ_y matrizea.
   (a) σ_y matrizea hermitearra al da? Kalkula bitez autobalioak eta autobektore normalizatuak.
   (b) Lor bitez σ_y-ren autobektoreetara proiektatzen duten proiektoreen matrizeak. Froga bedi proiektore horiek ortogonalak direla eta itxitura-erlazioa betetzen dutela.

   Kontsidera ditzagun orain hiru dimentsioko bektore-espazio baten $\{|1>, |2>, |3>\}$ oinarri ortonormala eta bektore-espazio horretako J_y matrizea.
   (c) J_y matrizea hermitearra al da? Kalkula bitez autobalioak eta autobektore normalizatuak.
   (d) Lor bitez J_y-ren autobektoreetara proiektatzen duten proiektoreen matrizeak. Froga bedi proiektore horiek ortogonalak direla eta itxitura-erlazioa betetzen dutela.

2. Zeeman bakarrik + eEx
   (a) Kontsidera bedi **E** eta **B** eremu estatiko eta uniformeen eraginpean kokaturiko hidrogeno-atomoa (**B** handia eta **E** txikia). Kalkula bitez, bigarren ordenako eta ordena altuagoko gaiak arbuiatuz, elektroiaren spin momentu angeluarra barne hartuta eta ekarpen erlatibistak (egitura mehea) alde batera utzita, $n = 2$ energiak eta egoera geldikorrak, **E** eta **B** paraleloak direnean nahiz **E** eta **B** perpendikularrak direnean. Zeeman + Stark
   (b) Kontsidera bedi **B** eremu estatiko eta uniformearen eraginpean kokaturiko hidrogeno-atomoa (**B** handia). Ekarpen erlatibistak (egitura mehea) perturbazio bezala hartuz gero, zeintzuk dira ordena txikieneko autobektoreak?

FISIKA KUANTIKOA 2. KUATRIA 1. partea

Gehen V. I : II (+1 eta 2 ariz.) + ~~VI~~ + II D, E, F + VI A, C + II A, B + IX A, B, C + X

V. II : XI A, B, C, (A. XI, C. XI, E. XI) + C. XI, E. XI, XII, E. XI

$\boxed{\mathcal{H}_{\vec{r}}}$ → Spin-ik ez (espazio espazioa)

$\langle u_i | u_j \rangle = \delta_{ij}$

- Autobektore bat oinarri baten garatu $\{|u_i\rangle\}$: $|\Psi\rangle = \sum_i c_i |u_i\rangle$

$* \; c_i = (u_i, \Psi) = \langle u_i | \Psi \rangle$ Oinarri diskretua $\Rightarrow \sum_i u_i(\vec{r}) u_i^*(\vec{r}') = \delta(\vec{r}-\vec{r}')$

$\sum_i |u_i\rangle\langle u_i| = \mathbb{1}$

Itxidura erlazioa

$|\Psi\rangle = \int g(\alpha) |w_\alpha\rangle d\alpha$ $\{|w_\alpha\rangle\}$ oinarri jarraitua

$\Rightarrow \int w_\alpha(\vec{r}) w^*_\alpha(\vec{r}') d\alpha = \delta(\vec{r}-\vec{r}')$; $\int |w_\alpha\rangle\langle w_\alpha| d\alpha = \mathbb{1}$

$* \; g(\alpha) = \langle w_\alpha | \Psi \rangle$ $\langle w_\alpha | w_{\alpha'} \rangle = \delta(\alpha-\alpha')$

- Bi autobektore oinarri berean garatuta badaude: $\langle \Psi_1 | \Psi_2 \rangle = \sum_i c_i^* d_i$ (diskretua)

$\langle \Psi_1 | \Psi_2 \rangle = \int g_1^*(\alpha) g_2(\alpha) d\alpha$ $|\vec{p}\rangle = |p_x, p_y, p_z\rangle$

- $\vec{p}$-ren autobektoreak: $|\vec{p}\rangle$, $\langle \vec{r} | \vec{p} \rangle = \Psi_p(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i(\vec{p}\cdot\vec{r})/\hbar}$ (Jarraitua)

$|\Psi\rangle = \int g(\vec{p}) |\vec{p}\rangle d^3p$, $\overset{\Psi(p)}{g}(\vec{p}) = \langle \vec{p} | \Psi \rangle$ Fourieren transformatua

$* \; g(\vec{p}) = \langle \vec{p} | \Psi \rangle = \langle \vec{p} | \underbrace{\int |\vec{r}\rangle\langle\vec{r}| d^3r}_{\mathbb{1}} | \Psi \rangle = \int \langle \Psi_p | \vec{r} \rangle \langle \vec{r} | \Psi \rangle d^3r =$

$\int \langle \vec{r} | \vec{p} \rangle^* \langle \vec{r} | \Psi \rangle d^3r = \int \Psi(\vec{r}) \frac{1}{(2\pi\hbar)^{3/2}} e^{-i(\vec{p}\cdot\vec{r})/\hbar}$ $\int |\vec{p}\rangle\langle\vec{p}| d^3p = \mathbb{1}$

- $\vec{r}$-ren autobektoreak: $|\vec{r}\rangle$ $\langle \vec{r} | \vec{r}' \rangle = \delta(\vec{r}-\vec{r}') = \xi_{\vec{r}'}$ (Jarraitua)

$* \; |\Psi\rangle = \int g(\vec{r}) |\vec{r}\rangle d^3r$, $g(\vec{r}) = \langle \vec{r} | \Psi \rangle = \Psi(\vec{r})$ $(|\vec{r}\rangle = |x, y, z\rangle)$

Itxidura erlazioa: $\int |\vec{r}\rangle\langle\vec{r}| d^3r = \mathbb{1}$

- $|\Psi\rangle \in \mathcal{H}$ "ket"; $\langle \Psi | \in \mathcal{H}^*$ "bra" $\rightarrow \langle \Psi | \Psi \rangle \in \mathbb{C}$, $|\Psi\rangle\langle\Psi|$ eragilea

- Oinarri mixtoa: $\{|u_i\rangle, |w_\alpha\rangle\} \Rightarrow \begin{cases} \langle u_i | u_j \rangle = \delta_{ij} \\ \langle w_\alpha | w_{\alpha'} \rangle = \delta(\alpha-\alpha') \\ \langle u_i | w_\alpha \rangle = 0 \end{cases}$

itxidura erlazioa

$\sum_i u_i(\vec{r}) u_i^*(\vec{r}') + \int d\alpha \, w_\alpha^*(\vec{r}') w_\alpha(\vec{r}) = \delta(\vec{r}-\vec{r}')$

$\delta(\vec{r}-\vec{r}') = \delta(x-x')\delta(y-y')\delta(z-z')$

• $\langle \lambda\psi| = \lambda^* \langle\psi|$, $|\lambda\psi\rangle = \lambda|\psi\rangle$; $\langle A\psi| = \langle\psi|A^+$, $|A\psi\rangle = A|\psi\rangle$ Eragileak

$\langle\psi|A^+|\phi\rangle = \langle\phi|A|\psi\rangle^*$ ↳ Eragile hermitikoa ↔ $A^+ = A$

Eragileak $AB|\psi\rangle = A(B|\psi\rangle)$, $[A,B] = AB - BA$ Eragile unitarioa $UU^+ = U^+U = \mathbb{1}$

Proiektoreak: * $P_\psi = |\psi\rangle\langle\psi|$ → $P_\psi^+ = P_\psi$, $|P_\psi|^2 = P_\psi$ Idempotentea

$(\|\psi\| = \sqrt{\langle\psi|\psi\rangle} = 1)$

$P_\psi|\phi\rangle = |\psi\rangle\langle\psi|\phi\rangle = \langle\psi|\phi\rangle|\psi\rangle$ $|\phi\rangle$-ren proiekzioa $|\psi\rangle$-ren gainean.

↘ biderkagarri bat da

* Azpiespazio batean ⇒ $\{|\psi_q\rangle\}$ H_q-ren oinarria: $P_q = \sum_q |\psi_q\rangle\langle\psi_q|$ →

↳ $\langle\psi_{q_1}|\psi_{q_2}\rangle = \delta_{q_1 q_2}$

$P_q^+ = P_q$, $\langle\psi_q|\psi_q\rangle = 1 \Rightarrow P_q^2 = P_q$

→ $\{|\psi_q\rangle\}$ oinarriko autobektoreen konbinazio lineala

$P_q|\phi\rangle = \sum_q \langle\psi_q|\phi\rangle|\psi_q\rangle$ → $|\phi\rangle$-ren proiekzioa H_q azpiespazioan.

Adjuntua: $(A^+)^+ = A$, $(\lambda A)^+ = \lambda^* A^+$, $(BA)^+ = A^+B^+$, $(A+B)^+ = A^+ + B^+$

$(|u\rangle\langle v|)^+ = |v\rangle\langle u|$

• Matrizialki ⇒ $\{|u_i\rangle\}$ oinarria eta $|\psi\rangle \in \mathcal{H}$: $|\psi\rangle = \sum_i c_i|u_i\rangle$ → $|\psi\rangle$-ri

$\begin{pmatrix} c_i \\ \vdots \end{pmatrix}$ c_i matrize zutabea dagokio ⟷ $\langle\psi|$-ri c_i^* lerro matrizea $(c_i^* \ldots)$

Oinarria jarraitua bada α balio bakoitzeko c_α bat (infinitu) $\begin{pmatrix} c_\alpha \\ \vdots \\ \vdots \end{pmatrix} \downarrow \alpha$

* $\langle\psi|\phi\rangle = (c_1^* \ldots c_n^*) \begin{pmatrix} d_1 \\ \vdots \\ d_n \end{pmatrix} = \sum_i c_i^* d_i$

edo $\langle\psi|\phi\rangle = (c_\alpha^* \ldots) \begin{pmatrix} d_\alpha \\ \vdots \end{pmatrix} = \int d_\alpha c^*_\alpha \, d\alpha$

* A ere matrize bat → $A = \begin{pmatrix} & \end{pmatrix}$ $\langle u_i|A|u_j\rangle = A_{ij}$

$\langle w_\alpha|A|w_{\alpha'}\rangle = A_{\alpha\alpha'}$

$A|\psi\rangle = (A_{ij})(c_j) = \sum_j A_{ij} c_j = (c_i)$ (Hermitikoa bada $A_{ij} = A_{ji}^*$)

$\langle\psi|A|\phi\rangle = \sum_i\sum_j c_i^* A_{ij} d_j$

$A|\psi\rangle = \int A(\alpha,\alpha') c(\alpha') d\alpha'$, $\langle\psi|A|\phi\rangle = \iint A(\alpha,\alpha') c^*(\alpha) d(\alpha') d\alpha' d\alpha$

Oinarriak lortu ⇒ Eragileen autobektoreak. $A|\psi\rangle = \lambda|\psi\rangle \Rightarrow |A-\lambda\mathbb{I}|=0$

A hermitikoa $\begin{cases} \lambda \in \mathbb{R} \\ \lambda \neq \mu \Rightarrow |\phi_\lambda\rangle \perp |\phi_\mu\rangle \text{ ortogonalak} \\ g \text{ ordenako endakapena } \lambda\text{-n} \Rightarrow \mathcal{H}_\lambda \text{ azpiespazioa } \{|\psi_\lambda^i\rangle\} \quad i=1,\dots,g \end{cases}$

Endakapena badago autobektore ortonormalak aukeratu daitezke ere ⇒ $\{|\psi_\lambda^i\rangle\}$ oinarri oton.

itxitura erlazioa endakapena dagoenean

- $\langle\psi_n^i|\psi_m^j\rangle = \delta_{nm}\delta_{ij}$
- $\sum_n \sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i| = \mathbb{1}$

(oinarri diskretua bada)

$$|\psi\rangle = \sum_n \sum_{i=1}^{g_n} \langle\psi_n^i|\psi\rangle |\psi_n^i\rangle$$ (endakapenean indizi gehiago behar badira serie gehiago jarri)

Eragile bat behagarria da bere autobektoreen sistema ortonormalak egoera-espazioan oinarri bat osatzen badu.

Endakapena badago ⇒ $\hat{P}_n = \sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i|$ $\mathcal{E}_n$ azpiespazioan proiektatu.

Orduan ⇒ $A = \sum_n a_n \hat{P}_n$ ($a_n \to$ autobalioak)

* R, P behagarriak:

$\vec{R} \Rightarrow \{|\vec{r}\rangle\}$ $\mathcal{H}_r$-ren oinarria: $\langle\vec{r}|\hat{R}|\psi\rangle = \vec{R}\langle\vec{r}|\psi\rangle$ $\to \hat{X}, \hat{Y}, \hat{Z}$

$\vec{P} \Rightarrow \{|\vec{p}\rangle\}$ $\mathcal{H}_r$-ren oinarria: $\langle\vec{p}|\hat{P}|\psi\rangle = \vec{P}\langle\vec{p}|\psi\rangle$, $\langle\vec{r}|\hat{P}|\psi\rangle$ $\{|\vec{r}\rangle\}$ adierazpidean (representation)

$\begin{cases} \langle\vec{r}|\hat{P}_x|\psi\rangle = \frac{\hbar}{i}\partial_x\langle\vec{r}|\psi\rangle \\ \langle\vec{r}|\hat{P}_y|\psi\rangle = \frac{\hbar}{i}\partial_y\langle\vec{r}|\psi\rangle \\ \langle\vec{r}|\hat{P}_z|\psi\rangle = \frac{\hbar}{i}\partial_z\langle\vec{r}|\psi\rangle \end{cases}$

$\hat{Y}, \hat{Z}$-rekin gauza bera

$x\,\delta(r-r_0) = x_0\langle r|r_0\rangle$

$\hat{X}$-ren autobektoreak ⇒ $\langle\vec{r}|\hat{X}|\vec{r}_0\rangle = x\langle\vec{r}|\vec{r}_0\rangle = x\,\underbrace{\delta(x-x_0)\delta(y-y_0)\delta(z-z_0)}_{\delta(r-r_0)} \Rightarrow \hat{X}|r_0\rangle = x_0|r_0\rangle$

$|\vec{r}_0\rangle$ autobektorea ⇒ $\mathcal{H}_x$-n x_0 balioari $|x_0\rangle$ balioa (ez-endakatua) baina

$\mathcal{H}_r$-n endakatua (y eta z zehaztugabe) : $|\vec{r}_0\rangle = |x_0, y, z\rangle$ → zehaztu gabe

$\hat{X}, \hat{Y}$ eta $\hat{Z}$-k autobektore komuna ⇒ $|\vec{r}\rangle$

$\langle p|\vec{p}_0\rangle = p_x\,\delta(\vec{p}-\vec{p}_0) = p_{x0}\,\delta(\vec{p}-\vec{p}_0)$

$\hat{P}_x$-ren autobektoreak ⇒ $\langle\vec{p}|\hat{P}_x|\vec{p}_0\rangle = \overset{p_x}{P_{x0}}\langle\vec{p}|\vec{p}_0\rangle = \langle\vec{p}|p_{x0}|\vec{p}_0\rangle \Rightarrow \hat{P}_x|\vec{p}_0\rangle = p_{x0}|\vec{p}_0\rangle$

Endakapena $\mathcal{H}_r$-n baina ez $\mathcal{H}_x$-n. ⇒ $\hat{P}_x, \hat{P}_y$ eta $\hat{P}_z$-k autobektore komuna: $|\vec{p}\rangle$

Behagarri trukakorrak: $[A,B]=0 \to$ A eta B-k autobektoreen oinarri komuna dute

$\{|\psi_n^i\rangle\}$ A-ren autobektoreen oinarria ⇒ $\underbrace{AB|\psi_n^i\rangle}= BA|\psi_n^i\rangle = Ba_n|\psi_n^i\rangle = a_n\,\underbrace{B|\psi_n^i\rangle}$

$B|\psi_n^i\rangle$ A-ren autobektorea da a_n autobalioarekin → $B|\psi_n^i\rangle \in \mathcal{E}_n \Rightarrow B|\psi_n^i\rangle = \sum_{i=1}^{g_n}\alpha_i|\psi_n^i\rangle$

Bi aukera: • $g_n = 1 \Rightarrow$ $B|\psi_n^i\rangle = b_n|\psi_n^i\rangle \rightarrow$ orduan $|\psi_n^i\rangle$ B-ren autobektorea da (bien autobektorea, A eta B-renak) ↳ B-ren autobalioak

• $g_n > 1 \Rightarrow$ (endakapena) $\Rightarrow$ B-ri dagokion matrizea $\{|\psi_n^i\rangle\}$ oinarrian blokeka diagonala da. *Blokeak ordenean ez dira diagonalak*

(Bloke bakoitza A-ren autobalio bakoitzari dagokion azpiespazioari dagokiona, ε_n) $\Rightarrow$ Hau diagonalizatuz A eta B-ren aldiberako oinarria lor dezakegu $|\varphi_n^i\rangle$

$$(B) = \begin{pmatrix} \boxed{\varepsilon_1} & & \\ & \boxed{\varepsilon_2} & \\ & & \boxed{\varepsilon_3} \end{pmatrix}$$

$* \langle\psi_n^i|B|\psi_m^j\rangle = \langle\psi_n^i|\sum_{k=1}^{g_m}\alpha_k|\psi_m^k\rangle = \sum_{k=1}^{g_m}\alpha_k\langle\psi_n^i|\psi_m^k\rangle$

$\sum_{k=1}^{g_m}\alpha_k\,\delta_{nm}\,\delta_{ik} = \alpha_i\,\delta_{nm} \rightarrow n \neq m$ matrize elementua nulua

$\{A, B, \ldots\}$ trukakorrak diren eragileen multzoa: $(a_n, b_n, \ldots)$ multzoari
($A \to a_n$, $B \to b_n$)
aldiberako autobektore bakarra badagokio $\rightarrow$ multzo betea $\Rightarrow$ BTMB

$*$ A ez-endakatua bada $\{A\}$ BTMB da

$|x_0\rangle \otimes |y_0\rangle \otimes |z_0\rangle$

Adibidez: $\{\hat{X}, \hat{Y}, \hat{Z}\}$-k BTMB osatzen dute $\mathcal{H}_{r}$-n $\Rightarrow$ (x_0, y_0, z_0) zehaztuz $\Rightarrow |r_0\rangle$ bakarra
$\{\hat{P}_x, \hat{P}_y, \hat{P}_z\}$-k BTMB osatzen dute $\mathcal{H}_{r}$-n $\Rightarrow (p_{x0}, p_{y0}, p_{z0})$ zehaztuz $\Rightarrow |p_0\rangle$ bakarra

Neurketak $\Rightarrow$ A behagarria neurtu $\rightarrow$ a_n autobalioak neur daitezke soilik $\Rightarrow$ a_n neurtzeko probabilitatea: $P_n = \sum_{i=1}^{g_n}|\langle\varphi_n^i|\psi\rangle|^2$ ($\{|\varphi_n^i\rangle\}$ A-ren autobekt. oinarria)

a_n neurtzen badugu $\rightarrow$ kolapsatu $\rightarrow$ Hasierako egoera ε_n espazioan proiektatu:

$$|\psi'\rangle = \frac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}} \quad \left(\hat{P}_n = \sum_{i=1}^{g_n}|\varphi_n^i\rangle\langle\varphi_n^i|\right)$$

$\rightarrow$ Normalizazioa

$*$ Bi behagarri trukakorrak badira aldiberean neur daitezke $\Rightarrow$ a_n eta b_n neurtzeko probabilitatea: $P_n = \sum_{i=1}^{g_n}|\langle\omega_n^i|\psi\rangle|^2$ non $\{|\omega_n^i\rangle\}$ A eta B-ren aldiberako autobektoreen oinarria den. a_n eta b_n neurtzen baditugu ε_n espazioan proiektatu:

$$|\psi'\rangle = \frac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}} \quad \left(\hat{P}_n = \sum_{i=1}^{g_n}|\omega_i^i\rangle\langle\omega_n^i|\right)$$

Trukakorrak ez badira ezin dira aldi berean neurtu.

Egoeraren denborarekiko garapena Schr. ekuazioaren soluzioa: $i\hbar\frac{\partial|\psi\rangle(t)}{\partial t} = H|\psi(t)\rangle$

Batez bestekoak ⇒ $\langle A \rangle = \sum_n P_n a_n$, $\left(P_n = \sum_{i=1}^{g_n} |\langle \varphi_n^i | \psi \rangle|^2 \right)$

* $\langle A \rangle_\psi = \sum_n \sum_{i=1}^{g_n} \langle \psi_n | a_n | \varphi_n^i \rangle \langle \varphi_n^i | \psi \rangle = \langle \psi | \hat{A} | \psi \rangle = \underbrace{(c_1^* \cdots c_n^*)}_{\text{oinarri berean}} (A_{ij}) \begin{pmatrix} c_1 \\ c_n \end{pmatrix}$

* $\Delta A^2 = \langle A^2 \rangle - \langle A \rangle^2$

Momentu angeluarra: $\hat{\vec{L}}$ momentu angelear orbitala → klasikoa ⇒ $\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$

$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$, $[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$, $[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$ $\quad \hat{L}_z \to \hat{L}_x \to \hat{L}_y \to \hat{L}_z$

$[\hat{L}^2, \hat{\vec{L}}] = 0$ $\quad ([\hat{L}_x, \hat{L}^2] = [\hat{L}_y, \hat{L}^2] = [\hat{L}_z, \hat{L}^2] = 0)$ edozein bektorek momentu angelear bat izateko bete behar dituen erlazioak.

L^2 eta L_z-k BTMB osatzen dutenez aldiberako oinarria osatzen dute:

* $|k\, l\, m_l\rangle \Rightarrow \langle \vec{r} | k\, l\, m_l \rangle = R_{kl}(r)\, Y_l^{m}(\theta, \varphi)$ → Harmoniko esferikoak

→ endekapena adierazteko indizea

$$\begin{cases} L^2 |k\, l\, m_l\rangle = l(l+1)\hbar^2 |k\, l\, m_l\rangle & l \in \mathbb{N} \\ L_z |k\, l\, m_l\rangle = \hbar m_l |k\, l\, m_l\rangle & m_l \in \mathbb{Z} \quad (|m_l| \le l) \end{cases}$$

* $V(r)$ zentrala bada $[L^2, H] = [L_x, H] = [L_y, H] = [L_z, H] = 0$

Orokortuz ⇒ $\hat{\vec{J}}$ momentu angeluarra $\quad (\hat{\vec{J}} = \hat{\vec{S}} + \hat{\vec{L}}$ → spin momentua + m. ang. orbitala)

$\hat{\vec{J}} \begin{cases} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{cases}$ Momentu angeluarraren erlazioak betetzen ditu (goikoak):

$\hat{\vec{J}} = \sum_{i=1}^{N} \hat{\vec{J}}_i$ $\quad$ (N → partikula kopurua)

(j, m) finkatuta balio hauek dituzten kopurua
↑ autobektore

• $\{\hat{J}^2, \hat{J}_z\}$ BTMB ⇒ aldiberako oinarria: $\{|k, j, m\rangle\}$ $\quad \begin{cases} \hat{J}^2 |k\, j\, m\rangle = \hbar^2 j(j+1) |k\, j\, m\rangle \\ J_z |k\, j\, m\rangle = m\hbar |k\, j\, m\rangle \end{cases}$

$\begin{cases} J_+ = J_x + iJ_y \\ J_- = J_x - iJ_y \end{cases} \Rightarrow (J_+)^+ = J_- \Rightarrow \begin{cases} J_x = \frac{J_+ + J_-}{2} \\ J_y = \frac{J_+ - J_-}{2i} \end{cases} \Rightarrow \begin{cases} J_+J_- = J^2 - J_z^2 + \hbar J_z \\ J_-J_+ = J^2 - J_z^2 - \hbar J_z \end{cases}$

• $J_\pm |k\, j\, m\rangle = \hbar \sqrt{j(j+1) - m(m\pm1)}$

$\mathcal{H}$ espazioa ⇒ $\mathcal{E}(j, m) \in \mathcal{H}$ azpiespazioa (j eta m finkoak ⇒ $\{|k\, \overbrace{j\, m}^{\text{finkoak}}\rangle\}$)

$\mathcal{H} = \underbrace{\mathcal{E}(j, j)}_{\text{dim } g(j,m) = g(j)} \oplus \cdots \oplus \mathcal{E}(j, m) \oplus \cdots \oplus \mathcal{E}(j, -j) \oplus \cdots$ → j-ren balio guztiak

$g(j, m)$ berezgina ⇒ $\mathcal{E}(k, j)$ azpiespazioa hartu ⇒ $\{|k\, \overbrace{j}^{\text{finkoak}}\, m\rangle\}$ → dim = 2j+1

$\mathcal{H} = \mathcal{E}(1, j) \oplus \mathcal{E}(2, j) \oplus \cdots \oplus \mathcal{E}(g(j), j) \oplus \cdots$ → j-ren beste balioak

$$F(\vec{J})|K\,j\,m\rangle = F(J_x, J_y, J_z)\underbrace{|K\,j\,m\rangle}_{\in \mathcal{E}(K,j)} \in \mathcal{E}(K,j)$$

→ edozein eragile

Aldatzen den gauza balioa m da

$\mathcal{E}(K,j)$ → $F(\vec{J})$-rekiko aldakorra → bere matrizea blokeka diagonala

⇒ H hauen batura zuzena da

$$(F(\vec{J})) = \begin{array}{c|c} & \mathcal{E}(1,1)\ \mathcal{E}(1,2)\ \cdots \\ \hline \begin{array}{c}\mathcal{E}(1,1)\\ \mathcal{E}(1,2)\\ \vdots\end{array} & \begin{pmatrix} \square & 0 \\ 0 & \square \end{pmatrix} \end{array}$$

$\langle K\,j\,m|F(\vec{J})|K'j'm'\rangle \propto \delta_{KK'}\delta_{jj'}$

→ azpiespazio bereko bektoreak konektatu

K aldatuz gero eta j ere mantenduz blokea ez da aldatzen (K-ren independentea → sistemaren menpekotasunik ez → unibertsala)

hurrengo bektore guztiak ~~ez~~ dira J_z-ren autobektoreak → m-ren eskuzko balioa badute soilik

$\ast\ j = 1/2$ → $(J_+) = \hbar\begin{pmatrix}0&1\\0&0\end{pmatrix}$, $(J_-) = \hbar\begin{pmatrix}0&0\\1&0\end{pmatrix}$, $(J_x) = \frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}$

$(J_y) = \frac{\hbar}{2}i\begin{pmatrix}0&-1\\1&0\end{pmatrix}$, $(J_z) = \frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$, $(J^2) = \frac{3\hbar^2}{4}\begin{pmatrix}1&0\\0&1\end{pmatrix}$

$\ast\ j = 1$ → $(J_x) = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}$, $(J_y) = \frac{\hbar i}{\sqrt{2}}\begin{pmatrix}0&-1&0\\+1&0&-1\\0&1&0\end{pmatrix}$ $\{1, 0, -1\}$

$(J_z) = \hbar\begin{pmatrix}+1&0&0\\0&0&0\\0&0&-1\end{pmatrix}$ $\qquad J^2 = \hbar^2 j(j+1)\mathbb{1}$ → identitate matrizea

Blokeak ⇒ hauen oinarritzat $\{|K\,j\,m\rangle\}$ hartu (J_z-ren autobektoreak)

→ aldakorra dena

j balio finko batekin ari bagara lan egiten $\mathcal{E}(j, K)$-ri dagokion blokea ordezkatu behar gara soilik i $F(\vec{J})$-rekiko aldakorra.

L^2 eta L_z-ren komunak diren neurketak: $\langle r|K\,l\,m\rangle = R_{K,l}(r)\,Y_l^m(\theta,\varphi) = \psi_{Klm}(r,\theta,\varphi)$

$$\psi(r) = \sum_K \sum_l \sum_{m=-l}^{l} c_{K,l,m} R_{K,l}(r)\,Y_l^m(\theta,\varphi) \ \ast \Rightarrow c_{K,l,m} = \int d^3r\, \psi^*_{Klm}(\vec{r})\,\psi(\vec{r}) =$$

$$|\psi\rangle = \sum_K \sum_l \sum_{m=-l}^{l} c_{K,l,m}|K\,l\,m\rangle \ ; \quad \int_0^\infty r^2 dr\, R^*_{K,l}(r)\int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\, d\theta\, \psi(r,\theta,\varphi)\,Y_l^m(\theta,\varphi)$$

L^2 eta L_z neurtu → l eta m neurtzeko probabilitatea ⇒ $P(l,m) = \sum_K |c_{Klm}|^2$

L^2 neurtzen badugu bakarrik ⇒ $P(l) = \sum_{m=-l}^{l} P(l,m) = \sum_K \sum_{m=-l}^{l} |c_{Klm}|^2$

$\ast$ L_z eta L_z-k r-n ez dute eragiten ⇒ $\psi(r) = \sum_l \sum_{m=-l}^{l} a_{l,m}(r)\,Y_l^m(\theta,\varphi)$

Beraz $\Rightarrow$ $P(l,m) = \int_0^\infty r^2 dr\, |a_{l,m}(r)|^2 \rightarrow P(l) = \sum_{m=-l}^{l} \int_0^\infty r^2 dr\, |a_{l,m}(r)|^2$,

$P(m) = \sum_{l \geq |m|} \int_0^\infty r^2 dr\, |a_{l,m}(r)|^2$

Spina $\Rightarrow$ $\mathcal{H}_s$ espazioa $(\mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_s)$ $\Rightarrow$ $\vec{S}$ spin momentu angeluarra

$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$, $[\hat{S}_y, \hat{S}_z] = i\hbar \hat{S}_x$, $[\hat{S}_z, \hat{S}_x] = i\hbar \hat{S}_y$

$\{S^2, S_z\}$ BTMB $\Rightarrow$ $\{|s\, m_s\rangle\}$ aldibereko oinarria $\begin{cases} S^2 |s, m_s\rangle = s(s+1)\hbar^2 |s, m_s\rangle \\ S_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle \end{cases}$

[Elektroia $\rightarrow$ $s = 1/2$ finkoa $\rightarrow$ $\{S_z\}$-k BTMB osatzen du $(-s \leq m_s \leq s)$] $\downarrow$ $g(s) = 2s+1$

* $\sum_s \sum_{m_s=-s}^{m_s=s} |s, m_s\rangle\langle s, m_s| = \mathbb{1}$; $\langle s, m_s | s', m'_s\rangle = \delta_{ss'}\delta_{m_s m'_s}$

* $|\chi\rangle = \sum_s \sum_{m_s=-s}^{s} c_{m_s} |s, m_s\rangle \Rightarrow c_{m_s} = \langle s\, m_s | \chi\rangle$

*' $m_s = \pm 1/2 \Rightarrow \{|1/2, 1/2\rangle, |1/2, -1/2\rangle\} = \{|+\rangle, |-\rangle\}$ $\begin{cases} |+\rangle\langle +| + |-\rangle\langle -| = \mathbb{1} \\ \langle + | - \rangle = 0 \end{cases}$

$s = 1/2 \Rightarrow S_+ = \begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix}$, $S_- = \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix}$, $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $S_y = \frac{\hbar i}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, $S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

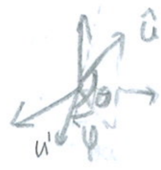
Matrizeak adierazteko $\Rightarrow$ $(\vec{S}) = \frac{\hbar}{2}\vec{\sigma} \rightarrow (S_x) = \frac{\hbar}{2}\sigma_x$, $(S_y) = \frac{\hbar}{2}\sigma_y$,

$(S_z) = \frac{\hbar}{2}(\sigma_z)$ $(\sigma_x, \sigma_y, \sigma_z \Rightarrow$ Paulinen matrizeak$)$

- $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \mathbb{1}$, $\sigma_x \sigma_y = \sigma_z$ $\begin{cases} [\sigma_x, \sigma_y] = 2i\sigma_z \\ \sigma_x\sigma_y + \sigma_y\sigma_x = 0 \end{cases}$, $\mathrm{Tr}\,\sigma_x = \mathrm{Tr}\,\sigma_y = \mathrm{Tr}\,\sigma_z = 0$
- $|\sigma_x| = |\sigma_y| = |\sigma_z| = -1$, $\{\mathbb{1}, \sigma_x, \sigma_y, \sigma_z\}$ 2x2-ko matrize oinarria

* u' bektorean u norabidean badugu $(s = 1/2)$ eta $\{|+\rangle_{u'}, |-\rangle_{u'}\}$ oinarria bada

$$\begin{array}{l} \hbar/2 \rightarrow \\ -\hbar/2 \rightarrow \end{array} \begin{cases} |+\rangle_u = \cos\frac{\theta}{2} e^{-i\varphi/2} |+\rangle_{u'} + \sin\frac{\theta}{2} e^{i\varphi/2} |-\rangle_{u'} \\ |-\rangle_u = \sin\frac{\theta}{2} e^{-i\varphi/2} |+\rangle_{u'} - \cos\frac{\theta}{2} e^{i\varphi/2} |-\rangle_{u'} \end{cases}$$



$\theta = (\widehat{\hat{u}, \hat{u}'})$

Partikulek spina badute (propietate intrintsekoa) $\Rightarrow$ $\mathcal{H}_r$-z gain $\mathcal{H}_s$ behar dugu $\Rightarrow$ $\mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_s$ $\Rightarrow$ $\{\hat{x}, \hat{y}, \hat{z}, \hat{S}^2, \hat{S}_z\}$ BTMB (edo $\vec{p}$-rekin ere)

$\mathcal{H}_r = \mathcal{H}_x \otimes \mathcal{H}_y \otimes \mathcal{H}_z$

(* $V(r)$ bada $\Rightarrow \{H, \hat{L}^2, \hat{L}_z, \hat{S}^2, \hat{S}_z\}$ re.)

$|\vec{r}\rangle \otimes |S, m_s\rangle = |r, S, m_s\rangle$

$\langle n\, s\, m_s | r\, s\, m_s\rangle = \langle n|r\rangle\langle s\, m_s|s\, m_s\rangle = \langle n|r\rangle$

$\{\hat{x}, \hat{y}, \hat{z}, \hat{S}^2, \hat{S}_z\}$ duguneen $\Rightarrow \{|\vec{r}\rangle \otimes |S, m_s\rangle\}$ oinarria.

oinarri jarraitua

* $|\psi\rangle = \sum_{i, m_s} c_{i, m_s} |\varphi_i\rangle \otimes |m_s\rangle \neq |\varphi\rangle \otimes |\chi\rangle$ $(|\varphi\rangle \in \mathcal{H}_r, |\chi\rangle \in \mathcal{H}_s)$

orokorrean

$\mathcal{H}_r$-ko oinarri bat.

* $|\vec{r}\rangle \otimes |S, m_s\rangle$ (S finkatuta) $\Rightarrow |\psi\rangle = \sum_{m_s} \int d^3r \underbrace{\psi(\vec{r})\, c_{m_s}}_{\psi_{m_s}(\vec{r})} (|\vec{r}\rangle \otimes |m_s\rangle)$

S finkatuta ez dago $\sum_S$

$\rightarrow \{|\vec{r}, \varepsilon\rangle\} \Rightarrow \sum_\varepsilon \int d\vec{r}\, |\vec{r}, \varepsilon\rangle\langle \vec{r}, \varepsilon| = \mathbb{1}$; $\langle \vec{r}, \varepsilon | \vec{r}\,', \varepsilon'\rangle = \delta(\vec{r} - \vec{r}\,')\, \delta_{\varepsilon\varepsilon'}$

$|\psi\rangle = \sum_\varepsilon \int d\vec{r}\, |\vec{r}, \varepsilon\rangle\, \psi_\varepsilon(\vec{r})$ $\quad (\psi_\varepsilon(\vec{r}) = \langle \vec{r}, \varepsilon|\psi\rangle)$

$S = 1/2 \rightarrow \varepsilon = +, - \Rightarrow |\psi\rangle = \int d^3r \underbrace{\psi_+(\vec{r})}_{\langle r,+|\psi\rangle} |\vec{r}, +\rangle + \int d^3r \underbrace{\psi_-(\vec{r})}_{\langle r,-|\psi\rangle} |\vec{r}, -\rangle$

- Spinorea: $[\psi](\vec{r}) = \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}$; $[\psi]^\dagger(\vec{r}) = (\psi^*_+(\vec{r}) \quad \psi^*_-(\vec{r}))$

$\langle \psi|\phi\rangle = \sum_\varepsilon \int d^3r\, \psi_\varepsilon^*(\vec{r})\, \phi_\varepsilon(\vec{r}) = \int d^3r\, [\psi]^*(\vec{r})\, [\phi(\vec{r})]$

↳ lehen bezala baina orain zutabe bat, ε re dugulako.

$\langle \psi| = \sum_\varepsilon \int d^3r\, \psi_\varepsilon^*(\vec{r})\, |\vec{r}, \varepsilon\rangle$

- Stern Gerlach $\Rightarrow$ $\vec{M}_S = -g_S \frac{\mu}{\hbar} \vec{S}$ $\qquad \mu = \frac{q\hbar}{2m}$

faktore giro-magnetikoa $\rightarrow e^- \simeq 2 \rightarrow \mu = \mu_B$ Bohr-en magnetoia

Elektroia $\rightarrow$ $M_S = \frac{2\mu_B}{\hbar} S$; Stern Gerlach dispositiboa adierazteko

$\boxed{SG}$ $\hat{u} \rightarrow$ Eremu magnetikoaren norabidea $\rightarrow S_u$ neurtu

* Stern Gerlach dispositiboa jarrita bateko $\Rightarrow$ norabide batean $\Rightarrow$ beti lortuko dugu $|+\rangle_u$ (edo $|-\rangle_u$) irteeran : $P_+ = 1$, $P_- = 0$ (irteeran)

* Irten eta gero $|\pm\rangle_{u'}$ neurtzeko probabilitatea $\Rightarrow$ $P_\pm = |{}_{u'}\langle \pm|+\rangle_u|^2$ $\begin{cases} P_+ = \cos^2\theta/2 \\ P_- = \sin^2\theta/2 \end{cases}$ $\quad \theta \equiv (\widehat{u, u'})$

- $\vec{B}$ eremu batenpean dagoen partikula: $H = -\vec{M}_S \cdot \vec{B} = -\gamma \vec{S} \cdot \vec{B} = -\gamma B\, \vec{S} \cdot \vec{u} = \omega S_u$

u-ren norabidea

$\begin{cases} \vec{\omega} = -\gamma \vec{B} \\ \vec{M}_S = \gamma \vec{S} \end{cases}$ $\quad \gamma = -\frac{2\mu_B}{\hbar}\ (e^-)$

H-ren autobektoreak S_u-renak : $|\pm\rangle_u \rightarrow$ autobalioak $\pm\omega\frac{\hbar}{2}$

Orduan denboraren garapena $\Rightarrow |\chi\rangle(0) = |+\rangle_{u'}$ adibidez;

$\hat{u}'$ $\hat{u}$-rekiko proiekzioan ari da

$|\chi\rangle(t) = \cos\left(\frac{\theta}{2}\right) e^{-i\frac{(\varphi+\omega t)}{2}} |+\rangle_u + \sin\left(\frac{\theta}{2}\right) e^{i\frac{(\varphi+\omega t)}{2}} |-\rangle_u = |+\rangle_{u'}(t)$

↓ lehenengo garatu $\{|+\rangle_u, |-\rangle_u\}$-n $|\chi\rangle(0)$ gero $\cdot\, e^{-i\frac{E}{\hbar}t}$

Spin eragileak: $|r, \varepsilon\rangle$ autobektoreek ε-n baino ez dute eragiten.

Eragile orbitalak: $|r, \varepsilon\rangle$ autobektoreek ε berdin uzten dute $\Rightarrow$ haien 2x2-ko matrizea $\mathbb{1}$ eragilearen proportzionala da. Adibidez:

$$[\![X]\!] = \begin{pmatrix} x & 0 \\ 0 & x \end{pmatrix} \Rightarrow [\psi'](r) = [\psi](r)\,[\![X]\!]$$

$$[\![P_x]\!] = \frac{\hbar}{i}\begin{pmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial x} \end{pmatrix} \nearrow \text{ gauza bera } [\![P_x]\!]\text{-rekin}$$

* Eragile guztiek 2x2-ko matrize bat dute lotuta ($s = 1/2$)

Eragile mixtoak: H_r-ri dagokiona r-n eragin eta H_s-ri dagokiona ε-n. Adibidez:

$$[\![L_z S_z]\!] = \frac{\hbar}{2}\begin{pmatrix} \frac{\hbar}{i}\frac{\partial}{\partial \varphi} & 0 \\ 0 & -\frac{\hbar}{i}\frac{\partial}{\partial \varphi} \end{pmatrix}$$

$*\{|p,\varepsilon\rangle\}$ adierazpidea ere existitzen da: $\langle r,\varepsilon|p,\varepsilon'\rangle = \langle r|p\rangle\langle\varepsilon|\varepsilon'\rangle =$

$$\delta_{\varepsilon\varepsilon'}\,\frac{1}{(2\pi\hbar)^{3/2}}\,e^{i\vec{p}\cdot\vec{r}/\hbar} \rightarrow |\psi\rangle\text{-k ere spinorea: } [\bar{\psi}](p) = \begin{pmatrix} \bar{\psi}_+(p) \\ \bar{\psi}_-(p) \end{pmatrix}$$

$$\bullet\begin{cases} \bar{\psi}_+(p) = \langle p,+|\psi\rangle = \dfrac{1}{(2\pi\hbar)^{3/2}}\displaystyle\int d^3r\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\,\psi_+(r) \\ \bar{\psi}_-(p) = \langle p,-|\psi\rangle \nearrow \text{ gauza bera } \psi_-(r)\text{-rekin.} \end{cases}$$

Probabilitateak $\Rightarrow$ • Elektroia r posizioan eta $S_z = \hbar/2$ neurtzeko probabilitatea:

$$dP(r,+) = |\psi_+(r)|^2 d^3r \Rightarrow \text{Edozein } r \text{ bada} \Rightarrow P(+) = \int |\psi_+(r)|^2 d^3r$$

- r posizioan aurkitzeko probabilitatea $\Rightarrow P(r) = \sum_{\varepsilon} |\psi_\varepsilon(r)|^2$
- p momentua neurtzeko probabilitatea $\Rightarrow P(p) = \sum_{\varepsilon} |\bar{\psi}_\varepsilon(p)|^2$
- A eragilea $\Rightarrow (a_n, \varepsilon)$ neurtzeko probabilitatea ($\{|n^i\,\varepsilon\rangle\}$ oinarria) $\Rightarrow P_n^\varepsilon = \sum_{i=1}^{g_n} |\langle n^i\,\varepsilon|\psi\rangle|^2$

a_n soilik $\Rightarrow$ $$P_n = \sum_\varepsilon \sum_{i=1}^{g_n} |\langle n^i\,\varepsilon|\psi\rangle|^2 \overset{*'}{=} \sum_\varepsilon \sum_{i=1}^{g_n} \Big|\int d^3r \langle\vec{r}|n^i\rangle^* \underbrace{\langle\vec{r},\varepsilon|\psi\rangle}_{\psi_\varepsilon(\vec{r})}\Big|^2$$

$$*' \quad |n^i\,\varepsilon\rangle = \sum_{\varepsilon'}\int \langle\vec{r}\,\varepsilon'|n^i\,\varepsilon\rangle|\vec{r}\,\varepsilon'\rangle d^3r = \sum_{\varepsilon'}\int \langle\vec{r}|n^i\rangle \underbrace{\langle\varepsilon'|\varepsilon\rangle}_{\delta_{\varepsilon'\varepsilon}} |\vec{r}\,\varepsilon'\rangle d^3r =$$

$$\int \langle\vec{r}|n^i\rangle|\vec{r},\varepsilon\rangle d^3r$$

$\rightarrow H = H_1 + H_2 + V(|\vec{r}_1 - \vec{r}_2|)$

Bi partikula $\Rightarrow$ Momentu angeluarrak gehitu : $\vec{J} = \vec{J}_1 + \vec{J}_2$ $\begin{cases} \vec{S} = \vec{S}_1 + \vec{S}_2 \\ \vec{L} = \vec{L}_1 + \vec{L}_2 \end{cases}$

(Klasikoki $\vec{J} = kte$)

* $[\vec{J}, H] = [\vec{L} + \vec{S}, H] = 0 \Rightarrow \vec{J}$ higidura konstantea ; $\langle \vec{J} \rangle = kte$

$([\vec{J}_1, H] = [\vec{J}_2, H] = 0$ soilik $V(|\vec{r}_2 - \vec{r}_1|) = 0$ denean) → bi partikulen elkarrekintza.

* Bi egoera espazio $\mathcal{H}_1, \mathcal{H}_2 \Rightarrow \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \Rightarrow \{ J_1^2, J_2^2, J_{1z}, J_{2z} \}$ trukakorrak baina

$\mathcal{H}$-n eragiten duenean hauek: $\{ J_1^2, J_2^2, J^2, J_z \}$ (BTMB) $\begin{cases} [J^2, J_{1z}], [J^2, J_{2z}] \neq 0 \\ \text{baina} \\ [J^2, J_{1z} + J_{2z}] = [J^2, J_z] = 0 \end{cases}$

↳ Gainera $(\vec{J}^2, J_z)$ H-rekin trukakorrak dira.

- $\{ J_1^2, J_2^2, J^2, J_z \} \Rightarrow \{ |j_1 j_2 j m\rangle \}$ oinarria ; H blokeka diagonala oinarri honetan, $\mathcal{E}(j, m)$ azpiespazioetan, J^2 eta J_z-rekin trukakorra delako

$$H = \begin{array}{c|c} & \mathcal{E}(j', m) \ \ldots \\ \hline \mathcal{E}(j', m) & \begin{pmatrix} \square & & \\ & \square & \\ & & \square \end{pmatrix} \\ \vdots & \end{array}$$

Hemendik errez diagonalizatu.

Baina oinarria hau kalkulatzeko $\{ |j_1 j_2 m_1 m_2 \rangle \}$-tik abiatu eta J^2 eta J_z diagonalizatu. $(J_z = J_{1z} + J_{2z}$, $J^2 = J_1^2 + J_2^2 + 2 J_1 \cdot J_2 = J_1^2 + J_2^2 + 2 J_{1z} J_{2z} + (J_{1+} J_{2-} + J_{1-} J_{2+}))$

- $\mathcal{H} = \sum_{\oplus} \mathcal{E}(K_1, K_2, j_1, j_2) = \sum_{\oplus} \underbrace{\mathcal{E}(K_1 j_1) \otimes \mathcal{E}(K_2, j_2)}_{dim = (2j_1+1)(2j_2+1)} = \sum_{\oplus} \Big(\sum_{\oplus} \mathcal{E}(K, j) \Big)$

↳ $F(J_1)$ eta $F(J_2)$-rekiko aldaerrna → $F(J)$

$K_i = 1, \ldots g(j_i)$ eta j_i aldakorra izango da

$\mathcal{E}(j)$ ↳ j-ren balioak

$\{ |K_1, K_2, j_1, j_2, K, j, m\rangle \} \rightarrow \{ |K\, j\, m\rangle \}$-ra laburtu (nahikoa K, j eta m zehaztea, lotuta daudelako)

$$\begin{cases} J^2 |K\, j\, m\rangle = j(j+1)\hbar^2 |K\, j\, m\rangle \\ J_z |K\, j\, m\rangle = m\hbar |K\, j\, m\rangle \\ J_\pm |K\, j\, m\rangle = \hbar\sqrt{j(j+1) - m(m\pm1)}\, |K, j, m\pm1\rangle \end{cases}$$

$\mathcal{E}(K_1, K_2, j_1, j_2)$ $F(J)$-rekiko aldaerrna denez J^2 eta J_z blokeka diagonalak izango dira $\Rightarrow$ blokeka diagonalizatuz $\{ |K\, j\, m\rangle \}$ oinarria lortu

- j_1 eta j_2 zehaztuta $\Rightarrow$ $|m_1, m_2\rangle$ bektoreak ($\mathcal{H}_2$, $\mathcal{H}_2$) $\begin{cases} \sum_{m_1 m_2} |m_1, m_2\rangle \langle m_1, m_2| = \mathbb{1} \\ m = m_1 + m_2 \end{cases}$

$$|j\, m\rangle = \sum_{m_1 m_2} |m_1 m_2\rangle \underbrace{\langle m_1 m_2 | j\, m\rangle}$$

↳ Clebsch-Gordan-en koefizienteak

$|j_1 - j_2| \leq j \leq \underbrace{j_1 + j_2}_{m_{max}}$ (K-nli ez, endekapenik ez) $\Rightarrow$ J balio bakoitzeko $\mathcal{E}(J)$ espazio bakarra

Diagonalizatu gabe, ipon kalkulatzen J_- eta J_+-en laguntzaz

$$\mathcal{E}(j_1, j_2) = \mathcal{E}(j_1 + j_2) \oplus \mathcal{E}(j_1 + j_2 - 1) \oplus \cdots \oplus \mathcal{E}(|j_1 - j_2|)$$

- $\mathcal{E}(j_1 + j_2) \Rightarrow m = j_1 + j_2 \Rightarrow$ autobektore bakarra * $|j_1 + j_2 = j, m = j_1 + j_2\rangle = |j_1 = m_1, m_2 = j_2\rangle$

  $\hookrightarrow \dim = (2j+1) = 2(j_1 + j_2) + 1$

* $$|j_1 + j_2, j_1 + j_2 - 1\rangle = \frac{J_- |j_1 + j_2, j_1 + j_2\rangle}{\hbar \sqrt{\underbrace{(j_1+j_2)(j_1+j_2+1) - (j_1+j_2)(j_1+j_2-1)}_{2(j_1+j_2)}}} = \sqrt{\frac{j_2}{j_1+j_2}} |j_1, j_2 - 1\rangle +$$

$$\sqrt{\frac{j_1}{j_1+j_2}} |j_1 - 1, j_2\rangle$$

$\vdots$

* Horrela beste autobektoreekin eta bat falta bozenigu ortonormaltasuna baldintzek oplikatu. (Ad: $m = j_1 + j_2 - 1$ badugu badakigu $m_1 = j_1 - 1$ eta $m_2 = j_2$ edo $m_1 = j_1$ eta $m_2 = j_2 - 1$ dela $\Rightarrow$ bi hauen konbinazio lineal bat)

Modu honetan $\Rightarrow$ $$|j_1\, j_2\, m_1\, m_2\rangle = \sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m=-j}^{j} |j\, m\rangle \langle j\, m | j_1\, j_2\, m_1\, m_2\rangle$$

Adibidea: $j_1 = j_2 = 1/2 \Rightarrow m_1, m_2 = \pm 1/2 \rightarrow \{|+,+\rangle, |+,-\rangle, |-,+\rangle, |-,-\rangle\} = \{|m_1\, m_2\rangle\}$ oinarria. Oinarri honetan:

$$(J_z) = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \Rightarrow m = 1, 0, -1 \text{ bana endekapena}$$

$\hookrightarrow J_z = J_{1z} + J_{2z}$

$$(J^2) = \hbar^2 \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \Rightarrow \text{Blokeka diagonala } \mathcal{E}(m)\text{-n.}$$

$\rightarrow m = 0$

Orduan (J^2) diagonalizatu edo lehen azaldutako metodoa oplikatu:

- $m = 1, 0, -1 \rightarrow j = \begin{cases} 1 \\ 0 \end{cases}$ • $j = 1 \Rightarrow |1, 1\rangle = |+, +\rangle$ Aukera bakarra)

$$|1, 0\rangle = \frac{1}{\hbar\sqrt{2}} J_- |1, 1\rangle = \frac{1}{\hbar\sqrt{2}} (J_{1-} + J_{2-}) |+, +\rangle = \frac{1}{\sqrt{2}} [|-, +\rangle + |+, -\rangle]$$

$\hookrightarrow$ 0 lortzeko $m_1 = 1/2$ eta $m_2 = -1/2$ edo alderantziz

• $|1,-1\rangle = |-,-\rangle$ (aukera bakarra $m=-1$ izateko $m_1 = m_2 = -1/2$) Tripletea

• $j=0 \Rightarrow$ $|0,0\rangle = \alpha|+,-\rangle + \beta|-,+\rangle \Rightarrow$ ortonormaltasuna aplikatu

$\alpha = -\beta \Rightarrow$ $|0,0\rangle = \frac{1}{\sqrt{2}}[|+,-\rangle - |-,+\rangle]$ Singletea

Diagonalizatuz (J^2) emaitza bera lortuko genuke.

Perturbazioen teoria: ("Stationary perturbation theory") $H \neq H(t)$

Orduan H-ren autobalio eta autobektoreak kalkulatzeko denborarekiko independentea den Schrödingeren ekuazioa planteatu $\rightarrow$ askotan oso zaila ebaztea $\Rightarrow$ Perturbazioen teoria. $\Rightarrow$ $H = H_0 + W \rightarrow$ Perturbazioa (H_0 baino askoz txikiagoa)
$\hookrightarrow$ ezaguna dugu bere soluzioa

* Perturbazioa: $W = \lambda\tilde{W}$ planteatu $(\lambda << 1)$

* $H_0 \Rightarrow$ bere autobektore/autobalioak ezagunak: $H_0|\varphi_n^{o\,i}\rangle = E_n^o|\varphi_n^{o\,i}\rangle$ Diskretuak direla onartu

• H-ren autobalio eta autobektoreak: $E(\lambda)$ eta $|\psi(\lambda)\rangle \Rightarrow H|\psi(\lambda)\rangle = E(\lambda)|\psi(\lambda)\rangle$
$\hookrightarrow H(\lambda) = H_0 + \lambda\tilde{W}$

• Problema $\Rightarrow$ H_0-ren autobalioak diren energia mailetan ematen diren aldaketak W perturbazioaren ondorioz.  $\lambda \to 0$ $E(\lambda) = E_n^o$

Perturbazioen teoria $\Rightarrow$ Hurbilketa batean $|\psi(\lambda)\rangle$ eta $E(\lambda)$ λ-ren potentzietan garatu:

$$\begin{cases} E(\lambda) = \varepsilon_0 + \lambda\varepsilon_1 + \lambda^2\varepsilon_2 + \dots \\ |\psi(\lambda)\rangle = |0\rangle + \lambda|1\rangle + \lambda^2|2\rangle + \dots \end{cases} \rightarrow \begin{cases} \langle 0|0\rangle = 1 \\ \langle 1|0\rangle = \langle 0|1\rangle = 0 \\ \langle 2|0\rangle = \langle 0|2\rangle = -\frac{1}{2}\langle 1|1\rangle \end{cases}$$ Frogatu daiteke

Orokorrean $E(\lambda)$-ren bigarren ordenako hurbilketa egiten da eta $|\psi(\lambda)\rangle$-ren bat ordenako hurbilketa.

$$(H_0 + \lambda\tilde{W})\left[\sum_{q=0}^{\infty}\lambda^q|q\rangle\right] = \left[\sum_{\ell=0}^{\infty}\lambda^\ell\varepsilon_\ell\right]\left[\sum_{q=0}^{\infty}\lambda^q|q\rangle\right]$$

• $\varepsilon_0, \varepsilon_1, |0\rangle, \dots$? E_n^o perturbatu eta gero nola mozkiltzen den jakin nahi badugu $\Rightarrow$ $\varepsilon_0 = E_n^o$ planteatu. Bi aukera: (n jakin bat)

1 * E_n^o ez-endekatua da: $|0\rangle = |\varphi_n^o\rangle$ izango da ($\lambda \to 0$; perturbaziorik ez $H = H_0$ denez emaitza berdina lortu)

• $\langle \varphi_n^0 | (H_0 - E_0) | 1 \rangle + \langle \varphi_n^0 | (\tilde{\omega} - \varepsilon_1) | 0 \rangle = \langle \varphi_n^0 | \cancel{E_0 - E_0} | 1 \rangle + \langle \varphi_n^0 | \tilde{\omega} | 0 \rangle - \varepsilon_1 \langle \varphi_n^0 | 0 \rangle =$

$\langle \varphi_n^0 | \tilde{\omega} | \varphi_n^0 \rangle - \varepsilon_1 \langle \varphi_n^0 | \varphi_n^0 \rangle = 0$ $\quad (\underbrace{(H_0 - E_0)|1\rangle + (\tilde{\omega} - E_1)|0\rangle = 0}_{\psi^1} \rightarrow$ potentziala

berdintzean) $\Rightarrow \quad \varepsilon_1 = \langle 0 | \tilde{\omega} | 0 \rangle = \langle \varphi_n | \tilde{\omega} | \varphi_n \rangle$

• $\langle \varphi_m^{0\,i} | (H_0 - E_0) | 1 \rangle + \langle \varphi_m^{0\,i} | (\tilde{\omega} - \varepsilon_1) | 0 \rangle = 0 \Rightarrow \langle \varphi_m^{0\,i} | 1 \rangle = \frac{1}{E_n^0 - E_m^0} \langle \varphi_m^{0\,i} | \tilde{\omega} | \varphi_n^0 \rangle$

$|1\rangle = |\varphi_n\rangle \underset{\langle 0|1\rangle = 0}{\cancel{\langle \varphi_n | 1 \rangle}} + \sum_{m \neq n}{}' \sum_i \langle \varphi_m^i | 1 \rangle |\varphi_m^i\rangle$ $\quad$ ($\{\varphi_m^i\}$ osoa delako)

$$|1\rangle = \sum_{m \neq n}{}' \sum_i \frac{\langle \varphi_m^{0\,i} | \tilde{\omega} | \varphi_n^0 \rangle}{E_n^0 - E_m^0} |\varphi_m^{0\,i}\rangle$$

• $\varepsilon_2 = \langle \varphi_n^0 | \tilde{\omega} | 1 \rangle \longrightarrow \quad \varepsilon_2 = \sum_{m \neq n}{}' \sum_i \frac{|\langle \varphi_m^{0\,i} | \tilde{\omega} | \varphi_n^0 \rangle|^2}{E_n^0 - E_m^0}$

↳ aurreko arguduo bera ε_1 lortzeko (potentziala berdinduz)

Beraz $\Rightarrow$ * $E(\lambda) = E_n^0 + \underbrace{\langle \varphi_n^0 | \tilde{\omega} | \varphi_n^0 \rangle \lambda + \sum_{m \neq n}{}' \sum_i \frac{|\langle \varphi_m^i | \tilde{\omega} | \varphi_n \rangle|^2}{E_n^0 - E_m^0} \lambda^2}_{\text{Perturbatzen dena}} + O(\lambda^3)$

* $|\psi(\lambda)\rangle = |\varphi_n^0\rangle + \sum_{m \neq n}{}' \sum_i \frac{\langle \varphi_m^i | \tilde{\omega} | \varphi_n^0 \rangle}{E_n^0 - E_m^0} |\varphi_m^i\rangle \lambda + O(\lambda^2)$

2* E_n^0 endekatua da: $|0\rangle \in \mathcal{E}_n^0$ -n egongo da $\Rightarrow |0\rangle = \sum_{i=1}^{g_n} \langle \varphi_n^i | 0 \rangle |\varphi_n^i\rangle$

• Potentzialen berdinketaz^{*1} $\Rightarrow \langle \varphi_n^{0\,i} | (H_0 - E_0) | 1 \rangle + \langle \varphi_n^{0\,i} | (\tilde{\omega} - \varepsilon_1) | 0 \rangle = \langle \varphi_n^i | \cancel{(E_0 - E_0)} | 1 \rangle + \langle \varphi_n^{0\,i} | \tilde{\omega} | 0 \rangle +$

$- \varepsilon_1 \langle \varphi_n^{0\,i} | 0 \rangle = 0 \Rightarrow \quad \varepsilon_1 \langle \varphi_n^i | 0 \rangle = \langle \varphi_n^i | \tilde{\omega} | 0 \rangle \quad \boxed{i = 1, 2, \ldots, g_n}$

↳ ezagutu nahi ditugun koefizienteak.

$\varepsilon_1 \langle \varphi_n^i | 0 \rangle = \sum_{j=1}^{g_n} \underbrace{\langle \varphi_n^i | \tilde{\omega} | \varphi_n^j \rangle}_{\text{matrize elementuak}} \langle \varphi_n^j | 0 \rangle \qquad i = 1, \ldots, g_n$

$\tilde{\omega}$-ren autobalio eta autobektoreen problema $\mathcal{E}_n$ espazioan $\Rightarrow \tilde{\omega}^{(n)}$ ($\tilde{\omega}$-ren murrizketa) diagonalizatu. $\rightarrow \left(\tilde{\omega}^{(n)}\right) \underbrace{\begin{pmatrix} \langle \varphi_n^1 | 0 \rangle \\ \vdots \\ \langle \varphi_n^{g_n} | 0 \rangle \end{pmatrix}}_{|0\rangle} = \varepsilon_1 \begin{pmatrix} \langle \varphi_n^1 | 0 \rangle \\ \vdots \\ \langle \varphi_n^{g_n} | 0 \rangle \end{pmatrix}$

Diagonalizatzean $\Rightarrow$ ε_j-k lortu eta haiekin lotutako autobektoreak, $|0\rangle_j$.

ε_j eta $|0\rangle_j$ bakoitzarekin perturbatutako autobalio eta autobektore bat egongo da.

• $E_j(\lambda) = E_n^0 + \lambda \varepsilon_1^j + O(\lambda^2)$ $\quad (j=1,2,\ldots, g_n^{(1)} \leq g_n)$

• $|\psi_j(\lambda)\rangle = |0\rangle_j + O(\lambda)$

Ordena handiagoan lortu nahi baditugu $|1\rangle$ eta ε_2 garatzeko antzeko prozedura bera, bana $|\varphi_n^0\rangle$ jarri beharrean $|0\rangle$ jarriz.

Adibideak:

Stark efektua: Hidrogeno atomoa $\vec{E}$ eremu uniforme batean $\Rightarrow H = H_0 + e\vec{E}\cdot\vec{r} = H_0 + Eez$

okiloa

$(\vec{r} = \vec{r}_1 - \vec{r}_2 \Rightarrow$ protoi eta elektroiaren arteko posizio erlatiboa)

• $W = +Eez = \lambda \tilde{W}$ perturbazioa $\Rightarrow \lambda = +\frac{eEa_0}{e^2/4\pi\varepsilon_0 a_0} = +\frac{E\,4\pi\varepsilon_0 a_0^2}{e}$

$$\tilde{W} = \frac{e^2}{4\pi\varepsilon_0 a_0^2} z$$

• H_0-ren autobektore eta autobalioak: $E_n^0 = -\frac{E_I}{n^2}$, $|\varphi_n^0\rangle = |n\,l\,m\rangle$

* Lehenengo energia mailaren perturbazioa: $n=0$

$$\varepsilon_0 = E_1^0 = -E_I = -\frac{e^2}{8\pi\varepsilon_0 a_0^2}, \quad |0\rangle = |\varphi_1^0\rangle = |1\,0\,0\rangle$$

$$\lambda\varepsilon_1 = \langle\varphi_1^0|W|\varphi_1^0\rangle = +Ee\langle 100|z|100\rangle = 0$$

$\int d^3r\,\underbrace{\overset{\text{bik}}{|\varphi_1|^2}}_{\text{bak}}\overset{\text{bak}}{z} = 0$

↳ paritatea, φ_1^0 bikoitia ($l =$ bikoitia)

(Ez dago lehen ordenako korrekziorik)

$$\lambda^2\varepsilon_2 = \sum_{n\neq 1}{}' \sum_{l} \sum_{m_l=-l}^{l} \frac{|\langle n\,l\,m_l|W|100\rangle|^2}{E_1^0 - E_n^0} = -\frac{9}{8}E_I\frac{e^2E^2a_0^2}{E_I^2}$$

$|\psi_1\rangle = |0\rangle + |1\rangle\lambda$ $\quad E_1 = \varepsilon_0 + \varepsilon_1\lambda + \varepsilon_2\lambda^2 + O(\lambda^3) = -E_I\left[1 + \frac{9}{8}\frac{(4\pi\varepsilon_0)^2}{e^2}E^2a_0^4 + O(E^3)\right]$

$$\lambda|1\rangle = +eE\sum_{n\neq 1}{}'\sum_{l}\sum_{m_l}\frac{\langle n\,l\,m|z|100\rangle}{E_1^0 - E_n^0}|n\,l\,m\rangle = eE\sum_{n\neq 1}{}'\frac{\langle n10|z|100\rangle}{E_1^0 - E_n^0}|n10\rangle$$

$l\neq 1$ eta $m_l \neq 0$ nulua

* Hemendik polarizabilitatea $\Rightarrow \langle\vec{p}\rangle_{n=1} = \langle e\vec{r}\rangle_{n=1}$

$$\langle p_x\rangle_{n=1} = \langle\psi_1|ex|\psi_1\rangle = 0 = \langle p_y\rangle_{n=1} \Rightarrow \langle p_z\rangle_{n=1} = e\langle\psi_1|z|\psi_1\rangle = \underbrace{\frac{9}{2}(4\pi\varepsilon_0)a_0^3}_{\alpha}E$$

polarizabilitatea

* Bigarren energia mailaren perturbazioa: $n=2$

$$\varepsilon_0 = E_2^0 = -E_I/4 \qquad g_2^0 = 4 \Rightarrow \text{endakatua} \qquad (E_2^0 \text{ apropazioa})$$

oinarria

$$\hat{W}^2 \text{ diagonalizatu} \Rightarrow \{|2\,1\,1\rangle, |2\,1\,0\rangle, |2\,1\,-1\rangle, |2\,0\,0\rangle\}$$

$$\hat{W}^{(1)} = a_0 e \mathcal{E} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 \\ 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \end{pmatrix} \Rightarrow \varepsilon_j = \begin{cases} 0 \Rightarrow \{|2\,1\,1\rangle, |2\,1,-1\rangle\} \text{ endakapena} \\ \pm 3 e a_0 E \Rightarrow |0\rangle = \frac{1}{\sqrt{2}}[|2\,1\,0\rangle \mp |2\,0\,0\rangle] \end{cases}$$

Zeeman bortitza: $\vec{B}$ eremu magnetiko oso bortitza dagoenean:

$$H = H_0 - (\vec{M}_L + \vec{M}_S)\cdot\vec{B} \Rightarrow \vec{M}_L + \vec{M}_S = -\frac{\mu_B}{\hbar}(\vec{L} + 2\vec{S})$$

$$H = H_0 + \frac{\mu_B}{\hbar}(\vec{L} + 2\vec{S})\cdot\vec{B} = H_0 + \underbrace{\frac{\mu_B}{\hbar}(L_z + 2S_z)B}_{W}$$

$$\vec{B} = B\hat{k}$$

$\{H_0, L^2, S^2, L_z, S_z\}$-ren aldibereko autobektoreak: $\{|n\,l\,m_l\,m_s\rangle\}$ eta

H_0-ren autobalioak $\quad E_n^0 = -E_I/n^2$

H_0 eta W trukakorrak direnez bien aldibereko autobektoreak ditugu eta beraz H-ren autobalioak zehatzak dira ere $\Rightarrow$ ez dugu perturbazioen teoria aplikatu behar.

$$H|n\,l\,m_l\,m_s\rangle = H_0|n\,l\,m_l\,m_s\rangle + \frac{\mu_B}{\hbar}B(L_z + 2S_z)$$

$$|n\,l\,m_l\,m_s\rangle = \left[E_n^0 + \frac{\mu_B B}{\cancel{\hbar}}\cancel{\hbar}(m_l + 2m_s)\right]|n\,l\,m_l\,m_s\rangle$$

* Endakapena apurtzen da guztiz edo partzialki.

• $n=1$ $\begin{cases} l=0 \\ m_l=0 \\ m_s=\pm 1/2 \end{cases} \rightarrow (m_l + 2m_s) = \pm 1 \Rightarrow$ $n=1$, $g=2$

$|1\,0\,0\,+\rangle$

$|1\,0\,0\,-\rangle$

$\frac{2\mu_B B}{\hbar\omega}$

biLtan banatu

• $n=2$ $\begin{cases} l=0,1 \\ m_l=0,1,-1 \\ m_s=\pm 1/2 \end{cases}$ $\quad n=2$, $g=8$

$m_l + 2m_s = 2, 1, 0, -1, -2$

5 energia mailatan banatu

$|2\,1\,1\,+\rangle$

$|2\,0\,0\,+\rangle, |2\,1\,0\,+\rangle$

$|2\,1\,1\,-\rangle, |2\,1\,-1,+\rangle$

$|2\,0\,0\,-\rangle, |2\,1\,0\,-\rangle$

$|2\,1\,-1\,-\rangle$

$4\mu_B B$

Van der Waals: Bi hidrogeno atomoren arteko elkarrekintza, R distantziaz banatuta:

- $R \sim a_0 \Rightarrow$ elektroien probabilitate dentsitateek estali ("overlap") $\Rightarrow$ bi atomoek erakarri; energia distantzia jakin baten minimizatu $\Rightarrow H_2$ molekulak sortu
- $R >> a_0 \Rightarrow$ bi elektroiak uhinen estalketa arbuiagarria $\to$ bi H atomo neutro $\to$ haien arteko elkarrekintza ahula; dipolo elektrikoen artekoa $\Rightarrow$ Van der Waals

$\vec{P}_2 = e\vec{r}_2$

$\vec{E}_1 = -\frac{1}{4\pi\varepsilon_0}\frac{[\vec{P}_1 - 3\vec{P}_1\cdot\vec{R}\,\vec{R}]}{R^3}$

$$\begin{cases} H = H_1^0 + H_2^0 + W = H_1^0 + H_2^0 - \vec{P}_2 \cdot \vec{E}_1(R) \\ W = \frac{e^2}{4\pi\varepsilon_0}\frac{(x_1x_2 + y_1y_2 - 2z_1z_2)}{R^3} \end{cases}$$

Perturbazioen teoria aplikatu $\Rightarrow$ Oinarrizko egoera $(n_1 = 1, n_2 = 1)$:

$$E_{1,1} = \varepsilon_0 + \varepsilon_1\lambda + O(\lambda^2) \quad ; \quad \varepsilon_0 = E_{1,1}^0 = -2E_I \quad , \quad |0\rangle = |100;100\rangle$$

$$\varepsilon_1\lambda = \langle 100;100|W|100;100\rangle = 0$$ $\to$ paritatea

Ez dago 1. ordeneko zuzenketarik

$$\varepsilon_2\lambda^2 = \sum_{n_1 l_1 m_1}\sum_{n_2 l_2 m_2}\frac{|\langle n_1 l_1 m_1; n_2 l_2 m_2|W|100;100\rangle|^2}{E_{11}^0 - (E_{n_1}^0 + E_{n_2}^0)} = -\frac{\tilde{C}}{R^6} =$$

$$-C\left(\frac{e^2}{4\pi\varepsilon_0 a_0}\right)\left(\frac{a_0}{R}\right)^6 \simeq -\frac{13}{2}\left(\frac{e^2}{4\pi\varepsilon_0 a_0}\right)\left(\frac{a_0}{R}\right)^6 \propto \frac{1}{R^6}$$

Egitura mehaen (laburpena): $[H_0, W] \neq 0$ $\{H_0, L^2, S^2, J, J_z\}$ BTMB

bada $[H_0, W] \neq 0 \to |n\,l\,s\,j\,m\rangle$ ez da aldiberako oinarria (H_0-rena bai)

- n finkatuta $\to W^{(n)}$ $|n\,l\,s\,j\,m\rangle$ oinarrian diagonala $\Rightarrow$ hemendik lortu ($l\,s\,j\,m$-k ere $\mathcal{E}_n$ sortu (ez soilik l, m_l, m_s-k))

ε_1 lehen ordeneko zuzenketak $\to \lambda\varepsilon_1 = \langle n\,l\,s\,j\,m|W^{(n)}|n\,l\,s\,j\,m\rangle$ (diagonaleko elementuak) $\to |0\rangle = |\underline{n}\,l\,s\,j\,m\rangle \in \mathcal{E}_n$ ($|\underline{n}\,l\,m_l\,m_s\rangle$-ren kob. lineala)

$\hookrightarrow$ finkoa

- W-k ez ditu nahasten l ezberdineko elementuak $\to [W, L^2] = 0 \to l$-ren azpiespazio ezberdinetan diagonala

$$E_n^0 = m_ec^2 + E_n^0 + \lambda\varepsilon_1 + O(\lambda^2) = m_ec^2 + E_n^0\left[1 + \left(\frac{2\alpha}{n}\right)^2\left(\frac{n}{j+1/2} - 3/4\right) + O((2\alpha)^4)\right]$$

Fisika kuantikoa, kontrola

17-03-21

Zimarekelo azterketa, 2014

1) El estado cuántico de un electrón viene dado por: $[\Psi](r) = \begin{bmatrix} \psi_+(r) \\ \psi_-(r) \end{bmatrix}$

¿Cuál es la probabilidad de que al medir S_y se obtenga el valor $\frac{\hbar}{2}$ independientemente de la posición del electrón? ¿Cuál es la probabilidad de que al medir el momento lineal resulte p_0 con componente de espín $S_z = -\frac{\hbar}{2}$?

$$\begin{cases} \psi_+(r) = \langle r, + | \psi \rangle, \quad \psi_-(r) = \langle r, - | \psi \rangle \\ |\psi\rangle = \int d^3r \left[\psi_+(r) |r, +\rangle + \psi_-(r) |r, -\rangle \right] \end{cases}$$

* S_y neurtu eta $\hbar/2$ lortu ⇒ elektroia $|+\rangle_y$ egoeran egongo da ondoren

$|r, +\rangle_y = \frac{1}{\sqrt{2}} [|r, +\rangle + i|r, -\rangle]$ ($\{|+\rangle, |-\rangle\}$ oinarrian garatuta)

$$\cancel{\left[dP_{S_y=\hbar/2} = |{}_y\langle r, + | \psi \rangle|^2 d^3r = d^3r \left| \frac{1}{\sqrt{2}} \int d^3r' [\psi_+(r')\, {}_y\langle r', + | r, + \rangle + \psi_- \, {}_y\langle r, + | r, - \rangle] \right|^2 = \frac{1}{2} d^3r \left| \int d^3r \left(\psi_+(r) \frac{1}{\sqrt{2}} - \frac{i}{\sqrt{2}} \psi_-(r) \right) \right|^2 = \frac{1}{2} \cdot \frac{1}{2} d^3r \left| \int d^3r \left(\psi_+(r) - i\psi_-(r) \right) \right|^2 \right]}$$

$$dP_{S_y=\hbar/2} = |{}_y\langle r, + | \psi \rangle|^2 d^3r \overset{*'}{=} \frac{1}{2} |\psi_+(r) - i\psi_-(r)|^2 d^3r$$

*' ${}_y\langle r, + | \psi \rangle = \int d^3r' \left(\psi_+(r')\, {}_y\langle r, + | r', + \rangle + \psi_-(r')\, {}_y\langle r, + | r', - \rangle \right) =$

$\int d^3r' \left(\psi_+(r') \frac{1}{\sqrt{2}} \langle r, + | r', + \rangle + \psi_-(r') \left(\frac{-i}{\sqrt{2}} \right) \langle r, - | r', - \rangle \right) =$

$\frac{1}{\sqrt{2}} \int d^3r' \left[\psi_+(r') \delta(r - r') - i\psi_-(r') \delta(r - r') \right] = \frac{1}{\sqrt{2}} [\psi_+(r) - i\psi_-(r)]$

Espacio orbital integrando $\hbar/2$ cálculo probabilidades, posiciones independientes, todas

da $\Rightarrow$ $P(s_y=+\hbar/2)=\int dP(s_y=\hbar/2)=\int d^3r\,\frac{1}{2}\left[\psi_+(r)-i\psi_-(r)\right]^2=$

$\int d^3r\cdot\frac{1}{2}\left(\psi_+(r)-i\psi_-(r)\right)\left(\psi_+^*(r)+i\psi_-^*(r)\right)=\frac{1}{2}\int d^3r\left(|\psi_+(r)|^2+|\psi_-(r)|^2+\right.$

$\left.i\psi_+(r)\psi_-^*(r)-i\psi_-(r)\psi_+^*(r)\right)=\frac{1}{2}\int d^3r\left(|\psi_+(r)|^2+|\psi_-(r)|^2-2\,\mathrm{Im}\,(\psi_+\psi_-^*)\right)=$

$$\frac{1}{2}\Big[\underbrace{\int d^3r\left(|\psi_+(r)|^2+|\psi_-(r)|^2\right)}_{1\,=\,P(\hbar/2)+P(-\hbar/2)}+2\int d^3r\,\mathrm{Im}\,(\psi_-(r)\psi_+^*(r))\Big]=\frac{1}{2}+\int d^3r\,\mathrm{Im}\,(\psi_-(r)\psi_+^*(r))$$

$*$ Po nuevo $S_z=\hbar/2$ igual $\Rightarrow$ $(p_0,+)$ nuevo

$$P(p_0,+)=|\langle p_0,+|\psi\rangle|^2\overset{*'}{=}|\bar{\psi}_+(p_0)|^2$$

$*'$ $\langle p_0,+|\psi\rangle=\int d^3r'\left[\psi_+(r')\langle p_0,+|r',+\rangle+\psi_-(r')\langle p_0,+|r',-\rangle\right]=$

$$\int d^3r\left[\psi_+(r)\langle p_0|r'\rangle\langle +|+\rangle+\psi_-(r)\langle p_0|r'\rangle\cancel{\langle -|+\rangle}\right]=\int d^3r\left[\psi_+(r)\underbrace{\langle p_0|r\rangle}_{=\langle r'|p_0\rangle^*}\right]=$$

$$\int d^3r'\,\psi_+(r')\frac{1}{(2\pi\hbar)^{3/2}}e^{-ip_0\cdot\vec{r}'/\hbar}=\frac{1}{(2\pi\hbar)^{3/2}}\int\psi_+(r')d^3r'\,e^{-ip_0\cdot\vec{r}'/\hbar}=\bar{\psi}_+(p_0)$$

2.) Considerar un sistema físico en cuyo espacio de estados se ha elegido una base ortonormal formada por los kets $|\varphi_1\rangle;|\varphi_2\rangle;|\varphi_3\rangle;|\varphi_4\rangle;|\varphi_5\rangle;|\varphi_6\rangle$. En la base de estos 6 vectores, tomados en ese orden, los observables H_0 y W vienen dados por:

$$H_0=\hbar\omega_0\begin{pmatrix}5&0&0&0&0&0\\0&3&0&0&0&0\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&0&0&0&6\end{pmatrix},\quad W=b\omega_0\begin{pmatrix}0&0&-1&-2&0&1\\0&0&0&0&0&0\\-1&0&1&1&0&2\\-2&0&1&1&0&-2\\0&0&0&0&1&1\\1&0&2&-2&1&1\end{pmatrix}$$

a) Considerando a W como una perturbación de H_0 ($b\ll1$) determinar los energías del sistema hasta el orden mas bajo ~~dado~~ en el parametro b.

$$[b\omega_0] = [E] \overset{\text{energia}}{=} [W] = [\tilde{W}][\lambda] \overset{[\lambda]=1}{=} [\tilde{W}] \Rightarrow \lambda = \frac{b}{\hbar} \quad , \quad \tilde{W} = \frac{1}{\lambda} W$$

H_0 $\{|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, |\varphi_4\rangle, |\varphi_5\rangle, |\varphi_6\rangle\}$ oinarrian diagonala denez bere autobektoreak izango dira eta autobalioak:

$$H_0|\psi_n^{0,i}\rangle = E_n^0|\psi_n^{0,i}\rangle$$

$$\begin{cases} E_1^0 = 5\hbar\omega_0 \rightarrow |\psi_1^0\rangle = |\varphi_1\rangle \\ E_2^0 = 3\hbar\omega_0 \rightarrow |\psi_2^0\rangle = |\varphi_2\rangle \\ E_3^0 = \hbar\omega_0 \rightarrow |\psi_3^0\rangle = |\varphi_3\rangle, |\psi_4^0\rangle = |\varphi_4\rangle, |\psi_5^0\rangle = |\varphi_5\rangle \\ E_4^0 = 6\hbar\omega_0 \rightarrow |\psi_6^0\rangle = |\varphi_6\rangle \end{cases}$$

$\hookrightarrow g_3 = 3$ endekatua

Perturbatutako energiak: $E_n(\lambda) = \varepsilon_0 + \lambda\varepsilon_1 + O(\lambda^2)$

- $E_1(\lambda) = \varepsilon_0 + \lambda\varepsilon_1$, $\varepsilon_0 = E_1^0 = 5\hbar\omega_0$, $|0\rangle = |\varphi_1\rangle = |\psi_1^0\rangle$

$$\varepsilon_1 = \langle 0|\tilde{W}|0\rangle = (1\ 0\ 0\ 0\ 0\ 0)\,\hbar\omega_0 \begin{pmatrix} 0 & 0 & -1 & -2 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 1 & 0 & 2 \\ -2 & 0 & 1 & 1 & 0 & -2 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 2 & -2 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} =$$

$$\hbar\omega_0\,(1\ 0\ 0\ 0\ 0\ 0) \begin{pmatrix} 0 \\ 0 \\ -1 \\ -2 \\ 0 \\ 1 \end{pmatrix} = \hbar\omega_0 \cdot 0 = 0$$

(Ez dago 1. ordenako zuzenketarik)

$$E_1(\lambda) = \underset{+O(\lambda^2)}{E_1^0} = 5\hbar\omega_0 + O(\lambda^2) \qquad (\lambda = b/\hbar)$$

- $E_2(\lambda) = \varepsilon_0 + \lambda\varepsilon_1 + O(\lambda^2)$, $\varepsilon_0 = E_2^0 = 3\hbar\omega_0$, $|0\rangle = |\psi_2^0\rangle = |\varphi_2\rangle$

$$\varepsilon_1 = \langle 0|\tilde{W}|0\rangle = (0\ 1\ 0\ 0\ 0\ 0)\,\hbar\omega_0 \begin{pmatrix} 0 & 0 & -1 & -2 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 1 & 0 & 2 \\ -2 & 0 & 1 & 1 & 0 & -2 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 2 & -2 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \hbar\omega_0 (0\ 1\ 0\ 0\ 0\ 0) \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} =$$

$\hbar\omega_0 \cdot 0 = 0$ (ez dago 1. ordenako zuzenketarik)

$$E_2(\lambda) = 3\hbar\omega_0 + O(\lambda^2) \qquad (\lambda = b/\hbar)$$

- $E_3^0 \Rightarrow$ endekatua $\Rightarrow E(\lambda) = \varepsilon_0 + \lambda\varepsilon_1$, $\varepsilon_0 = E_3^0$, $|0\rangle \in \mathcal{E}_3$

$\mathcal{E}_3 \Rightarrow \{|\varphi_3\rangle, |\varphi_4\rangle, |\varphi_5\rangle\}$ autobektoreak osatutako ~~oport~~ azpiespazioa

$\hat{W}^{(3)}$ diagonalizatu $\Rightarrow$ ε_1^j $\hat{W}^{(3)}$-ren autobalioak izango dira, j balioentzako

$E(\lambda)$-ren gorapen bat $(E_j(\lambda) = \varepsilon_0 + \lambda\varepsilon_1^j + O(\lambda^2))$

$\hat{W}^{(3)} \Rightarrow \hat{W}$-ren minorra ε_3 azpiespazioan $\Rightarrow$ $\tilde{W}^{(3)} = \hbar\omega_0 \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Diagonalizatu $\Rightarrow$ $|\hat{W}^{(3)} - \varepsilon_1^j \mathbb{1}| = \hbar\omega_0 \left| \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{\varepsilon_1^j}{\omega_0\hbar}\mathbb{1} \right| = 0 \Rightarrow$

$\downarrow$

$\tilde{\varepsilon}_1^j = \omega_0\hbar\varepsilon_1^j$

$$\begin{vmatrix} 1-\tilde{\varepsilon}_1^j & 1 & 0 \\ 1 & 1-\tilde{\varepsilon}_1^j & 0 \\ 0 & 0 & 1-\tilde{\varepsilon}_1^j \end{vmatrix} = (1-\tilde{\varepsilon}_1^j)^3 - (1-\tilde{\varepsilon}_1^j) = (1-\tilde{\varepsilon}_1^j)\left((1-\tilde{\varepsilon}_1^j)^2 - 1\right) = 0 \Rightarrow$$

$\tilde{\varepsilon}_1^1 = 1 \Rightarrow \varepsilon_1^1 = \omega_0\hbar$; $(1-\tilde{\varepsilon}_1^j) = \pm 1 \Rightarrow$

$\tilde{\varepsilon}_1^2 = 0 \rightarrow \varepsilon_1^2 = 0$, $\tilde{\varepsilon}_1^3 = 2 \rightarrow \varepsilon_1^3 = 2\hbar\omega_0$

- $E_3(\lambda) = E_3^0 + \lambda\tilde{\varepsilon}_1^1 \overset{+O(\lambda^2)}{=} \hbar\omega_0 + \lambda\hbar\omega_0 + O(\lambda^2) = \hbar\omega_0\left(1 + \frac{b}{\hbar}\right) + O(\lambda^2) =$

$\omega_0(\hbar + b) + O(\lambda^2)$

- $E_4(\lambda) = E_3^0 + \lambda\varepsilon_1^2 + O(\lambda^2) = \hbar\omega_0 + 0 + O(\lambda^2) = \hbar\omega_0 + O(\lambda^2)$
- $E_5(\lambda) = E_3^0 + \lambda\varepsilon_2^2 + O(\lambda^2) = \hbar\omega_0 + 2\hbar\omega_0\lambda + O(\lambda^2) = \hbar(\omega_0 + 2\omega_0\lambda) + O(\lambda^2) =$

$\hbar\omega_0\left(1 + 2\frac{b}{\hbar}\right) + O(\lambda^2) = \omega_0(\hbar + 2b) + O(\lambda^2)$

- $E_6(\lambda) = \varepsilon_0 + \varepsilon_1\lambda + O(\lambda^2) \rightarrow \varepsilon_0 = E_6^0 = 6\hbar\omega_0$ $|0\rangle = |\Psi_6^0\rangle = |\varphi_6\rangle$

$$\varepsilon_1 = \langle 0|\hat{W}|0\rangle = (0\,0\,0\,0\,0\,1)\,\hbar\omega_0 \begin{pmatrix} 0 & 0 & -1 & -2 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 1 & 0 & 2 \\ -2 & 0 & 1 & 1 & 0 & -2 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 2 & -2 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} =$$

$$(0\,0\,0\,0\,0\,1)\,\hbar\omega_0 \begin{pmatrix} 1 \\ 0 \\ 2 \\ -2 \\ 1 \\ 1 \end{pmatrix} = \hbar\omega_0$$

$E_6(\lambda) = 6\hbar\omega_0 + \lambda\hbar\omega_0 \overset{+O(\lambda^2)}{=} \hbar\omega_0(6+\lambda) \overset{+O(\lambda^2)}{=} \hbar\omega_0\left(6 + \frac{b}{\hbar}\right) + O(\lambda^2) =$

$\omega_0(6\hbar + b) + O(\lambda^2)$

b) Encontrándose el sistema en el estado $|\Psi\rangle = \frac{1}{\sqrt{6}}|\varphi_3\rangle + \frac{1}{\sqrt{6}}|\varphi_4\rangle + \frac{2}{\sqrt{6}}|\varphi_5\rangle$, se mide la energía. Determinar (para $b \neq 0$) la probabilidad de encontrar al sistema en el nivel fundamental? ¿Cuál es el estado cuántico después de la medida?

Oinarrizko egoera $\Rightarrow$ $E = E_4 = \hbar\omega_0 + O(\lambda^2)$ $\Rightarrow$ $|\phi\rangle = |0\rangle + O(\lambda)$

$|0\rangle \Rightarrow$ $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} b \\ a \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow a = b,$ c edozein $\Rightarrow$ $|0\rangle = |\varphi_5\rangle$

Orduan $P_{E=E_4} = |\langle\Psi|0\rangle|^2 = \left| \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right|^2 = \frac{4}{6} = \frac{2}{3}$

Neurketa eta gero $\Rightarrow$ $|\Psi\rangle = |\varphi_5\rangle$

3.) Estructura fina en el nivel $n=3$ del átomo de hidrógeno:

Los términos que constituyen el hamiltoniano de estructura fina W_f del átomo de hidrógeno son:

$$W_f = \underbrace{\frac{-P^4}{8m_e^3c^2}}_{W_{mv}} + \underbrace{\frac{1}{2m_e^2c^2}\frac{1}{R}\frac{dV(R)}{dR}\vec{L}\cdot\vec{S}}_{W_{SO}} + \underbrace{\frac{\hbar^2}{8m_e^2c^2}\nabla^2 V(R)}_{W_D}$$

¿En cuántos subniveles se desdobla el nivel $n=3$ si se prescinde del término ~~de la~~ spin-órbita? ¿Cuál es la degeneración de cada uno de estos subniveles?

$H = H_0 + W_f \Rightarrow H|\psi\rangle = E|\psi\rangle$

~~Lehenengo aurkituko ditugun bektoreak~~ $\Rightarrow$ $\{H_0, L^2, S^2, L_z, S_z\}$ - k BTMB osatzen dute

$|n\, l\, m_l\, m_s\rangle \rightarrow H_0$-ren autobektoreak eta $E_n^0 = -\frac{E_I}{n^2} = \frac{-Ze^2}{8\pi\varepsilon_0 a_0}\cdot\frac{1}{n^2}$ autobalioak.

$[W_{mv}, L^2] = [W_{mv}, S^2] = [W_{mv}, L_z] = [W_{mv}, S_z] = 0$

$[W_D, L^2] = [W_D, S^2] = [W_D, L_z] = [W_{mv}, S_z] = 0$

} Baina $W_{SO}=0$ denez $\{H, L^2, S^2, S_z, L_z\}$ -k BTMB osatzen dute

Orduan H-ren autobektoreak $|n\, l\, m_l\, m_s\rangle$ dira eta autobalioak:

n arruntak ez

$\hookrightarrow [H_0, W_D] \neq 0, [H_0, W_{mv}] \neq 0$

$H = H_0 + W_{mv} + W_D \Rightarrow H|n\, l\, m_l\, m_s\rangle = H_0|n\, l\, m_l\, m_s\rangle + W_{mv}|n\, l\, m_l\, m_s\rangle +$

$W_D|n\, l\, m_l\, m_s\rangle \overset{*1}{=} \left(-\frac{E_I}{n^2} + \right.$

$H_0 - V = T$

$*\; W_{mv}|n\, l\, m_l\, m_s\rangle = -\frac{p^4}{8m_e^3c^2}|n\, l\, m_l\, m_s\rangle = -\frac{1}{2m_ec^2}\left(\frac{p^2}{2m_e}\right)^2|n\, l\, m_l\, m_s\rangle =$

$-\frac{1}{2m_ec^2}\left(H_0^2 + V^2 - H_0V - VH_0\right)|n\, l\, m_l\, m_s\rangle = -\frac{1}{2m_ec^2}\left((E_n^0)^2 - E_n^0\right.$

Viriala $\Rightarrow \langle V\rangle = -2\langle T\rangle = 2E_n^0$

FISIKA KUANTIKOA

16-10-25

3. DIMENTSIO BAKARREKO POTENTZIALAK

• SARRERA: DIMENTSIO BAKARREKO POTENTZIALAK:

Hamiltondarren autobalio eta autofuntzioen kalkulua: (ezinbestekoa uhin-funtzio baten denboraren garapena kalkulatzeko):

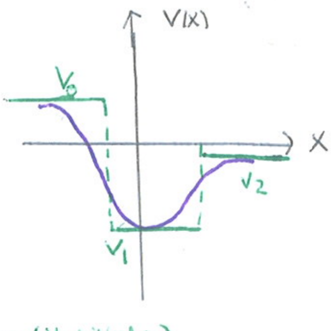
$$\hat{H}\psi_n = \varepsilon_n \psi_n \longleftrightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi_n = \varepsilon_n \psi_n$$

$$\{\psi_n\} \rightarrow \{\varepsilon_n\}$$

$$\Psi(x,t=0) = \sum_n c_n \psi_n \xrightarrow[V \neq V(x,t)]{} \Psi(x,t) = \sum_n c_n \psi_n e^{-\frac{i\varepsilon_n}{\hbar}t}$$

Hamiltondarraren autofuntzio eta autobalioak kalkulatzeko ekuazio diferentzial bat ebatzi behar dugu sistema bakoitzari dagokion energia potentziala ordezkatuz:

Ad:



* (Hurbilketa)

Baina V(x) edozein izan daitekenez, ekuazio diferentziala ebaztea nahiko zaila izaten da → hurbilketa bat egingo dugu tartekA V kte eginez. (horrela ekuazio diferentziala koefiziente konstantekoa izango da)

Neurri handi batean, hurbilketa horren bidez lortutako autobalio eta autofuntzioak benetakoen hurbilketa ona izango dira

• PARTIKULA ASKEA:

$$V=0 \rightarrow \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \longleftrightarrow \hat{H}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = \varepsilon \psi$$

$\psi = e^{rx}$ saiatu (koefiziente konstanteko delako) $\Rightarrow -\frac{\hbar^2}{2m} r^2 \cancel{e^{rx}} = \varepsilon \cancel{e^{rx}} \Rightarrow$

→ mekanika klasikoaren aldetik *

$r = \pm\sqrt{\frac{2m\varepsilon}{\hbar^2}}\, i$ ($\varepsilon \geq 0$ da derrigorrez $V=0$ delako eta $T \geq 0$ beti) $\Rightarrow K^2 = \frac{2m\varepsilon}{\hbar^2}$

* Mekanika kuantikoaren aldetik $\varepsilon < 0$ balitz esponentzialak ereduak izango lirateke eta uhin-funtzioa ez litzateke integragarria izango

→ $\hat{p}$-ren autofuntzioa, baina ψ_K ez

$\varepsilon = \frac{\hbar^2 K^2}{2m}$ $(K \in \mathbb{R}) \Rightarrow \psi_K = \underline{Ae^{iKx}} + Be^{-iKx} \Rightarrow$ aukera dezakegu autofuntzioak

ereduak izatea: $\begin{cases} \psi \Rightarrow \hat{H}\psi = \varepsilon\psi \\ \psi^* \Rightarrow \hat{H} = \hat{H}^* \Rightarrow \hat{H}\psi^* = \varepsilon\psi^* \end{cases} \Rightarrow \psi' = \psi + \psi^* \in \mathbb{R}$ (autofuntzioa)

$\psi_K' = A'\sin Kx + B'\cos Kx$ $(A', B' \in \mathbb{R})$ (Hau beti egin daiteke, eta nahi duguna erabili dezakegu)

• PARTIKULA-ASKEARI DAGOKION FARDEL-GAUSSIARRAREN DENBORA-GARAPENA:

* $\Psi(x,0) = \left(\frac{2}{\pi a^2}\right)^{1/4} e^{-\frac{x^2}{a^2}} e^{iK_0x}$ → funtzio konplexua $\rightarrow P(x,0) = \sqrt{\frac{2}{\pi a^2}}\, e^{-2\frac{x^2}{a^2}}$

→ Gaussiarra ($\Delta x = a/2$)

↳ normalizazio koefizientea

Denboran garatzeko, hasierako egoera hamiltondarraren autofuntzioetan garatu behar da.

Partikula askeari dagokion hamiltondarraren autofuntzioak: (uhin-lauak): $\left\{\frac{e^{iKx}}{\sqrt{2\pi}}\right\}\ \forall K \in \mathbb{R}$

* $\Psi(x,0) = \int_{-\infty}^{\infty} A(K,0)\frac{e^{iKx}}{\sqrt{2\pi}}\, dK$; $A(K,0) = \int_{-\infty}^{\infty} \Psi(x,0)\frac{e^{-iKx}}{\sqrt{2\pi}}\, dx = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}}\left(\frac{2}{\pi a^2}\right)^{1/4} e^{-\frac{x^2}{a^2}} e^{-i(K-K_0)x}\, dx =$

$$\left[*^1 \int_{-\infty}^{\infty} e^{-\alpha^2(\alpha+\beta)^2}\, d\alpha = \frac{\sqrt{\pi}}{\alpha} \right] \qquad \left(\frac{2}{\pi a^2}\right)^{1/4} \cdot \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\left[\frac{x^2}{a^2} - i(K_0-K)x\right]}\, dx =$$

$*^2$

$$\left(\frac{2}{\pi a^2}\right)^{1/4} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{a^2}\left(x - \frac{i(k_0-k)a^2}{2}\right)^2} e^{-\frac{(k_0-k)^2 a^2}{4}} dx = \frac{1}{\sqrt{2\pi}} \left(\frac{2}{\pi a^2}\right)^{1/4} e^{-\frac{(k_0-k)^2 a^2}{4}} \sqrt{\pi}\, a =$$

$$\left[* \; \frac{x^2}{a^2} - i(k_0-k)x = \left[\frac{x}{a} - i\frac{(k_0-k)a}{2}\right]^2 + \frac{(k_0-k)^2 a^2}{4} \right] \qquad \boxed{\frac{\sqrt{a}}{(2\pi)^{1/4}} e^{-\frac{a^2}{4}(k_0-k)^2}}$$

* $P(k) = |A(k,0)|^2 = \frac{a}{\sqrt{2\pi}} e^{-\frac{a^2}{2}(k_0-k)^2} \implies \langle p \rangle = \hbar \langle k \rangle = \hbar k_0$ hau funtzio konplexu honek zehaztu

$(\ast \;\; \psi \to \langle p \rangle = p \;\; ; \;\; \psi' = \psi e^{ik_0 x} \to \langle p \rangle' = p + \hbar k_0)$

* $\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\sqrt{a}}{(2\pi)^{1/4}} e^{-\frac{a^2}{4}(k_0-k)^2} e^{ikx} dk \xrightarrow{t} \cdot\, e^{-i\frac{E_k}{\hbar}t} = e^{-i\frac{\frac{\hbar^2 k^2}{2m}}{\hbar}t}$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\sqrt{a}}{(2\pi)^{1/4}} e^{-\frac{a^2}{4}(k_0-k)^2} e^{-i\frac{\hbar k^2}{2m}t} e^{ikx} dk = \left(\frac{2a^2}{\pi}\right) \frac{e^{i(\varphi + k_0 x)}}{\left(a^4 + \frac{4\hbar^2 t^2}{m^2}\right)^{1/4}} \cdot$$

$\to \in \mathbb{C}$ (a-ren nagusia)

*' estrategia erabiliz.

$$e^{-\left[\frac{x - \frac{\hbar k_0 t}{m}}{a^2 + \frac{2i\hbar t}{m}}\right]^2}$$

(Funtzioa moldatua)

* $P(x,t) = \sqrt{\frac{2}{\pi a^2}} \cdot \frac{1}{\sqrt{1 + \frac{4\hbar^2 t^2}{m a^4}}} e^{\frac{-2a^2\left(x - \frac{\hbar k_0 t}{m}\right)^2}{a^4 + \frac{4\hbar^2 t^2}{m}}} \implies x_{max} = \frac{\hbar k_0}{m} t \;;\; v_{max} = \frac{\hbar k_0}{m} = \frac{\langle p \rangle(0)}{m}$

probabilitate maximoko x

desplazatu

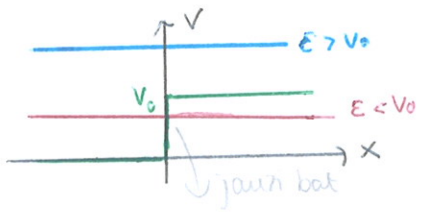
dentsitate maximoa duen abiadura

partikula klasikoak izango lukeen abiadura berdinarekin dagoela

$$\Delta x(t) = \frac{a}{2} \sqrt{1 + \frac{4\hbar^2 t^2}{m a^4}} = \Delta x(0) \cdot \sqrt{\frac{1 + 4\hbar^2 t^2}{m a^4}}$$

(zabaltzen joan)

- **POTENTZIAL-JAUZIA:**



Heaviside-n funtzioa

$$V(x) = V_0 \theta(x) = \begin{cases} V_0 & x > 0 \\ 0 & x < 0 \end{cases}$$

$$F(x) = -\frac{\partial V}{\partial x} = -V_0 \delta(x)$$

* Klasikoki bi aukera energiaren, $\varepsilon < V_0$ edo $\varepsilon > V_0$:

* $\varepsilon < V_0 \to$ $0 < x$ tartean energia osoa zinetikoa izango da eta $x = 0$-ra heltzean ezin izango da pasatu beste aldera, eta bota egingo da aurkako energiarekin.

energia zinetikoa ezin delako negatiboa izan.

* $E > V_0$ → energia osoa $x<0$ tartean zinetikoa izango da, eta orain $x=0$-ra heltzean $E>V_0$ denez pasatu ahal izango da, bere energia zinetikoa txikiuz

- POTENTZIAL-JAUZIA: ISLAPEN eta TRANSMISIO-KOEFIZIENTEAK, $E<V_0$:

$$\psi = \begin{cases} \frac{D}{2}\left(1+\frac{iK_2}{K_1}\right)e^{iK_1x} + \frac{D}{2}\left(1-\frac{iK_2}{K_1}\right)e^{-iK_1x} & x<0 \\ De^{-K_2x} & x>0 \end{cases}$$

$\hat{H}$-ren autof. potentzial jauziaren kasurako

(Hamiltondarraren autofuntzioak $V=0$; partikula askea)

$\left(K_1 = \frac{\sqrt{2mE}}{\hbar} \;,\; K_2 = \frac{\sqrt{2m|V_0-E|}}{\hbar} \right)$

* Korronte dentsitatea (probabilitate dentsitatearekin lotuta): $j = \frac{i\hbar}{2m}\left\{ \psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right\}$

$$\underset{p_1=\hbar K}{\psi = Ae^{iKx}} + \underset{p_2=-\hbar K}{Be^{-iKx}} \rightarrow j = |A|^2 \underset{v_1}{\frac{\hbar K}{m}} - |B|^2 \underset{v_2}{\frac{\hbar K}{m}}$$

(Bi eluxpen)
↳ bata aurreranzkoa (v_1) eta bestea atzerakarantza (v_2)
↳ jauzitik errebotatzen duena

* Islapen koefizientea:

errebotatu egiten duenaren korrontearen eluxpena (− duena)

$$R = \frac{|B|^2 \frac{\hbar K}{m}}{|A|^2 \frac{\hbar K}{m}} = \frac{\frac{|D|^2}{4}\left|1-\frac{iK_2}{K_1}\right|^2 \frac{\hbar K_1}{m}}{\frac{|D|^2}{4}\left|1+\frac{iK_2}{K_1}\right|^2 \frac{\hbar K_1}{m}} = \frac{1+\left(\frac{K_2}{K_1}\right)^2}{1+\left(\frac{K_2}{K_1}\right)^2} = 1$$

eraso egiten duenaren eluxpena

gure kasuan

(Islapena ari garenez aztertzen $x<0$-n egin behar dugu, errebotatzailea eluxpena hor dagoelako e^{-iK_1x} baita arazotzailea)

* Transmisio koefizientea:

Transmititutakoa → eskuinekoa uhin funtzioa $(x>0)$ → $j=0$ (ereala delako)

Eskuinean, nahiz eta dentsitate probabilitatea 0 ez izan, ez dago korronterik, ez dago fluxurik.

transmititutakoaren eluxpena

$$T = \frac{j_{x>0}}{|A|^2 \frac{\hbar K}{m}} = 0$$

eraso egiten duenaren eluxpena

⇒ Dena islatzen da nahiz eta uhin-funtzioa 0 ez izan eremu horretan

⇒ $R+T=0$

- POTENTZIAL-JAUZIA: ISLAPEN eta TRANSMISIO-KOEFIZIENTEAK, $E>V_0$:

$\hat{H}$-ren autofuntzioak

$$\psi = \begin{cases} \frac{1}{2}C\left(1+\frac{K_2}{K_1}\right)e^{iK_1x} + \frac{1}{2}C\left(1-\frac{K_2}{K_1}\right)e^{-iK_1x} & x<0 \\ Ce^{iK_2x} & x>0 \end{cases}$$

$\left(\frac{\sqrt{2Em}}{\hbar} = K_1 \quad \frac{\sqrt{2m(E-V_0)}}{\hbar} = K_2 \right)$

$$j = \begin{cases} \frac{1}{4}\left(1+\frac{k_2}{k_1}\right)^2 |C|^2 \frac{\hbar k_1}{m} - \frac{1}{4}\left(1-\frac{k_2}{k_1}\right)^2 |C|^2 \frac{\hbar k_1}{m} & x<0 \\ |C|^2 \frac{\hbar k_2}{m} & x>0 \end{cases}$$

erasoa   erreboteatu

* **Islapen koefizientea:**

erreboteatzen den fluxuaren eltapena

(x<0-n aztertu behi)

$$R = \frac{\cancel{\frac{1}{4}}\left(1+\frac{k_2}{k_1}\right)^2 \cancel{|C|^2} \cancel{\frac{\hbar k_1}{m}}}{\cancel{\frac{1}{4}}\left(1+\frac{k_2}{k_1}\right)^2 \cancel{|C|^2} \cancel{\frac{\hbar k_1}{m}}} = \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 = \left(\frac{\sqrt{2mE}-\sqrt{2m(E-V_0)}}{\sqrt{2mE}+\sqrt{2m(E-V_0)}}\right)^2 = \left(\frac{\sqrt{2mE/V_0}-\sqrt{2m(E/V_0-1)}}{\sqrt{2mE/V_0}+\sqrt{2m(E/V_0-1)}}\right)^2 =$$

$$\left(\frac{\sqrt{\frac{E}{V_0}}-\sqrt{\frac{E}{V_0}-1}}{\sqrt{\frac{E}{V_0}}+\sqrt{\frac{E}{V_0}-1}}\right)^2$$

erasotzen den fluxuaren eltapena

* **Transmisio koefizientea:**

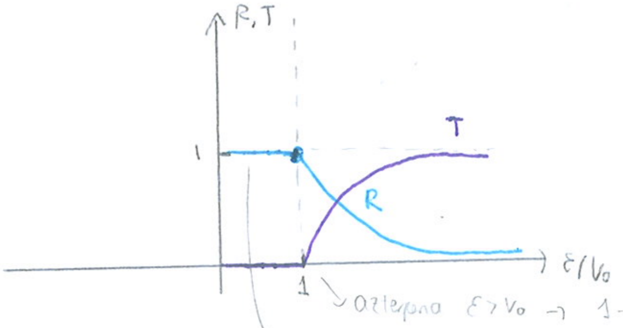
transmititutako fluxuaren eltapena

erasotzen den fluxuaren eltapena

$$T = \frac{\cancel{|C|^2} \frac{\hbar k_2}{\cancel{m}}}{\frac{1}{4}\left(1+\frac{k_2}{k_1}\right)^2 \cancel{|C|^2} \frac{\hbar k_1}{\cancel{m}}} = \frac{4k_2}{\left(1+\frac{k_2}{k_1}\right)^2 k_1} = \frac{4k_2k_1}{(k_1+k_2)^2} = \frac{4\sqrt{2m(E-V_0)}\sqrt{2mE}}{\left(\sqrt{2m(E-V_0)}+\sqrt{2mE}\right)^2} =$$

$$\frac{4\sqrt{E-V_0}\sqrt{E}}{\left(\sqrt{E-V_0}+\sqrt{E}\right)^2} = \frac{4\sqrt{E/V_0}\sqrt{\frac{E}{V_0}-1}}{\left(\sqrt{\frac{E}{V_0}-1}+\sqrt{E/V_0}\right)^2}$$

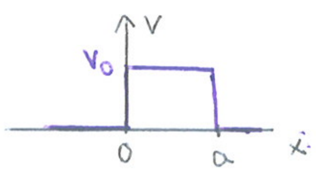
$(R+T=1)$



aztepna $E>V_0$ → 1-etik aurrera

$E<V_0$ (baina BETI $E>0$)

POTENTZIAL LANGA:



$$V(x) = \begin{cases} V_0 & x\in(0,a) \\ 0 & x\in(-\infty,0)\cup(a,\infty) \end{cases} \Rightarrow$$

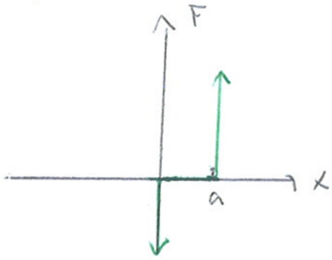
"Barrera" moduko bat dugu (0,a) tartean, $V=V_0$ denean

Klasikoki espero ko dugun portaera partikularen energiaren araberakoa izango da ($\varepsilon > V_0$, $\varepsilon < V_0$)

- Demagun $\varepsilon < V_0$ dela, orduan ezkerretik datorren partikula bat ($v = kte$ eramanda, $V = 0$ delako) langara iristerakoan ezin izango da beste aldera pasatu, energia zinetikoa negatiboa izan beharko litzatekelako ⇒ errebotatuko du eta ezkerrerantz joan.

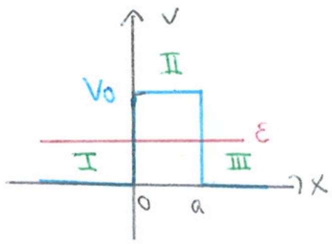
- Demagun $\varepsilon > V_0$ dela, orduan energia zinetiko konstante jakin batekin ezkerretik datorren partikula langara heltzean energia zinetikoaren jaitsiera jasango du (diferentzia hori $\varepsilon - V_0$ izanik) eta barneran, langan, energia zinetiko hori konstante mantendu eta gero barrera zeharkatzean jatorrizko energia zinetikoa berreskuratuko du. (partikula guztiek zeharkatuko dute langa)

Indarra ⇒ $F(x) = -\dfrac{\partial V}{\partial x} = -V_0\,\delta(x) + V_0\,\delta(x-a)$



Portaera kuantikoa aztertzeko ⇒ Schrödingeraren ekuazioa behar da.

POTENTZIAL LANGA, $E < V_0$



$$V(x) = \begin{cases} V_0 & x \in [0, a] \\ 0 & x \in (-\infty, 0) \cup (a, \infty) \end{cases}$$

Denboraren independentea den Schrödingeraren ekuazioa:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = \varepsilon\psi$$

- 3 tarte: I ⇒ $V = 0$ → $-\dfrac{\hbar^2}{2m}\dfrac{\partial^2 \psi}{\partial x^2} = \varepsilon\psi$ (partikula askea) → uhin laua → $\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$

$$k_1 = \sqrt{\frac{2m\varepsilon}{\hbar^2}} = \frac{\sqrt{2m\varepsilon}}{\hbar}$$

II $\Rightarrow$ $V = V_0 \rightarrow -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi}{\partial x^2} + V_0\psi = \mathcal{E}\psi \rightarrow \mathcal{E} < V_0$ denez $\rightarrow$ esponentzial errealak $\rightarrow$

$$\psi_2 = Ce^{K_2 x} + De^{-K_2 x} \quad ; \quad K_2 = \frac{\sqrt{2m(V_0-\mathcal{E})}}{\hbar}$$

III $\Rightarrow$ $V = 0 \rightarrow -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi}{\partial x^2} = \mathcal{E}\psi$ (partikula askea) $\rightarrow$ uhin lauak $\rightarrow$ $\psi_3 = Ee^{iK_1x} + Fe^{-iK_1x}$

$$\left(K_1 = K_3 = \frac{\sqrt{2m\mathcal{E}}}{\hbar}\right)$$

uhin funtzioa + deribatua jarraituak izatea

- Mugalde baldintzak: Ez dugu arrazoirik, uhin-funtzioa infinitura ez doa infinitura
- Jarraitasuna: $x=0$ eta $x=a$-n. $\Rightarrow$ 4 baldintza lortu eta 6 koefiziente ditugunez 2 aske geratzen zaizkigu.

$-K_1$ ezkerrerantz ekarpena delako

Guk aukeratuko dugu (2 askatasun gradu ditugulako) partikula ezkerretik datorrela: $\rightarrow$ $F=0$

$* \; x=0 \rightarrow \psi_1(0) = \psi_2(0) \rightarrow A+B = C+D$

$F=0$

$* \; x=a \rightarrow \psi_2(a) = \psi_3(a) \rightarrow Ce^{K_2a} + De^{-K_2a} = Ee^{iK_1a}$

$* \; x=0 \rightarrow \psi_1'(0) = \psi_2'(0) \rightarrow iK_1A - iK_1B = K_2(C-D) = iK_1(A-B)$

$* \; x=a \rightarrow \psi_2'(a) = \psi_3'(a) \rightarrow K_2(Ce^{K_2a} - De^{-K_2a}) = iK_1 e^{iK_1a}E$

Mathematica edo ordenagailuarekin ebatzi

Dena A-ren funtzioan jarri $\Rightarrow$ $B = \dfrac{(K_1^2+K_2^2)\sinh K_2a \; A}{(K_1^2-K_2^2)\sinh K_2a + 2iK_1K_2\cosh K_2a}$

$$C = \frac{K_1(iK_2-K_1)e^{-K_2a}A}{(K_1^2-K_2^2)\sinh K_2a + 2iK_1K_2\cosh K_2a} \quad ; \quad D = \frac{K_1(iK_1+K_1)e^{K_2a}A}{(K_1^2-K_2^2)\sinh K_2a + 2iK_1K_2\cosh K_2a}$$

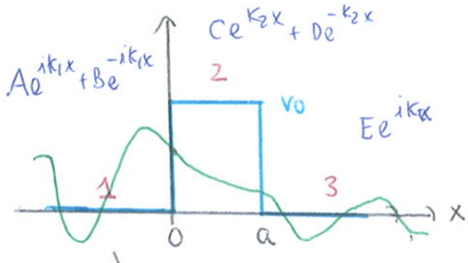
$$E = \frac{2iK_1K_2A}{(K_1^2-K_2^2)\sinh K_2a + 2iK_1K_2\cosh K_2a}$$

A normalizazio konstantea izan daiteke, baina uhin lauekin lortu dugunez arazoak egoten dira

Printzipioz energia edozein izan daiteke, ez dago mugatuta (balio diskretuak baliranak egoera lotuak ditugunean).

Kuantikoki, (0,a) tartean uhin-funtzioa txikia bada ere ez da nulua, ekarpen bat daukagu. Gainera, III. tartean ekarpen bat dugunez, partikula ezkerretik etorrita badago probabilitate bat langan egoteko ((0,a) tartean) baita langa zeharkatzeko.

POTENTZIAL-LANGA: ISLAPEN eta TRANSMISIO KOEFIZIENTEAK, $E < V_0$



uhin-funtzioaren zati ereala

uhin landa

$$1 \Rightarrow \vec{j}_1 = |A|^2 \frac{\hbar k_1}{m} - |B|^2 \frac{\hbar k_1}{m}$$

$$2 \Rightarrow \vec{j}_2 = 0 \quad \text{(uhin-funtzioa ereala delako)}$$

$$3 \Rightarrow \vec{j}_3 = |E|^2 \frac{\hbar k_1}{m}$$

korronte dentsitateak

Hauekin islapen eta transmisio koefizienteak kalkulatu:

Zenbat "igarotzen" den beste aldera

$$* \quad T = \frac{\vec{j}_3}{\vec{j}_{eraso}} = \frac{|E|^2 \cancel{\hbar k_1/m}}{|A|^2 \cancel{\hbar k_1/m}} = \frac{|E|^2}{|A|^2}$$

erasoaren ekarpena $|A|^2 \frac{\hbar k_1}{m}$ da ez $|B|^2$-rekin, islatutakoa delako

k_1, k_2 adierazpenak sartu

E eta A-ren adierazpenak jarriz $\Rightarrow$ $T = \dfrac{4k_1^2k_2^2}{4k_1^2k_2^2\cosh^2 k_2a + (k_1^2-k_2^2)^2\sinh^2 k_2a} =$

$$\frac{4E(V_0-E)}{4E(V_0-E) + V_0^2 \sinh^2\left[\frac{\sqrt{2m(V_0-E)}}{\hbar}a\right]}$$

$$* \quad R = 1 - T$$

$k_2a \gg 1$ badugu, $\sinh k_2a = \dfrac{e^{k_2a} - e^{-k_2a}}{2}$ denez $\rightarrow \sinh k_2a \approx \dfrac{e^{k_2a}}{2}$ izango da $\rightarrow$

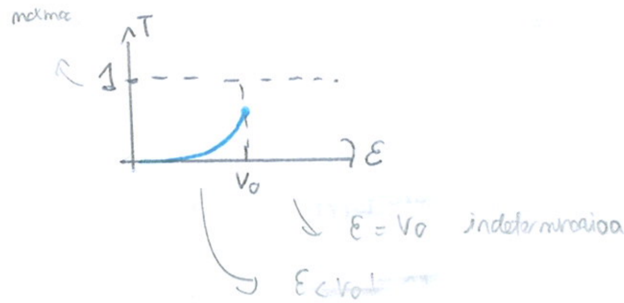
$T \approx \dfrac{16E(V_0-E)}{V_0^2} e^{-2k_2a} \neq 0$ $\Rightarrow$ esponentzialki txikia a eta k_2-rekin $\Rightarrow$ zenbat eta handiagoak izan gero eta gehiago txikitu transmisio koefizientea $\rightarrow$ langa zeharkatzeko probabilitatea txikia. ($k_2 \uparrow$ $V_0 - E \uparrow$)

Adibide numerikoa: • e^- bat, $E = 1\,eV$, $V_0 = 2\,eV$ $\Rightarrow$ $T_e = 0'78$ $\rightarrow$ langa zeharkatzeko probabilitatea %78-koa

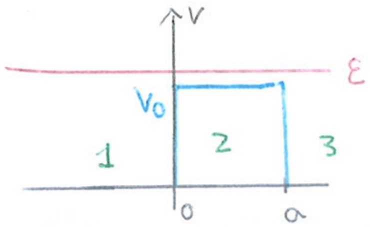
• p^+ bat, $E = 1\,eV$, $V_0 = 2\,eV$ $\Rightarrow$ $T_p \simeq 10^{-19}$ $\rightarrow$ probabilitate oso txikia $\Rightarrow$ masak eragin duela, bineduran barruan dagoelako $\left(k_2 = \frac{\sqrt{2m|V_0 - E|}}{\hbar} \right)$

Langa bat zeharkatzea $\Rightarrow$ TUNEL-EFEKTUA (Fenomeno erabat kuantikoa)

Nola aldatzen da T energiaren funtzioan?



POTENTZIAL-LANGA, $E > V_0$:



Uhin-funtzioa oszilakorra tarte guztietan

($0<x<a$ tartean k txikiagoa eta λ handiagoa)

V₀ ktea delako

* Schrödingeren ekuazioa: $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$

3 tarte: 1: $(x<0)$ $\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$ $\left(k_1 = \frac{\sqrt{2mE}}{\hbar} \right)$

2: $(0<x<a)$ $\psi_2 = Ce^{ik_2x} + De^{-ik_2x}$ $\left(k_2 = \frac{\sqrt{2m|E-V_0|}}{\hbar} \right)$

3: $(x>a)$: $\psi_3 = Ee^{ik_1x} + Fe^{-ik_1x}$ $(k_1 = k_3)$

* Mugalde baldintzak: Infinituarekin ez dugu arazorik, partikula askearen eremuan gaudelako ($-\infty$ edo $+\infty$-en ez da infinitura).

askatasuna hau aukeratuko

Jarraitasuna aztertzean $x=0$ eta $x=a$-n 4 baldintza lortuko ditugu eta sei konstante ditugunez bi aske geratuko dira $\Rightarrow$ suposatu lehen bezala ezkerretik datorrela (orduan ez du zentzurik eskuinean, $x>a$, ezkerrerantzko fluxurik izatea $\rightarrow F=0$)

• $\psi_1(0) = \psi_2(0)$ $\rightarrow$ $A+B = C+D$

• $\psi_2(a) = \psi_3(a) \rightarrow Ce^{ik_2a} + De^{-ik_2a} = Ee^{ik_1a}$

• $\psi_1'(0) = \psi_2'(0) \rightarrow ik_1(A-B) = ik_2(C-D) \rightarrow k_1(A-B) = k_2(C-D)$

• $\psi_2'(a) = \psi_3'(a) \rightarrow \cancel{i}k_2(Ce^{ik_2a} - De^{-ik_2a}) = \cancel{i}k_1 e^{-ik_1a}E$

Denak konstante beraren menpe jarriz:

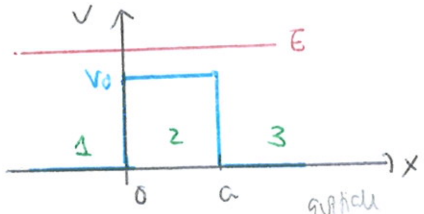
* $B = \dfrac{(k_1^2-k_2^2)\sin k_2a \; A}{\underbrace{(k_1^2+k_2^2)\sin k_2a + 2ik_1k_2\cos k_2a}_{Z}}$ Z (deitu honela luzeena delako gutxitzeko)

* $C = \dfrac{ik_1 e^{-k_2a} A(k_2+k_1)}{Z}$

* $D = \dfrac{ik_1 e^{ik_2a} A(k_2-k_1)}{Z}$

* $E = \dfrac{2ik_1k_2A}{Z}$

POTENTZIAL-LANGA, $E > V_0$: ISLAPEN eta TRANSMISIO KOEFIZIENTEAK:



guztiak esponentzial irudikariak baina λ ezberdinekin (k)

$1 \Rightarrow \quad \psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \qquad \left(k_1 = \dfrac{\sqrt{2mE}}{\hbar}\right)$

$2 \Rightarrow \quad \psi_2 = Ce^{ik_2x} + De^{-ik_2x} \qquad \left(k_2 = \dfrac{\sqrt{2m(E-V_0)}}{\hbar}\right)$

$3 \Rightarrow \quad \psi_3 = Ee^{ik_1x} \qquad (k_1 = k_3)$

$1 \Rightarrow \; j = |A|^2\dfrac{\hbar k_1}{m} - |B|^2\dfrac{\hbar k_1}{m} \qquad 2 \Rightarrow \; j = |C|^2\dfrac{\hbar k_2}{m} - |D|^2\dfrac{\hbar k_2}{m} \qquad 3 \Rightarrow \; j = |E|^2\dfrac{\hbar k_1}{m}$

• $T = \dfrac{|E|^2}{|A|^2}$ transmititutakoa / erasotzen duena $\Rightarrow$ E eta A-ren adierazpenak ordezkatuz $\Rightarrow$

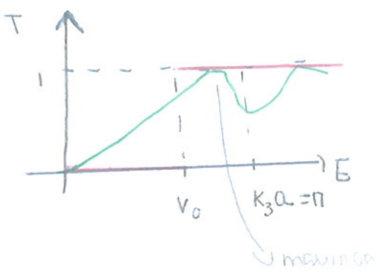
k_1, k_2 sartu

$$T = \frac{4k_1^2k_2^2}{(k_1^2+k_2^2)^2\sin^2 k_2a + 4k_1^2k_2^2\cos^2 k_2a} = \frac{4E(E-V_0)}{4E(E-V_0) + V_0^2\sin^2\Big(\underbrace{\frac{\sqrt{2m(E-V_0)}}{\hbar}a}_{k_2a}\Big)}$$

Energian balio batzuetarako $T = 1 \rightarrow \quad T = 1 \Leftrightarrow k_2a = n\pi \rightarrow T_{max}$

$T_{min} = \dfrac{4E(E-V_0)}{4E(E-V_0)+V_0^2}$; $k_2a = \dfrac{\pi}{2}(2n+1) \quad n \in \mathbb{N}$

$\lambda = \dfrac{2\pi}{k} \rightarrow \quad \lambda_2 = \dfrac{2\pi}{k_2}$ eta $k_2 = \dfrac{n\pi}{a}$ denean $(T=1) \rightarrow \dfrac{2a}{n} = \lambda \Rightarrow$ hau gertatzen denean partikula probabilitate osoz pasatu da beste aldera.

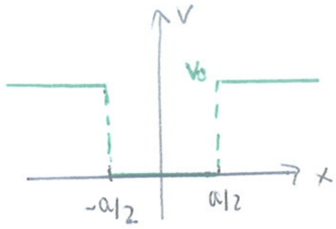


- Kuantikoki
- Klasikoki

$T_{max} = 1$ egiten duten energiaren balioei $\Rightarrow$ erresonantziak (anplitude maximoa)

POTENTZIAL-OSINA:

Potentzial-osina $\Leftrightarrow$ potentzial putzua



$$V(x) = \begin{cases} 0 & x \in [-a/2, a/2] \\ V_0 & |x| > a/2 \end{cases}$$

Daukagun energiaren arabera ($E < V_0$, $E > V_0$, ...) emaitza ezberdinak izango ditugu:

- klasikoki, $E < V_0$ bada putzuaren barruan baino ez da egongo partikula ($T < 0$ izan ez dadin) $\Rightarrow$ baimendutako zonaldea mugatuta eta finitua da $\Rightarrow$ energiaren diskretizazioa (egoera-lotuak) (kuantikoki)

  Klasikoki partikulak errebotatu egingo luke hormetan momentuaren ikurra aldatuz eta energia aldatu gabe.

- $E > V_0$ bada ez dago zonalde batean mugatuta egongo partikula klasikoki, zonalde guztian mugitu da (kanpoan $T = E - V_0$) $\Rightarrow$ kuantikoki ez dugu energiaren diskretizaziorik izango.

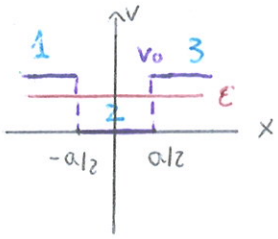
POTENTZIAL-OSINA, $E < V_0$:

$$V(x) = \begin{cases} V_0 & |x| < a/2 \\ 0 & |x| > a/2 \end{cases}$$

Badakigu klasikoki $E < V_0$ izanda partikula putzuaren barruan egongo dela eta kuantikoki egoera lotuak izango ditugula $\Rightarrow$ zer gertatzen den aztertzeko Schrödingeren ekuazioa ebatzi, denborarekiko independentea dena:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi=\varepsilon\Psi$$ Energiaren balioak diskretuak $\Rightarrow$ $\hat{H}$-ren autobalioak diskretuak.

3 tarte ezberdinetan banatu:



$1 \Rightarrow \Psi_1 = Ae^{K_1x}+Be^{-K_1x}$; $K_1=\frac{\sqrt{2m|V_0-E|}}{\hbar}$

$2 \Rightarrow \Psi_2 = Ce^{iK_2x}+De^{-iK_2x}$ edo $\sin K_2x$, $\cos K_2 x$

(egoera lotuak direnean erosoagoa sin, cos erabiltzea) $\Rightarrow$

uhin-funtzioen simetria hobeto ilustratzeko

$\Psi_2 = D\cos K_2x + C\sin K_2 x$; $K_2=\frac{\sqrt{2mE}}{\hbar}$

$3 \Rightarrow \Psi_3 = Ee^{K_1x}+Fe^{-K_1x}$

Mugalde baldintzak:

$x\to\infty$ $\Psi=\Psi_3$ dugulako

- $x\to\infty$ $\Psi\to 0$ $\longleftrightarrow$ $\Psi_3\to 0$ $\longleftrightarrow$ $E=0$; $\Psi_3=Fe^{-K_1x}$
  $x\to-\infty$ $\Psi\to 0$ $\longleftrightarrow$ $\Psi_1\to 0$ $\longleftrightarrow$ $B=0$; $\Psi_1=Ae^{K_1x}$

- Jarraitasuna: Ψ-ren jarraitasuna:

  * $\Psi_1(-a/2)=\Psi_2(-a/2) \leftrightarrow Ae^{-K_1a/2}=-C\sin K_2a/2+D\cos K_2a/2$
  * $\Psi_2(a/2)=\Psi_3(a/2) \leftrightarrow Fe^{-K_1a/2}=C\sin K_2a/2+D\cos K_2 a/2$

  Ψ'-ren jarraitasuna:

  * $\Psi_1'(-a/2)=\Psi_2'(-a/2) \leftrightarrow K_1Ae^{-K_1a/2}=K_2C\cos K_2a/2+K_2D\sin K_2 a/2$
  * $\Psi_2'(a/2)=\Psi_3'(a/2) \leftrightarrow -K_1Fe^{-K_1C/2}=K_2C\cos K_2a/2-K_2D\sin K_2a/2$

4x4-koa

Emaitza tribiala ez izateko $\Rightarrow$ determinantea koefizienteak eta zeroa berdindu edo sistemaren simetriaz baliatu: sistema simetrikoa denez uhin-funtzioak bakoitiak edo bikoitiak izango dira (hamiltondorraren eta inbertsio simetriaren aldibereko autofuntzioak izango ditugu eta inbertsio simetriaren autofuntzioak funtzio bakoitiak eta bikoitiak dira) $\Rightarrow$ Beraz $\Rightarrow$ $\hat{H}$-ren autofuntzioak bakoitiak / bikoitiak

izango dira:

- Simetrikoak: (bikoitiak). $\psi(x) = \psi(-x)$ $\Rightarrow$ ertzeten duguna bata bestearen berdina:

$A = F$ eta $C = 0$ ($\sin k_2 x$ bakoitia delako) $\Rightarrow$ ekuazioetan

sartu $\Rightarrow$ $\begin{cases} A e^{-k_1 a/2} = D \cos k_2 a/2 & (1) \\ k_1 A e^{-k_1 a/2} = k_2 D \sin k_2 a/2 & (2) \end{cases}$ $\Rightarrow \frac{(2)}{(1)} \Rightarrow k_2 \operatorname{tg} k_2 a/2 = k_1$

$\Downarrow$

ekuazio trastzendentala $\Leftarrow$ energiak bete behar duen baldintza ψ bikoitia denean

E ezin da zuzenean askatu

- Antisimetrikoak: (bakoitiak): $\psi(x) = -\psi(-x)$ $\Rightarrow$ $A = -F$ eta $D = 0$ ($\cos k_2 x$

bikoitia delako) $\Rightarrow$ ekuazioetan sartu $\Rightarrow$ $\begin{cases} A e^{-k_1 a/2} = -C \sin k_2 a/2 & (1) \\ k_1 A e^{-k_1 a/2} = k_2 C \cos k_2 a/2 & (2) \end{cases}$

$\Rightarrow \frac{(2)}{(1)} \Rightarrow -k_2 \operatorname{cotg} k_2 a/2 = k_1$ (ek. trastzendentala $\Rightarrow$ E ezin da zuzenean askatu) analitikoki

Ekuazio trastzendentalak $\Rightarrow$ ebatzpen grafikoa

Ebatzpen grafikoa (Kualitatiboa)

Aldagai aldaketa $\Rightarrow$ $k_2 a/2 = X$ $\quad k_1 a/2 = Y$

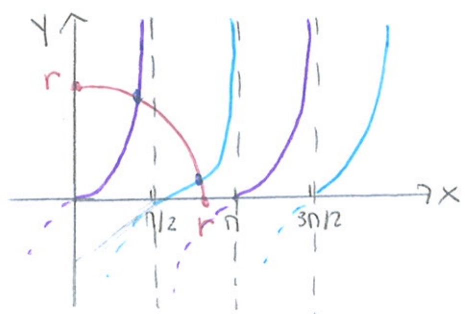
1: $Y = X \operatorname{tg} X$ (bik.)

2: $Y = -X \operatorname{cotg} X$ (bak.)

*'

3. $X^2 + Y^2 = \frac{a^2}{4}(k_1^2 + k_2^2) = \underbrace{\frac{a^2}{4}\left(\frac{2mV_0}{\hbar^2}\right)}_{r^2}$ (zirkunferentzia) $\Rightarrow r = \left(\frac{a}{2}\frac{\sqrt{2mV_0}}{\hbar}\right)$

X eta Y definituta dauden moduan, $X, Y \geq 0$ beti. (1. koadrantea soilik)



Bi ebaki puntu ebatzpen honetan (r-ren tamainaren arabera):

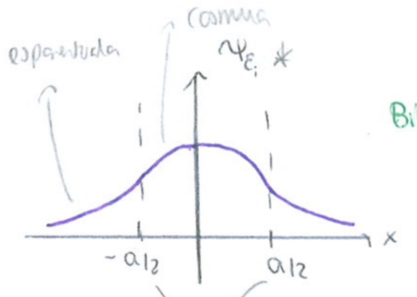
1. a $X < \pi/2$ denean eta 2. a $X \in (\pi/2, \pi)$

($X = k_2 \frac{a}{2}$ $\Rightarrow$ E lotu) $\Rightarrow$ 2 egoera lotu.

(V_0 zenbat eta handiagoa izan gero eta egoera lotu gehiago)

$\llcorner$) ez dira ebakitzen, funtzioak sim edo antis baina ezin direlako izan, ez biak

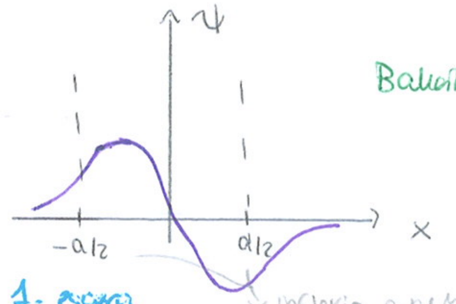
*' (3) beti bete behar da eta Y_1 eta Y_2 ((1) edo (2)) dugun arabera sim edo antis



Bikoitia

Oinarrizko egoera

(Kurbadurarea aldatu)



Bakoitia

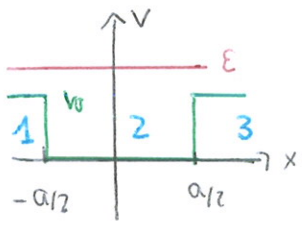
1. egoera kitzikatua

* oinarrizko egoera → ardatzik eta oszilazio gutxien

↳ bi ebaki puntuekin lortu ditugun energiekin (oinarrizko egoerak ⇒ bi ebaki puntu ⟷ bi egoera lotu

* Nahiz eta V_0 oso txikia izan gutxienez beti izango dugu ebaki puntu bat eta egoera lotu bat eta $V_0 \to \infty$ ∞ egoera lotu (ebaki puntuak $\pi/2, \pi, \ldots$; asintotak) ⇒ potentzial-osin infinitua

POTENTZIAL-OSINA, $E > V_0$:



$$V(x) = \begin{cases} V_0 & |x| < a/2 \\ 0 & |x| > a/2 \end{cases}$$

Klasikoki partikula zonalde guztietan egon daiteke (ez dago zonalde debekaturik)

egoera ez-lotuak → erasoaren esparrutik irudikariak ardatzilrea

3 zonalde:

1: $\psi_1 = A e^{iK_3 x} + B e^{-iK_3 x}$ $\qquad K_3 = \dfrac{\sqrt{2m(E-V_0)}}{\hbar}$

2: $\psi_2 = C e^{iK_2 x} + D e^{-iK_2 x}$ $\qquad K_2 = \dfrac{\sqrt{2mE}}{\hbar}$

3: $\psi_3 = E e^{iK_3 x} + F e^{-iK_3 x}$ $\qquad K_3 = \dfrac{\sqrt{2m(E-V_0)}}{\hbar}$

Kasu honetan infinituan uhin funtzioa ez doa infinitura ⇒ hori dagoelako eragozpik ez. Ez dugu beraz, zerora berdindu behar konstanteetako bat. Jarraitasuna inposatzean 4 baldintza lortu ditugu eta 6 konstante ditugunez bi "askatasun" izango dugu.
↳ gradu =

Beraz, aukeratuko dugu partikula ezkerretik datorrela → $F = 0$.

$F=0$ egitean simetria apurtu (simetria mantendu nahi badugu $F\neq 0$)

↳ orain ez da erreala izan

Jarraitasuna:

- $\psi_1(-a/2)=\psi_2(-a/2) \rightarrow A e^{-ik_3 a/2} + Be^{ik_3 a/2} = Ce^{-ik_2 a/2} + De^{+ik_2 a/2}$

- $\psi_2(a/2)=\psi_3(a/2) \rightarrow Ce^{ik_2 a/2} + De^{-ik_2 a/2} = Ee^{ik_3 a/2}$

- $\psi_1'(-a/2)=\psi_2'(-a/2) \rightarrow ik_3(Ae^{-ik_3 a/2} - Be^{ik_3 a/2}) = ik_2(Ce^{-ik_2 a/2} - De^{ik_2 a/2})$

- $\psi_1'(a/2)=\psi_2'(a/2) \rightarrow ik_2(Ce^{ik_2 a/2} - De^{-ik_2 a/2}) = ik_3 E e^{ik_3 a/2}$

Guztiak A-ren mempe jarri:

$Z=(k_2^2+k_3^2)\sin k_2 a + 2ik_2k_3\cos k_3 a$ definitu:

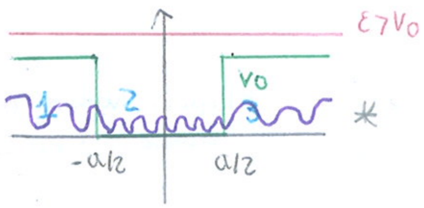
- $B=(k_3^2-k_2^2)\sin k_2 a \, e^{-ik_3 a}\dfrac{A}{Z}$; • $C= ik_3(k_2+k_3)e^{-ik_2 a/2}\dfrac{A}{Z}$

- $D= ik_3(k_2-k_3)e^{ik_2 a/2}\dfrac{A}{Z}$; • $E=2k_2k_3 i\, e^{-ik_3 a}\dfrac{A}{Z}$

Uhin-funtzioaren irudia egiteko hemen ez du zentzu handirik, konplexuak direlako

TRANSMISIO eta ISLAPEN KOEFIZIENTEAK; POTENTZIAL-OSINA $E>V_0$:

↳ egoera ez-lotua



Egoera lotuak ditugunean ez du zentzurik islapen, transmisio koefizienteak definitzea, egoerak potentzial osinaren barnean daudelako lotuta (ez du zentzurik esatea partikula ezkerretik datorrela, eskuinera doala...)

Uhin-funtzioa bera marrazteak ez du zentzu handirik, konplexua delako, baina bere modulua ↗ karratura onedala itengo da; dentsitate probabilitatea ⇒ oszilakorra. *

$k_2>k_3$ denez $\lambda_2<\lambda_3 \Rightarrow$ osziazio gehiago barnean.

1: $Ae^{ik_3x}+Be^{-ik_3x}=\psi_1$

2: $Ce^{ik_2x}+De^{-ik_2x}=\psi_2$

3: $Ee^{ik_3x}=\psi_3$

$k_2=\dfrac{\sqrt{2mE}}{\hbar}$; $k_3=\dfrac{\sqrt{2m(E-V_0)}}{\hbar}$

$1 \Rightarrow j_1 = |A|^2\dfrac{\hbar k_3}{m} - |B|^2\dfrac{\hbar k_3}{m}$ (−) ; $3 \Rightarrow j_3 = |E|^2\dfrac{\hbar k_3}{m}$ $\Rightarrow$ $T=\dfrac{j_3}{|A|^2\frac{\hbar k_3}{m}}=$

erasoaren eharpena ; islapenaren eharpena

T kalkulatzeko 2. tartekoa ez da garrantzitsua

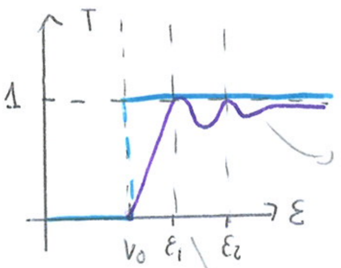
$$* \quad T = \frac{|E|^2 \frac{\hbar k_3}{m}}{|A|^2 \frac{\hbar k_3}{m}} = \frac{4k_2^2 k_3^2}{(k_2^2+k_3^2)^2 \sin^2 k_2 a + 4k_2^2 k_3^2 \cos^2 k_2 a} = \frac{4E(E-V_0)}{4E(E-V_0) + V_0^2 \sin^2\left(\frac{\sqrt{2mE}}{\hbar} a\right)}$$

k_2, k_3 ordezkatuz

Erresonantziak, E-ren balio batzuetarako $T = 1 \Rightarrow k_2 a = \frac{\sqrt{2mE}}{\hbar} a = n\pi$!

Erresonantzian $E \Rightarrow E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$ (potentzial osin infinituko energiak)

Klasikoki $T = 1$ da beti, kuantikoki islapen probabilitatea dago.



$E_i \Rightarrow T = 1$

• ⇒ kuantikoa

• ⇒ klasikoa

minimoa gero eta handiagoa E handiko delako

gure aztertuko $E > V_0$

DIRAC-EN DELTA POTENTZIALA:

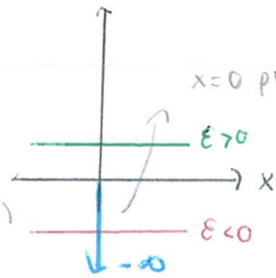
Hurbilketa zentzuz potentzial adierazteko

Energia potentzialaren idealizazioa, anplitudea infinitua duelako puntu batean ⇒ puntu batean kontzentratuta:

• $V(x) = -\alpha \delta(x) \Rightarrow$

gure aukera

x=0 puntuan kontzentratuta

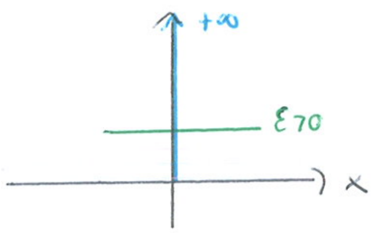


* Putzu baten limitea ⇒
{ zabalera → 0
{ anplitudea → ∞
(oso sakona)

• Klasikoki portaera E-ren arabera. $E < 0 \Rightarrow$ espazio lokala ⇒ $x \neq 0$ partikula ezin izango da egon, $V = 0$ delako; $x = 0$-n bakarrik $(T \to \infty)$

• $V(x) = \alpha \delta(x)$

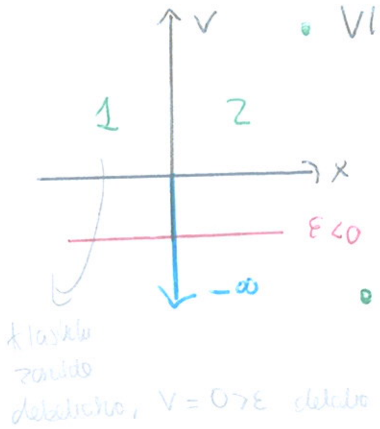
*Langa baten limitea, bakarra.



• $E > 0 \Rightarrow$ espazio osoan higi daiteke, $x \neq 0$ duen abiadura konstantez.

• Klasikoki ⇒ $E > 0 \Rightarrow$ Ezkerretik eskumara badoa $x = 0$-ra heltzean, $V > E$ denez ezin izango du zeharkatu eta errebotatu egingo da, kontrako zeinua duen momentu linealarekin.

DIRAC-EN DELTA, $E<0$:



- $V(x) = -\alpha\,\delta(x)$; $E<0$ denez klasikoki egoera lotuak izango ditugu beraz kuantikoki energiaren diskretizazioa espero dugu.

- Denboraren independentea den Schrödingeren ekuazioa aztertu:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - \alpha\,\delta(x)\psi = E\cdot\psi \qquad (E<0)$$

- Bi zonalde, 1 eta 2, (Dirac-en delta $x=0$-n zentratuta): partikula askearen soluzioak + mugalde baldintzak:

$$1 \Rightarrow \psi_1 = Ae^{Kx} + Be^{-Kx} \qquad K = \frac{\sqrt{2m|E|}}{\hbar}$$

$$2 \Rightarrow \psi_2 = Ce^{Kx} + De^{-Kx}$$

- Mugalde baldintzak. ψ ezin da infinitura joan $\pm\infty$-on $\Rightarrow B=C=0$
  ($x\to\infty$ $\psi_2\to 0$ eta $x\to-\infty$ $\psi_1\to 0$)

- Jarraitasuna: $\psi_1(0)=\psi_2(0) \Rightarrow A=D$
  ψ-ren deribatua ez da jarraia, $\frac{\partial^2\psi}{\partial x^2} \propto \delta(x)$ proportzionala delako eta beraz $\frac{\partial\psi}{\partial x}$-n Heaviside-n funtzioa bat egongo da $\Rightarrow$ ezin da aplikatu deribatuaren jarraitasuna.

- ψ'-ren ez-jarraitasuna: integrala 0-n inguruan, 0 puntuko ez jarraitasuna zehaztasunez aztertzeko

$$* \lim_{\varepsilon\to 0}\left\{-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{\partial^2\psi}{\partial x^2}dx - \int_{-\varepsilon}^{\varepsilon}\alpha\,\delta(x)\psi\,dx = \int_{-\varepsilon}^{\varepsilon}E\psi\,dx\right\} \simeq$$

0-ren inguruan $\psi \sim \psi(0)$
(integrala ez egiteko, ez dugulako ψ ezagutzen)

$$\lim_{\varepsilon\to 0}\left\{-\frac{\hbar^2}{2m}\left.\frac{\partial\psi}{\partial x}\right]_{-\varepsilon}^{\varepsilon} - \alpha\psi(0) = E\psi(0)x\Big]_{-\varepsilon}^{\varepsilon}\right\} = \lim_{\varepsilon\to 0}\left\{-\frac{\hbar^2}{2m}\left[\left.\frac{\partial\psi_2}{\partial x}\right]_{\varepsilon} - \left.\frac{\partial\psi_1}{\partial x}\right]_{-\varepsilon}\right] - \alpha\psi(0) =\right.$$

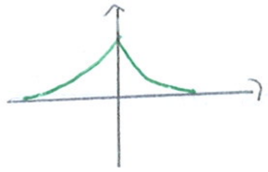
eskuinean ezkerrean

$$\left.E\psi(0)2\varepsilon\right\} = \lim_{\varepsilon\to 0}\left\{-\frac{\hbar^2}{2m}\left[-\overset{D}{A}Ke^{-K\varepsilon} - AKe^{-K\varepsilon}\right] - \alpha A \simeq EA\cdot 2\varepsilon\right\} = \frac{\hbar^2}{\cancel{2}m}\cancel{2}AK - \alpha A = 0$$

$$K = \frac{\alpha m}{\hbar^2} \Rightarrow E = -\frac{\hbar^2K^2}{2m} = -\frac{\hbar^2\alpha^2m^2}{2m\hbar^4} = -\frac{\alpha^2 m}{2\hbar^2}$$

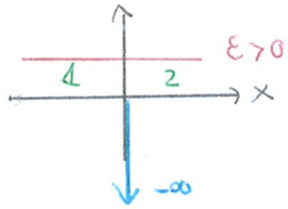
Egoera lotu bakarra
$\alpha\uparrow$ $E\downarrow$

K balin rehastuta $\Rightarrow$ $\Psi = \begin{cases} Ae^{Kx} & x<0 \\ Ae^{-Kx} & x>0 \end{cases}$ $\Rightarrow$ A lortu normalizazioa eginez.



$A = \frac{1}{K}$

DIRAC-EN DELTA, $E>0$:



- $V(x) = -\alpha\delta(x)$; Denboraren independentea den Schrödingeren ekuazioa: $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - \alpha\delta(x)\Psi = E\Psi$

- Bi zonalde:

1 $\Rightarrow$ $\Psi_1 = Ae^{iKx} + Be^{-iKx}$ 2 $\Rightarrow$ $\Psi_2 = Ce^{iKx} + De^{-iKx}$; $K = \frac{\sqrt{2mE}}{\hbar}$ $(E>0)$

- Honen infinitan ez dugu arazorik, beraz konstante bi izango ditugu libre: suposatuko dugu partikula ezkerretik datorrela $\leftrightarrow$ 2-zonaldean ez da egongo ezkerrerako fluxurik $\rightarrow$ $D=0$

- Jarraitasuna: $\Psi_1(0) = \Psi_2(0)$ $\Rightarrow$ $A+B=C$

- Ψ'-ren ez-jarraitasuna:

$$\lim_{\varepsilon\to 0}\left[-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{\partial^2\Psi}{\partial x^2}dx - \alpha\int_{-\varepsilon}^{\varepsilon}\delta(x)\Psi\,dx = \int_{-\varepsilon}^{\varepsilon}E\Psi\,dx\right] = \lim_{\varepsilon\to 0}\left[-\frac{\hbar^2}{2m}\left(\frac{\partial\Psi}{\partial x}\right)\Big|_{-\varepsilon}^{\varepsilon} - \alpha\Psi(0) \simeq E\Psi(0)x\Big]_{-\varepsilon}^{\varepsilon}\right] = \lim_{\varepsilon\to 0}\left[-\frac{\hbar^2}{2m}\left(\frac{\partial\Psi_2}{\partial x}\Big]_{\varepsilon} - \frac{\partial\Psi_1}{\partial x}\Big]_{-\varepsilon}\right) - \alpha\Psi(0) \simeq E\Psi(0)\cdot 2\varepsilon\right] =$$

$$\left[-\frac{\hbar^2}{2m}\left(iKC - (iKA - iKB)\right) - \alpha C = 0\right] \rightarrow -i\frac{\hbar^2 K}{2m}\left[C - A + B\right] - \alpha C = 0 \rightarrow$$

$$-i\frac{\hbar^2 K}{2m}\cdot(A+B-A+B) = \alpha(A+B) = -i\frac{\hbar^2 K}{2m}\cdot 2B = \alpha(A+B) \rightarrow -i\frac{\hbar^2 K}{m}B - \alpha B = \alpha A \Rightarrow$$

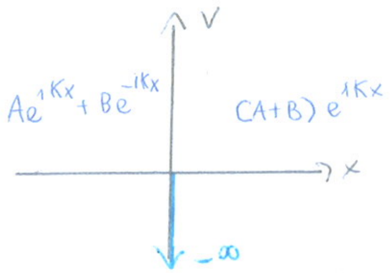
$$A = \left(-1 - \frac{i\hbar^2 K}{m\alpha}\right)B$$

orduan

$$\Rightarrow \Psi = \begin{cases} Ae^{iKx} + Be^{-iKx} & x<0 \\ (A+B)e^{iKx} & x>0 \end{cases}$$

$\hookrightarrow$ ezin dugu normalizatu.

DIRAC-EN DELTA ISLAPEN eta TRANSMISIO KOEFIZIENTEAK, E>0



- Egoera ez-lotuetan, $E>0$

$$A=\left(-1-\frac{i\hbar^2K}{m\alpha}\right)B$$

- $j=|A|^2\frac{\hbar K}{m}-|B|^2\frac{\hbar K}{m} \qquad x<0$

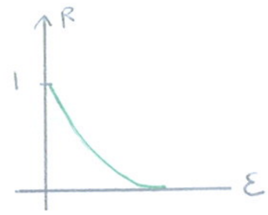
- $j=|A+B|^2\frac{\hbar K}{m} \qquad x>0$

uhin lauak

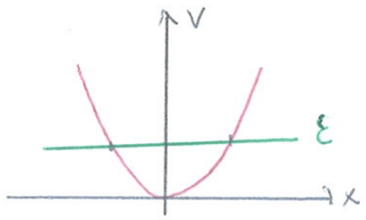
$$R+T=1$$

$$R=\frac{|B|^2\frac{\hbar K}{m}}{|A|^2\frac{\hbar K}{m}}=\frac{1}{1+\frac{\hbar^4K^2}{m^2\alpha^2}}=\frac{1}{1+\frac{2\hbar^2E}{m\alpha^2}}\Rightarrow$$

$$E=\frac{\hbar^2K^2}{2m}$$



OSZILADORE HARMONIKOA:



$$V(x)=\frac{1}{2}Kx^2$$

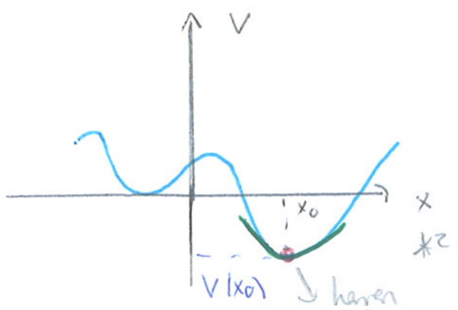
- Potentziala infinitura doanean egoera lotuak izango ditugu eta klasikoki partikula $E>V$ gunean baino ez da egongo.

hasierako baldintzen menpekoa

- Adibidez, malguki bat. (adibide klasikoa)

$F=-Kx$; $X=A\sin(wt+\varphi)$ $\quad w=\sqrt{\frac{K}{m}}$

- Demagun partikula baten sistemako energia potentziala (edozeinekoa izan daiteke) hauxe dela (arbitrario bat):



Partikulak energia potentzialeko minimora joateko joera izango du, non $T=0$ (oreka) $\Rightarrow$ bere gaineko indarra nulua ($\vec{F}=-\vec{\nabla}V$)

Oreka puntu horren inguruan desplazatu oso gutxi $\Rightarrow$ Taylor $\Rightarrow$

$$V(x)=V(x_0)+\cancel{\underbrace{\frac{dV}{dx}\Big|_{x_0}}_{\text{minimoa}}(x-x_0)}+\frac{1}{2}\frac{d^2V}{dx^2}\Big|_{x_0}(x-x_0)^2+\cancel{\theta^3}$$

2. ordeneko hurbilpenekin geratu bakarrik $\Rightarrow V(x)=V_0+\frac{1}{2}\frac{d^2V}{dx^2}\Big|_{x_0}(x-x_0)^2=\frac{1}{2}K(x-x_0)^2+V_0$

- Jatorria aldatzen badugu eta x_0-n zentratu, $x - x_0 = x'$, $V(x') = \frac{1}{2}k(x')^2$ $\Rightarrow$ parabola batez ordezkatu eta $V(x_0)$-n.

k^2

- Hurbilketa honetan x_0-n dagoen partikulak (edo inguruan) potentzial harmonikoa ikusten du. → balioanik baliagarria partikula oreka posizio honetako gehiegi urruntzen ez bada.
- Malgukiaren ordezkatzeko tresneria osoa aplika dezakegu.

OSZILODORE HARMONIKOAREN AUTOFUNTZIOAK eta AUTOBALIOAK:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2\psi = E\psi$$

* Aldagai aldaketa: $u = \sqrt{\alpha}\,x$, $\alpha = \frac{\sqrt{mk}}{\hbar}$ $[\alpha] = L^{-2}$; $\beta = \frac{2mE}{\hbar\sqrt{mk}}$ $[\beta]$ adimentsionala.

$$\frac{d^2\psi}{du^2} + (\beta - u^2)\psi = 0 \quad ; \quad u \to \pm\infty \quad \psi \sim e^{-u^2/2} \quad \left(\frac{d^2\psi}{du^2} - u^2\psi = 0\right)$$

infinituan 0-ra doana

* $\psi(u) = H(u)e^{-u^2/2}$ $\Rightarrow$ $\frac{d}{du}\left(e^{-u^2/2}H'(u) - u e^{-u^2/2}H(u)\right) + (\beta - u^2)H(u)e^{-u^2/2} =$

$$-u\cancel{e^{-u^2/2}}H'(u) + \cancel{e^{-u^2/2}}H''(u) + u^2\cancel{e^{-u^2/2}}H(u) - u\cancel{e^{-u^2/2}}H'(u) - \cancel{e^{-u^2/2}}H(u) +$$

$$(\beta - u^2)H(u)\cancel{e^{-u^2/2}} = H''(u) - 2uH'(u) + (\beta - 1)H(u) = 0$$

Hermiteren polinomioak soluzioa

Hermiteren ekuazio diferentziala

- Polinomioen metodoa: $H(u) = \sum_{i=0}^{\infty} a_i u^i$ $\Rightarrow$ sartu ekuazioan $\Rightarrow$

$j = i-2$

$$\sum_{i=2}^{\infty} i(i-1)a_i u^{i-2} - \sum_{i=1}^{\infty} 2i a_i u^i + (\beta-1)\sum_{i=0}^{\infty} a_i u^i = \sum_{i=0}^{\infty}(i+2)(i+1)a_{i+2}u^i - \sum_{i=0}^{\infty} 2i a_i u^i + (\beta-1)\sum_{i=0}^{\infty} a_i u^i =$$

$$\sum_{i=0}^{\infty}\left[(i+2)(i+1)a_{i+2} + (\beta - 1 - 2i)a_i\right]u^i = 0 \quad \longleftrightarrow \quad (i+2)(i+1)a_{i+2} + (\beta - 1 - 2i)a_i = 0 \quad \forall i$$

$$a_{i+2} = \frac{2i+1-\beta}{(i+2)(i+1)}a_i$$

(a_0 eta a_1 finkatu a_i guztiak lortu)

$a_0 \downarrow$ bik, $a_1 \downarrow$ bak

$$H(u) = a_0\left[1 + \frac{1-\beta}{2}u^2 + \frac{(5-\beta)(1-\beta)}{24}u^4 + \dots\right] + a_1\left[u + \frac{3-\beta}{6}u^3 + \frac{(7-\beta)(3-\beta)}{120}u^5 + \dots\right]$$

2. ordenako ekuazio diferentziala $\Rightarrow$ zehazki gabeko bi konstante (a_0, a_1)

* Polinomioan ordena infinitua denez $u \to \pm\infty$ badoa infinitura joango litzateke eta Ψ ez litzateke fisikoki esanguratsua izango. Fisikoki esanguratsua izateko polinomioa eten egin behar da unaren batean $\Longleftrightarrow$ n baterako

$2n+1-\beta = 0$ izan behar da $\left(a_{i+2} = \frac{2i+1-\beta}{(i+2)(i+1)} a_i \right) \Leftrightarrow \beta = 2n+1 \quad n \in \mathbb{N}$

$$\beta = 2n+1 = \frac{2mE}{\hbar\sqrt{mK}} \Rightarrow E = \left(\frac{1}{2}+n\right)\hbar\sqrt{\frac{K}{m}} = \left(\frac{1}{2}+n\right)\hbar\omega \quad n\in\mathbb{N}$$

Energiak bete behar duen baldintza Ψ fisikoki esanguratsua izateko

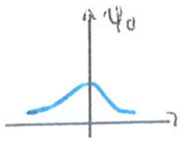
- Lehenengo soluzio sinpleena: $n=0$; $\beta=1 \Rightarrow H(u) = a_0 + a_1 \underbrace{\left[u + \frac{2}{6}u^3 + \dots\right]}_{\neq 0}$

beraz, fisikoki esanguratsua izateko $a_1 = 0$ izan beharko da: $H_0(u) = a_0 \rightarrow$

$$\Psi_0(u) = a_0 e^{-u^2/2} \Rightarrow \Psi_0(x) = a_0 e^{-\alpha x^2/2} = a_0 e^{-\frac{\sqrt{mK}x^2}{2\hbar}} \Rightarrow \text{Normalizatuz} \Rightarrow$$

normalizazio ktea

* $\Psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} \quad \left(\omega = \sqrt{\frac{K}{m}}\right)$



simetrikoa

* $E_0 = \frac{\hbar^2 K^2}{2m^2} = \frac{1}{2}\hbar\omega \quad \left(\beta = \frac{2mE}{\hbar\sqrt{mK}}\right)$

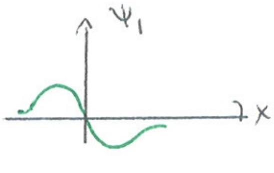
Gaussiana

- Bigarrena: $n=1$; $\beta=3 \Rightarrow H(u) = \underbrace{a_0\left[1 + \frac{-2}{2}u^2 + \frac{2(-2)}{24}u^4 + \dots\right]}_{\neq 0} + a_1 u$

beraz fisikoki esanguratsua izateko $a_0 = 0 \Rightarrow H_1(u) = a_1 u \rightarrow$

$$\Psi_1(u) = H_1(u)e^{-u^2/2} = a_1 u e^{-u^2/2} \Rightarrow \Psi_1(x) = \left(\frac{mK}{\hbar^2}\right)^{1/4} x \cdot a_1 e^{-\frac{\sqrt{mK}x^2}{2\hbar}} \Rightarrow \text{normalizatuz} \Rightarrow$$

* $\Psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\, x\, e^{-\frac{m\omega x^2}{2\hbar}} \quad \left(\omega = \sqrt{\frac{K}{m}}\right)$ antisimetrikoa



* $E_1 = \frac{3}{2}\hbar\omega$

$n=2$, $n=3$, ... Kalkulatzeko modu berean jarraitu genuke. Hermiteren polinomioak direnez tauletan egoten dira. (guztiek dute $e^{-\frac{m\omega x^2}{2\hbar}}$ esponentzial hori eta polinomioaren ordena n-ren berdina da ; n bikoitia bada simetrikoa izango da funtzioa eta bakoitia bada antisimetrikoa)

SORTZE- eta DEUSEZTATZE-ERAGILEAK:

Osziladore harmonikoaren hamiltondarraren autofuntzioak kalkulatzeko erabilgarriak izango diran eragileak.

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}\underbrace{m\omega^2}_{K}\hat{x}^2 \qquad \left(\omega = \sqrt{\frac{K}{m}}\right)$$

- Eragile berriak definitu: Badakigu $(a^2+b^2) = (a+ib)(a-ib)$ dela eta honetan oinarrituz eragile hauek definitu zituen Dirac-ek:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \quad \text{(ez da hermitikoa)}$$

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) \Rightarrow \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^+), \quad \hat{p} = -i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}-\hat{a}^+)$$

$$[\hat{a},\hat{a}]=0, \quad \boxed{[\hat{a},\hat{a}^+] = \frac{m\omega}{2\hbar}\left[\hat{x}+\frac{i}{m\omega}\hat{p}, \hat{x}-\frac{i}{m\omega}\hat{p}\right] = \frac{m\omega}{2\hbar}\left\{\frac{i}{m\omega}[\hat{p},\hat{x}] - \frac{i}{m\omega}[\hat{x},\hat{p}]\right\} =}$$

$$\boxed{\frac{m\omega}{2\hbar}\left\{\frac{i}{m\omega}(-i\hbar) - \frac{i}{m\omega}\cdot(i\hbar)\right\} = \frac{m\omega}{2\hbar}\left\{\frac{\hbar}{m\omega}+\frac{\hbar}{\omega m}\right\} = 1}$$

Hamiltondarra bi eragile hauen funtzioan idatzi, bi zatitan banatu ahal izateko eta emaitzeko.

$$\boxed{\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}\omega^2 m\hat{x}^2} = \frac{1}{2m}\left\{-\frac{\hbar m\omega}{2}(\hat{a}^2+\hat{a}^{+2}-\hat{a}\cdot\hat{a}^+-\hat{a}^+\cdot\hat{a})\right\} + \frac{1}{2}m\omega^2\left(\frac{\hbar}{2m\omega}(\hat{a}^2+\hat{a}^{+2}+\hat{a}\cdot\hat{a}^++\hat{a}^+\hat{a})\right) =$$

$$-\frac{\hbar\omega}{4}(\cancel{\hat{a}^2}+\cancel{\hat{a}^{+2}}-\hat{a}\cdot\hat{a}^+-\hat{a}^+\hat{a}) + \frac{\hbar\omega}{4}(\cancel{\hat{a}^2}+\cancel{\hat{a}^{+2}}+\hat{a}\cdot\hat{a}^++\hat{a}^+\cdot\hat{a}) =$$

$$\frac{\hbar\omega}{4}\left(\hat{a}\cdot\hat{a}^{+}+\hat{a}^{+}\hat{a}+\hat{a}\cdot\hat{a}^{+}+\hat{a}^{+}\cdot\hat{a}\right)=\frac{\hbar\omega}{2}\left(\hat{a}\cdot\hat{a}^{+}+\hat{a}^{+}\hat{a}\right)=\frac{\hbar\omega}{2}\left(1+2\hat{a}^{+}\hat{a}\right)=\boxed{\hbar\omega\left(\hat{a}^{+}\hat{a}+\frac{1}{2}\right)}$$

$$[\hat{a},\hat{a}^{+}]=\hat{a}\cdot\hat{a}^{+}-\hat{a}^{+}\cdot\hat{a}=1\rightarrow\hat{a}\cdot\hat{a}^{+}=1+\hat{a}^{+}\hat{a}$$

konstante bat baino ez da, ez da ordezko handirik izango (ia-ia bi faktoreen biderketa izango dugu, konstantea arbuiatzen bada)

- Eragile berria definitu: $\hat{N}=\hat{a}^{+}\hat{a}$ ⟹ honen autofuntzioak $\hat{H}$-ren berdinak izango dira → honekin errazagoa da.

  $\hat{A}$-ren autobalio eta autofuntzioak kalkulatzea

OSZILADORE HARMONIKOAREN AUTOFUNTZIOAK eta AUTOBALIOAK $\hat{a}^{+}$ eta $\hat{a}$

ERAGILEEN PROPIETATEAK APLIKATUZ:

$$\hat{a}=\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}+\frac{i}{m\omega}\hat{p}\right)\quad;\quad\hat{a}^{+}=\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}-\frac{i}{m\omega}\hat{p}\right)\qquad[\hat{a},\hat{a}^{+}]=1$$

$$\hat{H}=\hbar\omega\left(\hat{a}^{+}\hat{a}+\frac{1}{2}\right)=\hbar\omega\left(\hat{N}+\frac{1}{2}\right)\Rightarrow\hat{N}\Psi_\lambda=\lambda\Psi_\lambda\quad\lambda\in\mathbb{R}\ \text{(Hermitikoa delako)}$$

$$\hat{H}\Psi_\lambda=\hbar\omega\lambda\Psi_\lambda+\frac{\hbar\omega}{2}\Psi_\lambda=\hbar\omega\left(\lambda+\frac{1}{2}\right)\Psi_\lambda$$

→ $\hat{H}$-ren autofuntzioa, autobalioa $\hbar\omega\left(\lambda+\frac{1}{2}\right)$

- $\hat{a}\Psi_\lambda\Rightarrow\hat{N}(\hat{a}\Psi_\lambda)=\hat{a}^{+}\cdot\hat{a}\,(\hat{a}\Psi_\lambda)=\hat{a}^{+}\hat{a}\cdot\hat{a}\Psi_\lambda=[\hat{a}\cdot\hat{a}^{+}-1]\,\hat{a}\Psi_\lambda=\hat{a}\cdot\underbrace{\hat{a}^{+}\hat{a}}_{\hat{N}}\Psi_\lambda+$

$$-\hat{a}\Psi_\lambda=\hat{a}\hat{N}\Psi_\lambda-\hat{a}\Psi_\lambda=\hat{a}\cdot\lambda\Psi_\lambda-\hat{a}\Psi_\lambda=\hat{a}\Psi_\lambda(\lambda-1)\Rightarrow\hat{a}\Psi_\lambda\ \text{autofuntzioa da.}$$

$\hat{a}\Psi_\lambda$-ren autobalioa $(\lambda-1)$ denez ⟹ $\hat{a}\Psi_\lambda\propto\Psi_{\lambda-1}$ (proportzionala)

kte bat

$$[\hat{a}\Psi_\lambda=c_\lambda\Psi_{\lambda-1}]\Rightarrow(\hat{a}\Psi_\lambda,\hat{a}\Psi_\lambda)=(\Psi_\lambda,\hat{a}^{+}\hat{a}\Psi_\lambda)=(\Psi_\lambda,\hat{N}\Psi_\lambda)=$$

$$(\Psi_\lambda,\lambda\Psi_\lambda)=\lambda(\Psi_\lambda,\Psi_\lambda)=\lambda\ =(c_\lambda\Psi_{\lambda-1},c_\lambda\Psi_{\lambda-1})=|c_\lambda|^2(\Psi_{\lambda-1},\Psi_{\lambda-1})\Rightarrow$$

↳ ortonormalak direla suposatuz.

ez du esangura fisikoa aldatzen

$$|c_\lambda|^2=\lambda\Rightarrow c_\lambda=\sqrt{\lambda}\,e^{i\alpha}\quad\alpha\in\mathbb{R}\Rightarrow\text{hartu }\alpha=0\Rightarrow$$

$$\boxed{c_\lambda=\sqrt{\lambda}}\Rightarrow\hat{a}\Psi_\lambda=\sqrt{\lambda}\,\Psi_{\lambda-1}$$

$\hat{a}$-k 1 ean jaitsi λ-ren baloa eta hari dagokion autofuntzio bat ematen du ⟹ $\hat{a}\Psi_\lambda$-ren gainean berriz aplikatu $\hat{a}$ $\Psi_{\lambda-2}$ lortuko genuke

Honela λ-ren balioa jaitsiz joan gaitezke negatibo egin arte $\Rightarrow$

negatibo denean energia negatiboa izango litzatekeelako:

- Gogoratu $\varepsilon_\lambda = \hbar\omega(\lambda + \frac{1}{2})$ dela $\lambda \geq -\frac{1}{2}$ (1)

(V eta T beti $\geq 0 \leftrightarrow E \geq 0$)

λ-ren balioa jaitsiz joan ahal gara horietako bat 0 ez bada egiten, λ

0 bada ezin dugu gehiago jaitsi, hurrengoa -1 izango litzatekeelako eta

$\hat{a}\Psi_\lambda = 0$

$\lambda \geq -1/2$ izan behar da (1) $\Rightarrow \lambda_{min} = 0$!! $\rightarrow \lambda \in \mathbb{N} \rightarrow \lambda = n = 0, 1, 2, 3, \ldots \Rightarrow$

$E > 0$ izateko!

$$\boxed{\varepsilon_n = \hbar\omega(n + \tfrac{1}{2}) \quad n \in \mathbb{N}}$$

Autofuntzioak kalkulatzeko:

- $\hat{a}\Psi_0 = 0 \Rightarrow$ ekuazioa ; $\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)\Psi_0 = 0 \rightarrow x\Psi_0 + \frac{\hbar}{m\omega}\frac{\partial\Psi_0}{\partial x} = 0 \Rightarrow$

$$\frac{\partial\Psi_0}{\partial x} = -\frac{m\omega}{\hbar}x\Psi_0 \rightarrow \frac{d\Psi_0}{\Psi_0} = -\frac{m\omega}{\hbar}x\,dx \Rightarrow \ln\Psi_0 = -\frac{m\omega}{2\hbar}x^2 + C \Rightarrow$$

$$\Psi_0 = Ae^{-\frac{m\omega}{2\hbar}x^2}$$ (A normalizazio ktea)

$\hookrightarrow$ aurrekoan lortutakoa!

- Hurrengoak kalkulatzeko $\hat{a}^+$ aplikatu:

- $\hat{a}\Psi_n = \sqrt{n}\,\Psi_{n-1}$ → deuseztatze eragilea: (jaitsi)

$\hat{a}^+\Psi_n = \sqrt{1+n}\,\Psi_{n+1}$ → sortze eragilea (igo)

$\hookrightarrow \hat{a}^+\Psi_0 = \Psi_1 \Rightarrow \Psi_1$ lortu, eta horrela $\hat{a}^+\Psi_1 = \sqrt{2}\,\Psi_2 \ldots$ eginez

Ψ_n orokorki: $\Rightarrow$ $$\boxed{\Psi_n = \frac{\hat{a}^+\Psi_{n-1}}{\sqrt{n}} = \frac{1}{\sqrt{n!}}(\hat{a}^+)^n\Psi_0}$$

$\hat{a}$, $\hat{a}^+$ eragileekin, abstraktuagoak badira ere, askoz sinpleagoak kalkuluak!

SORTZE- eta DEUSEZTATZE-ERAGILEEN BESTE APLIKAZIO BATZUK:

$$* \begin{cases} \hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) & \text{deuseztatze-eragilea} \\ \hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) & \text{sortze-eragilea} \end{cases} \Rightarrow \begin{cases} \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^{+}\right) \\ \hat{p} = -i\sqrt{\frac{\hbar\omega m}{2}}\left(\hat{a} - \hat{a}^{+}\right) \end{cases}$$

Eragile gehienak $\hat{x}$ eta $\hat{p}$-ren mende egoten direnez oso erabilgarria notazio hau $\Rightarrow$ $\hat{a}$ eta $\hat{a}^{+}$-ren mende adieraz ditzakegu, gainera badakigu:

$$\left.\begin{aligned} \hat{a}\,\psi_n &= \sqrt{n}\,\psi_{n-1} \\ \hat{a}^{+}\psi_n &= \sqrt{1+n}\,\psi_{n+1} \end{aligned}\right\}$$ hau kontuan hartuz eragileen batezbestekoak kalkulatu ditzakegu

* Gure egoera, uhin-funtzioa hamiltondarraren autofuntzioetan garatzen dugu:

$\Psi = \sum_n c_n \psi_n$; $\hat{A}$ behagarria badugu ($\hat{x}$ eta $\hat{p}$-ren mendekoa $\Rightarrow$ $\hat{a}$ eta $\hat{a}^{+}$-ren mendekoa) $\Rightarrow \hat{A}(\hat{a}, \hat{a}^{+}) \Rightarrow \langle \hat{A} \rangle = (\Psi, \hat{A}\Psi)$

eta $\hat{a}\psi_n$ eta $\hat{a}^{+}\psi_n$ nolakoak diren kontuan hartuz oso simplea kalkulatzea. → bestela hermiteren polinomioak etab...

* Adibide konkretua: Demagun $\Delta x \Delta p$ kalkulatu nahi dugula ψ_n autofuntzioan.

$(\Delta x)_n = \left(\overline{x^2} - \bar{x}^2\right)^{1/2}$; $(\Delta p)_n = \left(\overline{p^2} - \bar{p}^2\right)^{1/2}$

- $\langle x \rangle_n = (\psi_n, x\psi_n) = \left(\psi_n, \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^{+})\psi_n\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\psi_n, (\hat{a}+\hat{a}^{+})\psi_n\right) =$

$$\sqrt{\frac{\hbar}{2m\omega}}\left[(\psi_n, \hat{a}\psi_n) + (\psi_n, \hat{a}^{+}\psi_n)\right] = \sqrt{\frac{\hbar}{2m\omega}}\left[\overset{\text{ort.}}{(\psi_n, \cancel{\sqrt{n}\,\psi_{n-1}})} + \overset{\text{ort}}{(\psi_n, \cancel{\sqrt{n+1}\,\psi_{n+1}})}\right] = 0$$

bi jaisi

- $\langle x^2 \rangle_n = (\psi_n, x^2\psi_n) = \frac{\hbar}{2m\omega}\left(\psi_n, (\hat{a}+\hat{a}^{+})^2\psi_n\right) = \frac{\hbar}{2m\omega}\Big[\overset{0}{(\psi_n, \cancel{\hat{a}^2}\psi_n)} +$

bi igo

$$\overset{0}{(\psi_n, \cancel{\hat{a}^{+2}}\psi_n)} + (\psi_n, \hat{a}\hat{a}^{+}\psi_n) + (\psi_n, \hat{a}^{+}\hat{a}\psi_n)\Big] = \frac{\hbar}{2m\omega}\left[(\psi_n, \hat{a}\sqrt{n+1}\,\psi_{n+1}) + \right.$$

$(\psi_n, \hat{a}^+ \sqrt{n}\psi_{n-1})] = \frac{\hbar}{2m\omega}[\sqrt{1+n}(\psi_n, \sqrt{1+n}\psi_n) + \sqrt{n}(\psi_n, \sqrt{n}\psi_n)] =$

$\frac{\hbar}{2m\omega}[n+1+n] = \frac{\hbar}{2m\omega}(1+2n)$ Askoz errazagoa!

- $\langle \hat{p} \rangle_n = 0$ (Hamiltondaraen autofuntzioen degradakuntza)

- $\langle \hat{p}^2 \rangle_n = (\psi_n, \hat{p}^2 \psi_n) = -\frac{\hbar m\omega}{2}(\psi_n, (\hat{a}-\hat{a}^+)^2\psi_n) = -\frac{\hbar m\omega}{2}[(\psi_n, \cancel{\hat{a}^2}\psi_n) +$

$(\psi_n, \cancel{\hat{a}^{+2}}\psi_n) + (\psi_n, -\hat{a}^+\hat{a}\psi_n) + (\psi_n, -\hat{a}\hat{a}^+\psi_n)] = +\frac{\hbar m\omega}{2}[(\psi_n, \hat{a}^+\hat{a}\psi_n) +$

$(\psi_n, \hat{a}\hat{a}^+\psi_n)] = \frac{\hbar m\omega}{2}[(\psi_n, \hat{a}^+\sqrt{n}\psi_{n-1}) + (\psi_n, \hat{a}\cdot\sqrt{n+1}\psi_{n+1})] =$

$\frac{\hbar\omega m}{2}[n\cdot(\psi_n, \psi_n) + (n+1)(\psi_n, \psi_n)] = \frac{\hbar\omega m}{2}(2n+1)$ Askoz errazagoa!

$\Delta x = \sqrt{\frac{\hbar}{2m\omega}(1+2n)}$, $\Delta p = \sqrt{\frac{\hbar\omega m}{2}(1+2n)} \Rightarrow \Delta x \Delta p = \sqrt{\frac{\hbar}{2m\omega}(1+2n)} \cdot \sqrt{\frac{\hbar\omega m}{2}(1+2n)} =$

$\frac{\hbar}{2}\sqrt{(1+2n)^2} = \frac{\hbar}{2}(1+2n) \geq \frac{\hbar}{2}$

$n=0$ egitez $\Delta x \Delta p = \hbar/2$ minimoa $\Rightarrow \psi_0 \propto e^{-\alpha x^2}$ (Gaussiarra)

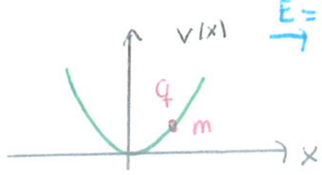
Beste edozein n-rna $\Rightarrow \Delta x \Delta p \geq \hbar/2$

ziurgabetasun txikienekoa

- $\psi = \sum_n c_n \psi_n$ funtzioaren ziurgabetasuna $(\Delta x \Delta p)$ beti izango da $\hbar/2$ baino handiagoa $c_n \neq 0$ $n \neq 0$ bada.

OSZILATZAILE HARMONIKOAREN GAINEKO EREMU BATEN ERAGINA:

- Demagun m masadun eta q kargako partikula bat oszilatzaile harmoniko baten eraginpean higitzen dela.



$\vec{E} = E_0 \hat{i}$

Partikulak jasango duen potentziala $\frac{1}{2}Kx^2$ da.

Bana demagun honetaz gain eremu elektriko bat aplikatzen dugula: Eremu horri bate energia potentzial bat egokituko zaio: $-qE_0 x$

- Beraz energia potentzial osoa $V = \frac{1}{2}Kx^2 - qE_0 x$ izango da. Zer gertatzen da kasu honetan? Denboraren independentea den Schrödingeren ekuazioa garatu:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \left(\frac{1}{2}Kx^2 - qE_0 x\right)\psi = E\psi$$

- Mundu klasikoan, halako problemaren aurrean Newtonen 2. legea aplikatzen da:

$$m\frac{d^2x}{dt^2} = -Kx + qE_0 \rightarrow \text{Aldagai-aldaketa} \rightarrow m\frac{d^2x}{dt^2} = -K\underbrace{\left(x - \frac{qE_0}{K}\right)}_{x'} = -Kx' = m\frac{d^2x'}{dt^2} \rightarrow$$

$$x' \rightarrow dx = dx'$$

Hemendik zuzenean ebatzi $\rightarrow$ $x' = A\sin(wt+\varphi_0)$, $x = A\sin(wt+\varphi_0) + \frac{qE_0}{K}$

- Antzeko ideia aplikatuko dugu. Karratuak osatu:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \left(\frac{1}{2}Kx^2 - qE_0x + \frac{q^2E_0^2}{2K}\right)\psi - \frac{q^2E_0^2}{2K}\psi = \varepsilon\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - \frac{q^2E_0^2}{2K}\psi +$$

$$\left(\sqrt{\frac{K}{2}}x - \frac{qE_0}{\sqrt{2K}}\right)^2 = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - \frac{q^2E_0^2}{2K}\psi + \frac{K}{2}\left(x - \frac{qE_0}{K}\right)^2$$

Aldagai aldaketa: $x - \frac{qE_0}{K} = x'$, $\varepsilon' = \varepsilon + \frac{q^2E_0^2}{2K}$ $\Rightarrow$ $\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2\psi}{\partial x'^2}$ $\Rightarrow$

autobalioak

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x'^2} + \frac{1}{2}Kx'^2 = \varepsilon'\psi \Rightarrow$$ Oszilatzaile harmonikoari dagokion berdina!

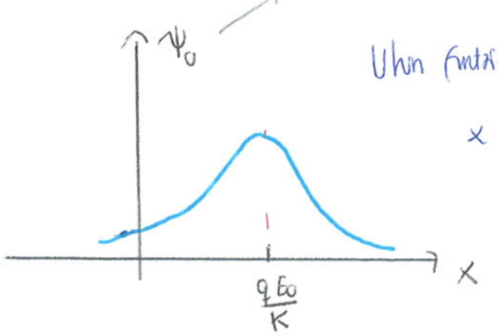
Hermiteren polinomioak: $\psi_n = A H_n\left(\sqrt{\frac{m\omega}{\hbar}}x'\right)e^{-\frac{m\omega}{2\hbar}x'^2}$, $\varepsilon'_n = \left(\frac{1}{2}+n\right)\hbar\omega$

Aldagai-aldaketa desegin $\Rightarrow$ $\Psi_n = A H_n\left(\sqrt{\frac{m\omega}{\hbar}}\left(x-\frac{qE_0}{K}\right)\right) e^{-\frac{m\omega}{2\hbar}\left(x-\frac{qE_0}{K}\right)^2}$

$$\mathcal{E}_n = \mathcal{E}' - \frac{q^2E_0^2}{2K} = \left(\frac{1}{2}+n\right)\hbar\omega - \frac{q^2E_0^2}{2K}$$

- Forma berdina dute, baina desplazatuta daude uhin-funtzioak, $\frac{qE_0}{K}$-n zentratuta.

Gaussiarra.



Uhin funtzioak simetrikoak edo antisimetrikoak dira baina $\frac{qE_0}{K}$ x puntuarekiko!

- Energiak txikiagoak dira, ekarpen negatibo bat dugulako $\Rightarrow$ daukagun energia potentziala (eremu elektrikoa dela eta) negatiboa delako. $\Rightarrow$ energia potentzial osoa txikiagoa da.

1D-TIK 3D-RAKO TRANTSIZIOA:

3 dimentsiotan (3D) askatasun handiagoa dugu baina ondorioz endakapena ere handiagoa izan daiteke. Hala ere, kontzeptualki, 1D eta 3D-n gauzak ez dira hain ezberdinak. Orain arte garatutako ideiak aplikagarriak izango dira:

1D		3D
$\hat{x} = x$	$\longrightarrow$	$\hat{\vec{r}} = \hat{x}\hat{\imath} + \hat{y}\hat{\jmath} + \hat{z}\hat{k} = x\hat{\imath} + y\hat{\jmath} + z\hat{k}$
$\hat{p} = -i\hbar\frac{\partial}{\partial x}$	$\longrightarrow$	$\hat{\vec{p}} = \hat{p}_x\hat{\imath} + \hat{p}_y\hat{\jmath} + \hat{p}_z\hat{k} = -i\hbar\left(\frac{\partial}{\partial x}\hat{\imath} + \frac{\partial}{\partial y}\hat{\jmath} + \frac{\partial}{\partial z}\hat{k}\right) = -i\hbar\vec{\nabla}$

Beste eragile gehienak hauen funtzioan garatu.

3D-KO SCHRÖDINGERREN EKUAZIOA:

$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$ 3D-n ekuazio bera $\rightarrow$ $\hat{H}$-ren adierazpena ezberdina, eragile ezberdina:

Laplacearra

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + V = \frac{(-i\hbar\vec{\nabla})\cdot(-i\hbar\vec{\nabla})}{2m} + V(\vec{r},t) = -\hbar^2\frac{\nabla^2}{2m} + V(\vec{r},t)$$

biderkadura eskalarra.

3D-ko Schrödingeren ekuazioa: $-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$

Hau aztertzeko prozedura bera:

- $V(\vec{r},t) = V(\vec{r})$ bada $\Rightarrow$ $\Psi(\vec{r},t) = \psi(\vec{r})\,\varphi(t)$ $\Rightarrow$

$$\hat{H}\psi_n = \varepsilon_n \psi_n \quad \text{eta} \quad \varphi(t) = A e^{-i\frac{\varepsilon_n}{\hbar}t}$$

(egoera geldikorren adierazpen orokora ez da aldatzen)

$$\Downarrow$$

$$\Psi_n = \psi_n e^{-i\frac{\varepsilon_n}{\hbar}t}$$

$$\Downarrow$$

$$\Psi(\vec{r},t) = \sum_n c_n \psi_n e^{-i\frac{\varepsilon_n}{\hbar}t}$$

Ezberdintasun bakarra ekuazio diferentziala 3D-koa dela eta orduan zailagoa dela ebaztea.

BIDERKADURA ESKALARRA eta NEURKETEN PROBABILITATEAK 3D-n:

- Demagun bi uhin funtzio ditugula, $\Psi(\vec{r},t)$ eta $\varphi(\vec{r},t)$, bi uhin funtzioen arteko biderkadura eskalarra hauxe da: $\int \Psi^*(\vec{r},t)\,\varphi(\vec{r},t)\,d^3r$ $\Rightarrow$
$d^3r = dx\,dy\,dz$
aukeratuko $\vec{r}$ nola dugun koordenatuetan jarriko (kartesiarrak, esferikoak...)

- Demagun A behagarria dugula eta hari dagozkion autofuntzioak $\hat{A}\psi_n^A = a_n \psi_n^A$ direla. $\Rightarrow$ $\{\psi_n^A\}$ oinarria, $\{a_n\}$ autobalioak.

Beti bezala, edozein egoera badugu, garatu dezakegu nahi dugun oinarrian $\Rightarrow$ $\hat{A}$-ren autofuntzioen oinarrian $\Rightarrow$ $\Psi(\vec{r},t) = \sum_n c_n(t)\,\psi_n^A(\vec{r},t)$ $\Rightarrow$ $c_n(t)$-ak lortzeko 1D-ko prozedura bera $\Rightarrow$ $c_n(t) = (\psi_n^A, \Psi(\vec{r},t))$ $\Rightarrow$ Haueek izango dira a_n lortzeko probabilitateak: $P(a_n) = |c_n(t)|^2$

3D-n, kontzeptualki biderkadura eskalarra eta probabilitatean neurketa berdina!

3D-KO MOMENTU LINEALAREN AUTOFUNTZIOAK:

$$\hat{\vec{p}}\,\psi = \underset{\text{autobalioa (bektorea)}}{\vec{p}}\,\psi = \hbar\vec{k}\,\psi = -i\hbar\vec{\nabla}\psi = \hbar\vec{k}\,\psi$$

Hemendik 3 ekuazio aterako dira, ekuazio bektoriala delako: $(\vec{k} = k_x\hat{i} + k_y\hat{j} + k_z\hat{k})$

$$-i\hbar\frac{\partial\psi}{\partial x} = \hbar k_x \;(1) \quad ; \quad -i\hbar\frac{\partial\psi}{\partial y} = \hbar k_y \;(2) \quad ; \quad -i\hbar\frac{\partial\psi}{\partial z} = \hbar k_z \;(3)$$

1D-ton genuenan ekuazio bera, ezberdintasun bakarra ψ-k $x, y,$ eta z-ren menpekotasuna

duela:

$(1) \Rightarrow \psi = f(y,z)\,e^{ik_x x}$ $\qquad (2) \Rightarrow \psi = g(y,z)\,e^{ik_y y}$ $\qquad (3) \Rightarrow \psi = h(y,z)\,e^{ik_z z}$

↳ badakigu menpekotasun hau esponentzial horrela izango duela.

Beraz $\Rightarrow$ $\psi_{\vec{k}}(\vec{r}) = Ae^{ik_x x}e^{ik_y y}e^{ik_z z} = Ae^{i(k_x x + k_y y + k_z z)} = Ae^{i\vec{k}\cdot\vec{r}}$

3D-KO FOURIER-EN GARAPENA:

$\vec{r}$ espaziotik $\vec{k}$ espaziora pasatzea: bektoreak ditugu $\begin{cases} \vec{r} = x\hat{i} + y\hat{j} + z\hat{k} \\ \vec{k} = k_x\hat{i} + k_y\hat{j} + k_z\hat{k} \end{cases}$

$$\psi(\vec{r}) \rightarrow A(\vec{k})\;?$$

Dimentsio bakoitzeko Fourieren transformatu bat egingo dugu aldagai bakoitzeko

$$* \quad \psi(\vec{r}) = \frac{1}{\sqrt{2\pi}}\cdot\frac{1}{\sqrt{2\pi}}\cdot\frac{1}{\sqrt{2\pi}}\int A(\vec{k})\,e^{ik_x x}\cdot e^{ik_y y}\,e^{ik_z z}\,dk_x dk_y dk_z = \frac{1}{(2\pi)^{3/2}}\int A(\vec{k})\,e^{i\vec{k}\cdot\vec{r}}\,d^3\vec{k}$$

$$* \quad A(\vec{k}) = \frac{1}{(2\pi)^{3/2}}\int \psi(\vec{r})\,e^{-i\vec{k}\cdot\vec{r}}\,d^3\vec{r}$$

$*$ $\int |\psi(\vec{r})|^2 d^3\vec{r} = 1$ badugu $\int |A(\vec{k})|^2 d^3\vec{k} = 1$ izango dugu 3D-tan ere!

Definitu $P(\vec{k}) = |A(\vec{k})|^2$ $\Rightarrow$ ezberdintasun bakarra 3D-tako integralak direla,

kontzeptualki gauza bera da.

3D-KO DENTSITATE-PROBABILITATEAREN KORRONTE DENTSITATEA:

Ezberdintasun bakarra ⇒ 3 osagai ditugu beraz bektore bat izango dugu:

$$* \ \vec{j} = \frac{i\hbar}{2m}\left\{ \Psi \vec{\nabla} \Psi^* - \Psi^* \vec{\nabla} \Psi \right\} = j_x \hat{i} + j_y \hat{j} + j_z \hat{z} \quad ; \quad \Psi(\vec{r}, t)$$

Froga:

partikulen dentsitatea

Fluidoetan $\frac{\partial n}{\partial t} + \vec{\nabla} \cdot \vec{j} = \frac{\partial n}{\partial t} + \mathrm{div}\, \vec{j} = 0$ da ⇒ horretan oinarritu:

Gure kasuan $\frac{\partial n}{\partial t}$, partikulen dentsitatea baino $P(x,t)$ dentsitate probabilitatea:

- $n \equiv P(x,t) = \Psi(\vec{r},t) \cdot \Psi^*(\vec{r},t) \Rightarrow \frac{\partial P}{\partial t} = \frac{\partial \Psi}{\partial t}\Psi^* + \Psi \frac{\partial \Psi^*}{\partial t}$

Schrödinger ⇒ $-\frac{\hbar^2}{2m}\left\{ \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right\} + V\Psi = i\hbar \frac{\partial \Psi}{\partial t}$ ⇒ orduan $\frac{\partial \Psi}{\partial t}$

bakandu, eta $\frac{\partial \Psi^*}{\partial t}$ modu berean bakandu fluidoan ekuazioan

ordezkatzea baino ez dugu goiko adierazpena lortzeko.

TRUKATZAILEAK:

Trukatzaileen definizioan ez da dimentsioa aipatzen beraz definizioa berdina

izango da: $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

Hala ere 3D-tan aldagai gehiago ditugunez trukatzaile gehiago izango ditugu, eragile

gehiago ditugulako.

Asko erabiltzen den trukatzailea: $[\hat{x}, \hat{p}_x] = i\hbar \quad ; \quad [\hat{y}, \hat{p}_y] = i\hbar \quad ; \quad [\hat{z}, \hat{p}_z] = i\hbar \ *$

$$* \ [\hat{z}, \hat{p}_z] = z\left(-i\hbar \frac{\partial}{\partial z}\right) - \left(-i\hbar \frac{\partial}{\partial z}\right) z = -i\hbar \cancel{z \frac{\partial}{\partial z}} + i\hbar + \cancel{i\hbar z \frac{\partial}{\partial z}} = i\hbar$$

$[\hat{x}, \hat{p}_y] = 0$ ($\vec{r}$-ren osagaia eta $\vec{k}$-rena ezberdinak badira trukatzailea nulua) ⇒

$$* \ [\hat{x}, \hat{p}_y] = -i\hbar x \frac{\partial}{\partial y} - \left(-i\hbar \frac{\partial}{\partial y} x\right) = -i\hbar \cancel{x \frac{\partial}{\partial y}} + \cancel{i\hbar x \frac{\partial}{\partial y}} = 0$$

Beraz, neurtu ahal dugu x eta p_x aldi berean zehaztasun osoarekin, baita $\vec{r}$ eta $\vec{k}$-ren osagaiak ezberdinak diren konbinazioak.

osagai ezberdinen trukatzaileak nuluak

$$[\hat{r}^2, \hat{p}^2] = [\hat{x}^2 + \hat{y}^2 + \hat{z}^2, \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2] = [\hat{x}^2, \hat{p}_x^2] + [\hat{y}^2, \hat{p}_y^2] + [\hat{z}^2, \hat{p}_z^2]$$

* $[\hat{x}^2, \hat{p}_x^2] = \hat{x}[\hat{x}, \hat{p}_x^2] + [\hat{x}, \hat{p}_x^2]\hat{x} = 2i\hbar(\hat{x}\hat{p}_x + \hat{p}_x\hat{x})$

* $[\hat{x}, \hat{p}_x^2] = \hat{p}_x[\hat{x}, \hat{p}_x] + [\hat{x}, \hat{p}_x]\hat{p}_x = 2i\hbar\hat{p}_x$

$$\Rightarrow [\hat{r}^2, \hat{p}^2] = 2i\hbar(\hat{x}\hat{p}_x + \hat{p}_x x + \hat{y}\hat{p}_y + \hat{p}_y\hat{y} + \hat{z}\hat{p}_z + \hat{p}_z\hat{z})$$

3D-KO EHRENFEST-EN TEOREMAK:

1D-tan: $\dfrac{d\langle\hat{x}\rangle}{dt} = \dfrac{\langle\hat{p}\rangle}{m}$; $\dfrac{d\langle\hat{p}\rangle}{dt} = \left\langle -\dfrac{\partial V}{\partial x}\right\rangle$

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{i}{\hbar}\overline{[\hat{H}, \hat{A}]} + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle$$

hemendik.

- Adierazpen hau orokor orokorra da, beraz 3D-tan ere aplikatu ahal izango dugu ($\hat{H}$-k eta $\hat{A}$-k forma ezberdina baina ez dute izango). Hortaz, 3D-tan:

x-ren osagaia

* $\dfrac{d\langle\hat{x}\rangle}{dt} = \dfrac{\langle\hat{p}_x\rangle}{m}$; $\dfrac{d\langle\hat{p}_x\rangle}{dt} = \left\langle -\dfrac{\partial V}{\partial x}\right\rangle$ ⇒ logika bera jarraitu. ⇒

* $\dfrac{d\langle\hat{y}\rangle}{dt} = \dfrac{\langle\hat{p}_y\rangle}{m}$; $\dfrac{d\langle\hat{p}_y\rangle}{dt} = \left\langle -\dfrac{\partial V}{\partial y}\right\rangle$

* $\dfrac{d\langle\hat{z}\rangle}{dt} = \dfrac{\langle\hat{p}_z\rangle}{m}$; $\dfrac{d\langle\hat{p}_z\rangle}{dt} = \left\langle -\dfrac{\partial V}{\partial z}\right\rangle$

3 Ehrenfest-en erlazio hauek batera ditzakegu adierazpen bakar batean, adierazpen bektoriala erabiliz.

- $$\frac{d\langle\hat{\vec{r}}\rangle}{dt} = \frac{d\langle\hat{x}\vec{i} + \hat{y}\vec{j} + \hat{z}\vec{k}\rangle}{dt} = \frac{d\langle\hat{x}\rangle}{dt}\vec{i} + \frac{d\langle\hat{y}\rangle}{dt}\vec{j} + \frac{d\langle\hat{z}\rangle}{dt}\vec{k} =$$

$$\frac{\langle \hat{p}_x \rangle}{m}\hat{i} + \frac{\langle \hat{p}_y \rangle}{m}\hat{j} + \frac{\langle \hat{p}_z \rangle}{m}\hat{k} = \frac{\langle \hat{\vec{p}} \rangle}{m}$$

- $$\frac{d\langle \hat{\vec{p}} \rangle}{dt} = \frac{d\langle \hat{p}_x \rangle}{dt}\hat{i} + \frac{d\langle \hat{p}_y \rangle}{dt}\hat{j} + \frac{d\langle \hat{p}_z \rangle}{dt}\hat{k} = \left\langle -\frac{\partial V}{\partial x}\right\rangle \hat{i} + \left\langle -\frac{\partial V}{\partial y}\right\rangle \hat{j} + \left\langle -\frac{\partial V}{\partial z}\right\rangle \hat{k} = \langle -\vec{\nabla} V \rangle$$

3D-KO VIRIALAREN TEOREMA:

$\Psi_\mathcal{E}(\vec{r},t) = \psi_\mathcal{E}(\vec{r})\, e^{-i\frac{\mathcal{E}}{\hbar}t}$; Egoera horretan neurtuko T-ren batezbestekoa:

egoera geldikorra

* $$\langle \hat{T} \rangle_{\psi_\mathcal{E}} = \frac{1}{2}\langle \hat{\vec{r}} \cdot \vec{\nabla} V \rangle_{\psi_\mathcal{E}} = -\frac{1}{2}\langle \hat{\vec{r}} \cdot \hat{\vec{F}} \rangle$$

Froga: $\frac{d\langle \hat{A} \rangle}{dt} = \frac{i}{\hbar}\overline{[\hat{H},\hat{A}]} + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$ adierazpenean oinarrituz, eraikat ondorengo deslako:

hermitikoa izateko

* $$\hat{A} = \frac{\hat{\vec{r}}\cdot\hat{\vec{p}} + \hat{\vec{p}}\cdot\hat{\vec{r}}}{2} = \underbrace{\frac{\hat{x}\hat{p}_x + \hat{p}_x\hat{x}}{2}}_{\hat{A}_x} + \underbrace{\frac{\hat{y}\hat{p}_y + \hat{p}_y\hat{y}}{2}}_{\hat{A}_y} + \underbrace{\frac{\hat{z}\hat{p}_z + \hat{p}_z\hat{z}}{2}}_{\hat{A}_z}$$

1D-ren jarraituko garapen berdina:

* $\frac{d\langle \hat{A} \rangle_{\psi_\mathcal{E}}}{dt} = 0$ da egoera iraunkor, geldikor, batean $\Rightarrow$ beraz $\overline{[\hat{H},\hat{A}]} = 0$

1D-ko emaitzak osagai bakoitzeko

$\left(\left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle = 0 \text{ delako}\right) \Rightarrow [\hat{H},\hat{A}] = [\hat{H},\hat{A}_x] + [\hat{H},\hat{A}_y] + [\hat{H},\hat{A}_z] = x\frac{\partial V}{\partial x} - \frac{P_x^2}{m} +$

$$y\frac{\partial V}{\partial y} - \frac{P_y^2}{m} + z\frac{\partial V}{\partial z} - \frac{P_z^2}{m} = x\frac{\partial V}{\partial x} + y\frac{\partial V}{\partial y} + z\frac{\partial V}{\partial z} - \frac{1}{m}\left(P_x^2 + P_y^2 + P_z^2\right) = \hat{\vec{r}}\cdot\vec{\nabla} V - 2\hat{T}$$

$$\langle [\hat{H},\hat{A}] \rangle_{\psi_\mathcal{E}} = \langle \hat{\vec{r}}\cdot\vec{\nabla} V \rangle_{\psi_\mathcal{E}} - 2\langle \hat{T} \rangle_{\psi_\mathcal{E}} = 0 \Rightarrow \langle \hat{T} \rangle_{\psi_\mathcal{E}} = \frac{1}{2}\langle \hat{\vec{r}}\cdot\vec{\nabla} V \rangle_{\psi_\mathcal{E}}$$

zentrala

Adierazpen hau nahiko interesatzea $V = \alpha r^n$ denean, koordenatu esferikoak erabiliz adibidez:

$$\vec{\nabla} V = \alpha n r^{n-1}\hat{r} \Rightarrow \vec{r}\cdot\vec{\nabla} V = \alpha n r^n = nV \Rightarrow \langle \hat{T} \rangle_{\psi_\mathcal{E}} = \frac{n}{2}\langle V \rangle_{\psi_\mathcal{E}}$$

$\hat{T}$ eta V zuzenean erlazionatuta, gainera $\langle \hat{T} \rangle_{\psi_\mathcal{E}} + \langle \hat{V} \rangle_{\psi_\mathcal{E}} = \mathcal{E}$

hemendik T eta V lortu

HIRU DIMENTSIOKO POTENTZIAL BANANGARRIAK:

$\Psi(\vec{r},t)$; $-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = \varepsilon\Psi$

- Baldin eta $V(\vec{r})$ banangarria bada ; $V(\vec{r}) = V_1(x) + V_2(y) + V_3(z)$ ekuazioa errazteko da eta dimentsio bakarreko ekuazioak lortuko ditugu.

  $\hat{T}$ beti da banangarria, orduan:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right] + V_1(x)\psi + V_2(y)\psi + V_3(z)\psi = \varepsilon\psi$$

- Aldagaien banantzea aplikatu: $\psi(\vec{r}) = X(x)\,Y(y)\,Z(z)$ $\rightarrow$ ordezkatu ekuazioan $\rightarrow$

$$-\frac{\hbar^2}{2m}\left[YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2}\right] + V_1XYZ + V_2XYZ + V_3XYZ = \varepsilon XYZ$$

$$\rightarrow \cdot\frac{1}{\psi} \rightarrow -\frac{\hbar^2}{2m}\left[\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2}\right] + V_1 + V_2 + V_3 = \varepsilon \rightarrow$$

$$\underbrace{-\frac{\hbar^2}{2m}\cdot\frac{1}{X}\frac{d^2X}{dx^2} + V_1(x)}_{\varepsilon_1}\ \underbrace{-\frac{\hbar^2}{2m}\cdot\frac{1}{Y}\frac{d^2Y}{dy^2} + V_2(y)}_{\varepsilon_2}\ \underbrace{-\frac{\hbar^2}{2m}\cdot\frac{1}{Z}\frac{d^2Z}{dz^2} + V_3(z)}_{\varepsilon_3} = \varepsilon$$

Guztien batura konstante bat denez, aldagai bakoitzari dagokion eskarpena konstante bat izan behar da ere. $\Rightarrow$ Hemendik 3 ekuazio lortzen ditugu, dimentsio bakarrekoak:

autobalioak　　autofuntzioak

$*$ $-\frac{\hbar^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2} + V_1 = \varepsilon_1 \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2X}{dx^2} + V_1X = \varepsilon_1X \Rightarrow X_{n_1}$ lortu, ε_{n_1} energiarekin

$*$ $-\frac{\hbar^2}{2m}\cdot\frac{1}{Y}\frac{d^2Y}{dy^2} + V_2 = \varepsilon_2 \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2Y}{dy^2} + V_2Y = \varepsilon_2Y \Rightarrow Y_{n_2}$ lortu, ε_{n_2} energiarekin

$*$ $-\frac{\hbar^2}{2m}\cdot\frac{1}{Z}\frac{d^2Z}{dz^2} + V_3 = \varepsilon_3 \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2Z}{dz^2} + V_3Z = \varepsilon_3Z \Rightarrow Z_{n_3}$ lortu, ε_{n_3} energiarekin

$\searrow$ Dimentsio bakarrekoak!

Beraz $\Rightarrow \begin{cases} \Psi_{n_1,n_2,n_3}(\vec{r}) = X_{n_1}(x)\, Y_{n_2}(y)\, Z_{n_3}(z) \\ E_{n_1,n_2,n_3} = \varepsilon_{n_1} + \varepsilon_{n_2} + \varepsilon_{n_3} \end{cases}$ $\Rightarrow$ zenbaki kuantiko gehiago ditugunez endakapena agertuko da errazago!

zenbaki kuantikoak

PARTIKULA ASKEA HIRU DIMENTSIOTAN:

$$V=0 \;;\quad -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial y^2} - \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial z^2} = \varepsilon\Psi$$

- Aldagaien banantzea $\Rightarrow \Psi = X(x)\,Y(y)\,Z(z) \Rightarrow$ 3 ekuazio:

$$\begin{cases} -\frac{\hbar^2}{2m}\frac{\partial^2 X}{\partial x^2} = \varepsilon_1 X \;,\quad \varepsilon_1 = \frac{\hbar k_x^2}{2m} \Rightarrow X_{k_x} = Ae^{ik_x x} + Be^{-ik_x x} \\ -\frac{\hbar^2}{2m}\frac{\partial^2 Y}{\partial y^2} = \varepsilon_2 Y \;,\quad \varepsilon_2 = \frac{\hbar k_y^2}{2m} \Rightarrow Y_{k_y} = Ce^{ik_y y} + De^{-ik_y y} \\ -\frac{\hbar^2}{2m}\frac{\partial^2 Z}{\partial z^2} = \varepsilon_3 Z \;,\quad \varepsilon_3 = \frac{\hbar k_z^2}{2m} \Rightarrow Z_{k_z} = Ee^{ik_z z} + Fe^{-ik_z z} \end{cases} \qquad k_x, k_y, k_z \in \mathbb{R}$$

- Beraz, $\Psi_{k_x,k_y,k_z}(\vec{r}) = \left(Ae^{ik_x x} + Be^{-ik_x x}\right)\left(Ce^{ik_y y} + De^{-ik_y y}\right)\left(Ee^{ik_z z} + Fe^{-ik_z z}\right)$

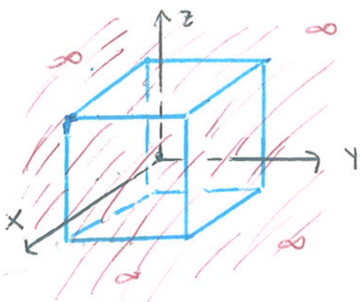
Kasu partikularra!

- Askatasuna dugunez konstanteetan, orokorrean, $B=D=F=0$ direneko kasua hartzen da $\Rightarrow$ $\Psi_{\vec{k}} = A'\, e^{ik_x x + ik_y y + ik_z z} = A'\, e^{i(\vec{k}\cdot\vec{r})}$

Hauek hartu momentu linealaren autofuntziotzat (1D-n bezala)

↳ ez orokorrean, kasu partikular hauetan.

HIRU DIMENTSIOKO POTENTZIAL OSIN KARRATUA:



$$V(x) = \begin{cases} 0 & x \in (-a/2, a/2) \cup y \in (-b/2, b/2) \cup z \in (-c/2, c/2) \\ \infty & , \text{ bestela} \end{cases}$$

V banangarria da, beraz $\Psi = X_{n_1} Y_{n_2} Z_{n_3}$ (zenbaki kuantikoak n_1, n_2, n_3)

V = 0 den gunean

Bakoitzak betetzen duen ekuazioa: $-\frac{\hbar^2}{2m}\frac{\partial^2 X_{n_1}}{\partial x^2} = \varepsilon_{n_1} X_{n_1}$,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 Y_{n_2}}{\partial y^2} = \varepsilon_{n_2} Y_{n_2} \quad , \quad -\frac{\hbar^2}{2m}\frac{\partial^2 X_{n_3}}{\partial z^2} = \varepsilon_{n_3} Z_{n_3}$$

- Aztertu baliotza bere aldetik eta gero mugalde baldintzak aplikatu:

$$X_{n_1}(-a/2) = X_{n_1}(a/2) = 0 \quad , \quad Y_{n_2}(-b/2) = Y_{n_2}(b/2) \quad , \quad Z_{n_3}(-c/2) = Z_{n_3}(c/2)$$

Hau da, dimentsio bakarreko emaitzak lortuko ditugu:

* $X_{n_1} = \sqrt{\frac{2}{a}} \sin\left[\frac{n_1 \pi}{a}(x - a/2)\right] \quad , \quad \varepsilon_{n_1} = \frac{\hbar^2 \pi^2 n_1^2}{2ma^2}$

* $Y_{n_2} = \sqrt{\frac{2}{b}} \sin\left[\frac{n_2 \pi}{b}(y - b/2)\right] \quad , \quad \varepsilon_{n_2} = \frac{\hbar^2 \pi^2 n_2^2}{2mb^2}$

* $Z_{n_3} = \sqrt{\frac{2}{c}} \sin\left[\frac{n_3 \pi}{c}(z - c/2)\right] \quad , \quad \varepsilon_{n_3} = \frac{\hbar^2 \pi^2 n_3^2}{2mc^2}$

Modu normalen antzekoa

- Beraz $\rightarrow \Psi_{n_1, n_2, n_3} = \sqrt{\frac{8}{abc}} \sin\frac{n_1\pi}{a}(x-a/2) \sin\frac{n_2\pi}{b}(y-b/2) \sin\frac{n_3\pi}{c}(z-c/2)$

$$\varepsilon = \varepsilon_{n_1} + \varepsilon_{n_2} + \varepsilon_{n_3} = \varepsilon_{n_1, n_2, n_3} = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\right) \qquad n_1, n_2, n_3 \in \mathbb{N} - \{0\}$$

Kasu berezia; kubo bat badugu, $a = b = c \Rightarrow$ itxelezko endakapena:

$$\varepsilon_{211} = \varepsilon_{121} = \varepsilon_{112} = \frac{\hbar^2 \pi^2}{2ma^2} \cdot 6 = \frac{3\hbar^2 \pi^2}{ma^2} \qquad (g = 3)$$

endakapena

3D-ko osziladore harmonikoa:

bestela isotropoa $k = k_1 = k_2 = k_3$

Kasurik orokorrena, osziladore anisotropoa: $V = \frac{1}{2}k_1 x^2 + \frac{1}{2}k_2 y^2 + \frac{1}{2}k_3 z^2$
$(k_1 \neq k_2 \,,\, k_2 \neq k_3 \,,\, k_1 \neq k_3)$

k_i balioiberekin ω_i definitu $\Rightarrow \omega_i = \sqrt{\frac{k_i}{m}} \qquad i = 1, 2, 3$

Potentzial banangarria ere kasu honetan: $\Psi_{n_1, n_2, n_3}(\vec{r}) = X_{n_1}(x)\, Y_{n_2}(y)\, Z_{n_3}(z) \Rightarrow$

- $-\frac{\hbar^2}{2m}\frac{\partial^2 X_{n_1}}{\partial x^2} + \frac{1}{2}m\omega_1^2 x^2 X_{n_1} = \varepsilon_{n_1} X_{n_1}$ — Dimentsio bakarreko emaitza! O-barne!

$$X_{n_1}(x) = H_{n_1}\left(\sqrt{\frac{m\omega_1}{\hbar}}\, x\right) e^{-\frac{m\omega_1}{2\hbar}x^2} \quad , \quad \varepsilon_{n_1} = \left(\frac{1}{2} + n_1\right)\hbar\omega_1 \qquad n_1 \in \mathbb{N}$$

Hermiteren polinomioa

- $Y_{n_2}(y) = H_{n_2}\left(\sqrt{\frac{m\omega_2}{\hbar}}\, y\right) e^{-\frac{m\omega_2}{2\hbar} y^2}$, $\quad \varepsilon_{n_2} = \left(\frac{1}{2} + n_2\right)\hbar\omega_2 \qquad n_2 \in \mathbb{N}$

- $Z_{n_3}(z) = H_{n_3}\left(\sqrt{\frac{m\omega_3}{\hbar}}\, z\right) e^{-\frac{m\omega_3}{2\hbar} z^2}$, $\quad \varepsilon_{n_3} = \left(\frac{1}{2} + n_3\right)\hbar\omega_3 \qquad n_3 \in \mathbb{N}$

$$\Rightarrow \Psi_{n_1,n_2,n_3} = H_{n_1} H_{n_2} H_{n_3}\, e^{-\frac{m}{2\hbar}(\omega_2 y^2 + \omega_3 z^2 + \omega_1 x^2)}$$

$$\Rightarrow \varepsilon_{n_1,n_2,n_3} = \varepsilon_{n_1} + \varepsilon_{n_2} + \varepsilon_{n_3} = \hbar\omega_1\left(\frac{1}{2}+n_1\right) + \hbar\omega_2\left(\frac{1}{2}+n_2\right) + \hbar\omega_3\left(\frac{1}{2}+n_3\right)$$

- Osziladore harmonikoa isotropoa denean $\Rightarrow \omega_1 = \omega_2 = \omega_3 \equiv \omega$

$$\varepsilon_{n_1,n_2,n_3} = \hbar\omega\left(\frac{1}{2}+\frac{1}{2}+\frac{1}{2}+n_1+n_2+n_3\right) = \hbar\omega\left(\frac{3}{2}+n_1+n_2+n_3\right) = \hbar\omega\left(\frac{3}{2}+n\right)$$

$n_1+n_2+n_3 = n$

$n \in \mathbb{N}$ $\quad$ * $\varepsilon_{n=0} = \frac{3}{2}\hbar\omega$, $\quad \varepsilon_{101} = \varepsilon_{011} = \varepsilon_{110} = \varepsilon_{n=2} = \hbar\omega\left(\frac{3}{2}+2\right)$ $(g=3)$

Egoera endakatuak!

Ariketa ebatziak, 3. Kuatria

(Ordenean)

- Froga ezazu bi partikulen arteko truke-eragilea hermitikoa dela.

$\Psi(\vec{r}_1,\vec{r}_2)$; $\hat{T}\Psi(\vec{r}_1,\vec{r}_2) = \Psi(\vec{r}_2,\vec{r}_1) \rightarrow \hat{T}^2\Psi(\vec{r}_1,\vec{r}_2) = \Psi(\vec{r}_1,\vec{r}_2)$

$\Rightarrow \hat{T}\cdot\hat{T} = \mathbb{1}$ (identitatea) (orokorrean $\hat{A}\cdot\hat{A}^{-1} = \mathbb{1} \rightarrow \hat{T}^{-1} = \hat{T}$)

* Truke eragilearen autobalioak: $\hat{T}\varphi(\vec{r}_1,\vec{r}_2) = \lambda\varphi(\vec{r}_1,\vec{r}_2) = \varphi(\vec{r}_2,\vec{r}_1)$

$\Rightarrow \lambda = \pm 1 \rightarrow \varphi(\vec{r}_1,\vec{r}_2)$ autofuntzio simetriko eta antisimetrikoak

↳ $\in \mathbb{R}$ baina horrek ez du frogatzen hermitikoa denik

(hermitiko $\rightleftarrows$ $\lambda \in \mathbb{R}$)

* $(\Psi, \hat{T}\varphi) = (\hat{T}\Psi, \varphi)$ Hermitikoa izateko baldintza ($\hat{T}^+ = \hat{T}$)

$$\boxed{(\Psi, \hat{T}\varphi)} = \iint \Psi^*(\vec{r}_1,\vec{r}_2)\,\hat{T}\varphi(\vec{r}_1,\vec{r}_2)\,d\vec{r}_1 d\vec{r}_2 = \iint \Psi^*(\vec{r}_1,\vec{r}_2)\,\varphi(\vec{r}_2,\vec{r}_1)\,d\vec{r}_1 d\vec{r}_2 =$$

aldagai aldaketa $\vec{r}_1 \leftrightarrow \vec{r}_2$

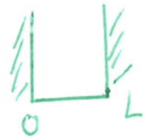
$$\iint \Psi^*(\vec{r}_2,\vec{r}_1)\,\varphi(\vec{r}_1,\vec{r}_2)\,d\vec{r}_1 d\vec{r}_2 = \left[\iint \Psi(\vec{r}_2,\vec{r}_1)\,\varphi^*(\vec{r}_1,\vec{r}_2)\,d\vec{r}_1 d\vec{r}_2\right]^* =$$

$$\left[\iint \varphi^*(\vec{r}_1,\vec{r}_2)\,\hat{T}\Psi(\vec{r}_1,\vec{r}_2)\,d\vec{r}_1 d\vec{r}_2\right]^* = (\varphi, \hat{T}\Psi)^* = \boxed{(\hat{T}\Psi, \varphi)}$$

- Izan bedi spinik gabeko ($s=0$) bi boson berdinez osaturiko sistema (simetrikoak espazioan). Sistema $\Rightarrow$ 1D-ko potentzial osin-infinituan dago, L zabalerakoa.

a) Bi basoren artean elkarrekintzarik ez → oinarrizko egoera eta lehen bi egoera kitzikatuak? Haien energiak?

* Partikula bakarra potentzial osin-infinituan ⇒ $|n\rangle$ $\quad n \in \mathbb{N}-\{0\}$



$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2 \quad , \quad \langle x | n \rangle = \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}$$

* Hamiltondar osoaren uhin-funtzioak: $\psi_{n_1,n_2} = \frac{2}{L} \sin \frac{\pi n_1 x_1}{L} \sin \frac{\pi n_2 x_2}{L}$

eta $E_{n_1,n_2} = \frac{\hbar^2 \pi^2}{2mL^2} (n_1^2 + n_2^2)$ $\quad \hookrightarrow |n_1, n_2\rangle$

Energia-mailak: n=3 → Bigarren egoera kitzikatua → $E_2 = \frac{4\hbar^2\pi^2}{mL^2}$

n=2 → Lehenengo egoera kitzikatua → $E_1 = \frac{\hbar^2\pi^2}{2mL^2} 5$

n=1 → oinarrizko egoera → $E_0 = \frac{\hbar^2\pi^2}{mL^2}$

$E_0 \Rightarrow |\psi_0\rangle = |\overset{n_1}{1}, \overset{n_2}{1}\rangle$ Simetrikoa

$\hookrightarrow \psi_0 = \frac{2}{L} \sin \frac{\pi x_1}{L} \sin \frac{\pi x_2}{L}$

$E_1 \Rightarrow |\psi_1\rangle = \frac{1}{\sqrt{2}} [|1,2\rangle + |2,1\rangle]$ Simetrizatu

$\hookrightarrow \psi_1 = \frac{2}{L} \cdot \frac{1}{\sqrt{2}} \left[\sin \frac{\pi x_1}{L} \sin \frac{2\pi x_2}{L} + \sin \frac{2\pi x_1}{L} \sin \frac{\pi x_2}{L} \right]$

$E_2 \Rightarrow |\psi_2\rangle = |2\,2\rangle$ Simetrikoa

$\hookrightarrow \psi_2 = \frac{2}{L} \sin \frac{2\pi x_1}{L} \sin \frac{2\pi x_2}{L}$

b) Basoen arteko elkarrekintza ⇒ $W(x_1, x_2) = -L V_0 \delta(x_1 - x_2)$

Lehen ordenako perturbazioa aplikatuz → oinarrizko egoeraren energia?

* Oinarrizko energia perturbaziorik gabe ⇒ $E_0 = \frac{\hbar^2\pi^2}{mL^2}$

* Perturbatzean → $\Delta E = \langle \psi_0 | W | \psi_0 \rangle \to E_0' = E_0 + \Delta E$

$$\langle \psi_0 | W | \psi_0 \rangle = -L V_0 \langle \psi_0 | \delta(x_1 - x_2) | \psi_0 \rangle = -L V_0 \int_0^L \int_0^L |\psi_0|^2 \delta(x_1 - x_2)\, dx_1 dx_2 =$$

$$-LV_0 \int_0^L \int_0^L \left(\frac{2}{L}\right)^2 \sin^2 \frac{\pi x_1}{L} \sin^2 \frac{\pi x_2}{L}\, \delta(x_1 - x_2)\, dx_2\, dx_1 = -LV_0 \int_0^L \left(\frac{2}{L}\right)^2 \sin^4 \frac{\pi x_1}{L}\, dx_1 =$$

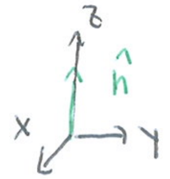
$$-\frac{4V_0}{L} \int_0^L \sin^4 \frac{\pi x_1}{L}\, dx_1 = -\frac{4V_0}{\cancel{L}} \cdot \frac{3\cancel{L}}{8} = -\frac{3V_0}{2} \Rightarrow \boxed{E_0' = \frac{\hbar^2\pi^2}{mL^2} - \frac{3V_0}{2}}$$

• Spina 1/2 duten bi partikula ($s_1 = s_2 = 1/2$) → ondoko eragilea:

$$* \quad \hat{S}_{12} = 3(\underbrace{\hat{S}_1 \cdot \hat{n}}_{\hat{S}_{1n}})(\underbrace{\hat{S}_2 \cdot \hat{n}}_{\hat{S}_{2n}}) - \hat{S}_1 \cdot \hat{S}_2$$

$\hat{n}$ ≡ bektore unitarioa.

Zenbat balio du $(\hat{S}_{12} - \frac{\hbar^2}{2})(\hat{S}_{12} + \hbar^2) | \chi_{triplet} \rangle$?



Tripletea ⇒ $s = 1$, $m_s = \pm 1, 0$ → $|1, m_s\rangle$

Lehenengo $\hat{S}_{12}$-ren adierazpena lortu: $\hat{n}$ hori edozein izan daiteke

eta gure erreferentzia sistema nahi dugun moduan aukeratu dezakegunez

Z ardatzean kokatuko dugu: $\hat{S}_1 \cdot \hat{n} = \hat{S}_{1z}$, $\hat{S}_2 \cdot \hat{n} = \hat{S}_{2z}$

Gainera → $\hat{S}_1 \cdot \hat{S}_2 = [S^2 - S_1^2 - S_2^2] \cdot \frac{1}{2}$ $\quad (\vec{S} = \vec{S_1} + \vec{S_2})$

$$\hat{S}_{12} = 3 \hat{S}_{1z} \hat{S}_{2z} - \frac{1}{2}(S^2 - S_1^2 - S_2^2)$$

Gainera $\rightarrow$ $S_z^2 = (S_{1z} + S_{2z})^2 = S_{1z}^2 + S_{2z}^2 + 2 S_{1z} S_{2z} \rightarrow$

$$S_{1z} S_{2z} = \frac{1}{2} [S_z^2 - \underbrace{S_{1z}^2 - S_{2z}^2}] = \frac{1}{2} [S_z^2 - \frac{\hbar^2}{2}]$$

$\hookrightarrow$ finkoa, karratua delako $(\frac{\hbar^2}{4})$

$$\Rightarrow \quad \hat{S}_{12} = \frac{3}{2} (S_z^2 - \cancel{\hbar^2}/2) - \frac{1}{2} (S^2 - \cancel{\hbar^2} \frac{3}{2}) = \frac{1}{2} (3 S_z^2 - \hat{S}^2)$$

$$\hat{S}_{12} | \chi_{mplete} \rangle = \frac{\hbar^2}{2} (3 m_s^2 - 2)$$

$$* \; (\hat{S}_{12} - \frac{\hbar^2}{2}) (\hat{S}_{12} + \hbar^2) | \chi_{mplete} \rangle = (\cancel{\hbar^2} + \frac{\hbar^2}{2} (3 m_s^2 - \cancel{2})) (\frac{\hbar^2}{2} (3 m_s^2 - 2) - \frac{\hbar^2}{2}).$$

$$| \chi_{mplete} \rangle = (\frac{\hbar^2}{2} (3 m_s^2 \quad)) (\frac{\hbar^2}{2} (3 m_s^2 - 3)) | \chi_{mplete} \rangle = | \psi \rangle$$

- $m_s = 0 \rightarrow \boxed{|\psi\rangle = 0}$ • $m_s = \pm 1 \rightarrow \boxed{|\psi\rangle = 0}$

- Bereizgaiak diren $S_1 = S_2 = 1/2$-ko bi partikula:

$$\hat{H} = g \left(\frac{\hat{S}_1 \cdot \hat{S}_2}{\hbar^2} + \frac{3}{4} \right)^2 + g \left(\frac{\hat{S}_1 \cdot \hat{S}_2}{\hbar^2} + \frac{3}{4} \right) + b \frac{(S_{1z} + S_{2z})}{\hbar}$$

$g, b > 0 \Rightarrow$ Badakigu: $S_{1z} + S_{2z} = S_z$ eta $\hat{S}_1 \cdot \hat{S}_2 = \frac{1}{2} (S^2 - \underbrace{S_1^2 - S_2^2}_{\text{finkoak}}) =$

$$\frac{1}{2} (S^2 - \frac{3\hbar^2}{2})$$

bereizgaiak ; ez dira simetrizatu / antisimetrizatu behar

$* \; t = 0 \rightarrow | \psi(t=0) \rangle = |+\rangle_1 |-\rangle_2 \rightarrow \langle S_1(t) \rangle ?$

Denboran garatu $\rightarrow$ $$\hat{H} = g \left(\frac{S^2 - \cancel{3\hbar^2/2}}{2\hbar^2} + \cancel{\frac{3}{4}} \right)^2 + g \left(\frac{S^2 - \cancel{3\hbar^2/2}}{2\hbar^2} + \cancel{3/4} \right) + b \frac{S_z}{\hbar} =$$

$$g \left(\frac{S^2}{2\hbar^2} \right) \left(1 + \frac{S^2}{2\hbar^2} \right) + b \frac{S_z}{\hbar}$$

- Autobeltereak $\Rightarrow$ $|s\ m_s\rangle$

- Autobaloreak $\Rightarrow$ $E = \frac{g}{2\cancel{\hbar^2}}\left(\cancel{\hbar^2}(s+1)s\right)\left(1+\frac{\cancel{\hbar^2}s(s+1)}{2\cancel{\hbar^2}}\right) + b\frac{\cancel{\hbar}m_s}{\cancel{\hbar}} =$

$$\frac{g}{2}s(s+1)\left(1+\frac{s(s+1)}{2}\right)+bm_s$$

Orduan $\Rightarrow$ $|+\rangle_1|-\rangle_2$ $\{|s,m_s\rangle\}$ oinarrian garatuko dugu:

$$|+\rangle_1|-\rangle_2 = \frac{1}{\sqrt{2}}[\underset{\downarrow s\ \downarrow m_s}{|1,0\rangle} + |0,0\rangle]$$

Beraz $\Rightarrow$ $|\psi(t)\rangle = \frac{1}{\sqrt{2}}[e^{-2git/\hbar}|1,0\rangle + |0,0\rangle]$

- $\vec{S}_1 = S_{1x}\hat{\imath} + S_{1y}\hat{\jmath} + S_{1z}\hat{k} \rightarrow \langle\vec{S}_1(t)\rangle = \langle S_{1x}(t)\rangle\hat{\imath} + \langle S_{1y}(t)\rangle\hat{\jmath} +$

$\langle S_{1z}(t)\rangle\hat{k}$

* $S_{1x} = \frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}\otimes \mathbb{1} = \frac{\hbar}{2}\begin{pmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{pmatrix}$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{-2git/\hbar}\frac{1}{\sqrt{2}}(|+-\rangle+|-+\rangle) + \frac{1}{\sqrt{2}}(|+-\rangle-|-+\rangle)\right) =$$

$$\frac{1}{2}\left[|+-\rangle(e^{-2git/\hbar}+1) + |-+\rangle(e^{-2git/\hbar}-1)\right] \rightarrow \vec{c} = \frac{1}{2}\begin{pmatrix}0\\1+e^{-2git/\hbar}\\e^{-2git/\hbar}-1\\0\end{pmatrix}$$

$$\langle S_{1x}\rangle = \frac{\hbar}{8}\left(e^{2git/\hbar}-1\quad 0\quad 0\quad 1+e^{2git/\hbar}\right)\begin{pmatrix}0\\1+e^{-2git/\hbar}\\e^{-2git/\hbar}-1\\0\end{pmatrix} = 0$$

$*\ \hat{S}_{1y} = \frac{\hbar i}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \otimes \mathbb{1} = \frac{\hbar i}{2}\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$

$$\langle \hat{S}_{1y} \rangle = \frac{\hbar i}{8}\left(e^{2igt/\hbar}-1 \quad 0 \quad 0 \quad -(1+e^{2igt/\hbar}) \right)\begin{pmatrix} 0 \\ 1+e^{-2igt/\hbar} \\ e^{-2igt/\hbar}-1 \\ 0 \end{pmatrix} = 0$$

$*\ \hat{S}_{1z} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \Rightarrow \langle \hat{S}_{1z} \rangle = \frac{\hbar}{8}\left(0 \quad 1+e^{2igt/\hbar} \quad 1-e^{2igt/\hbar} \quad 0 \right) \cdot$

$$\begin{pmatrix} 0 \\ 1+e^{-2igt/\hbar} \\ e^{-2igt/\hbar}-1 \\ 0 \end{pmatrix} = \frac{\hbar}{8}\left(\cancel{1} + e^{2igt/\hbar} + e^{-2igt/\hbar} \cancel{+1} + e^{-2igt/\hbar} \cancel{-1} \cancel{-1} + e^{2igt/\hbar} \right) =$$

$$\frac{\hbar}{8} \cdot 2\left(e^{2igt/\hbar} + e^{-2igt/\hbar} \right) = \frac{\hbar}{2} \cdot \cos\left(\frac{2gt}{\hbar}\right)$$

$$\Rightarrow \quad \langle \vec{S}_1(t) \rangle = \frac{\hbar}{2}\cos\left(\frac{2gt}{\hbar}\right)\hat{k}$$

- Elektroi (e) eta positroi (p) (bereizgarriak) baten spin-egoera zehazten duen Hamiltondarra $\Rightarrow$ $\hat{H} = J(\hat{S}_x^e \hat{S}_x^p + \hat{S}_y^e \hat{S}_y^p)$

$$\vec{S}_e \cdot \vec{S}_p = S_x^e S_x^p + S_y^e S_y^p + S_z^e S_z^p = \frac{1}{2}(S^2 - S_e^2 - S_p^2) \Rightarrow \text{bandatzi } \hat{H}$$

$$\hat{H} = J\left[\frac{1}{2}(S^2 - S_e^2 - S_p^2 - S_z^e S_z^p) \right]$$

$$S_z^e S_z^p = \frac{1}{2}(S_z^2 - S_z^{e\,2} - S_z^{p\,2}) \rightarrow \text{bandatzi } \hat{H}$$

$$\hat{H} = \frac{J}{2}(S^2 - S_e^2 - S_p^2 + S_z^{e\,2} + S_z^{p\,2} - S_z^2)$$

$t=0 \rightarrow |\psi(t=0)\rangle = |+\rangle_e |-\rangle_p$ $\quad$ ($\{|\pm\rangle_i\}$ $\hat{S}_z^i$-ren autofuntzioak, $i = e, p$)

* $\hat{H}$-ren autofuntzioak : $|S\ m_S\rangle$

↳ S_z^e edo S_z^p egitean BETI lortuko dugu $\frac{\hbar^2}{4}$; eta S_e^2 edo

S_p^2 egitean $\frac{3\hbar^2}{4}$

* $\hat{H}$-ren autobalioak: $E = \frac{J}{2}\hbar^2\left(S(S+1) - \frac{3}{2} + \frac{1}{2} - m_S^2\right) = \frac{J}{2}\hbar^2\left(S(S+1)\right.$ +

$\left.-1 - m_S^2\right)$

Orain hasierako egoera $\{|S\ m_S\rangle\}$ oinarrian garatu beharko dugu:

* $|+\rangle_e|-\rangle_p = \frac{1}{\sqrt{2}}\left[|\underbrace{1}_{S}\ \underbrace{0}_{m_S}\rangle + |0\ 0\rangle\right]$

$\left(|1\ 0\rangle = \frac{1}{\sqrt{2}}\left[|+\rangle_e|-\rangle_p + |-\rangle_e|+\rangle_p\right]\right.$ eta $\left.|0\ 0\rangle = \frac{1}{\sqrt{2}}\left[|+\rangle_e|-\rangle_p - |-\rangle_e|+\rangle_p\right]\right)$

• $|\Psi(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{-J\hbar i t/2}|1\ 0\rangle + e^{\hbar J i t/2}|0\ 0\rangle\right] = \frac{1}{2}\left[e^{\hbar J i t/2}\left(|+-\rangle + \right.\right.$

$\left.|-+\rangle\right) + e^{\hbar J i t/2}\left.\left(|+-\rangle - |-+\rangle\right)\right] = \frac{1}{2}\left(e^{\hbar J i t/2} + e^{\hbar J i t/2}\right)|+-\rangle +$

$\frac{1}{2}\left(e^{-\hbar J i t/2} - e^{\hbar J i t/2}\right)|-+\rangle = \cos\left(\frac{\hbar J t}{2}\right)|+-\rangle - i\sin\left(\hbar\frac{Jt}{2}\right)|-+\rangle$

↗ berdin digu $-i$ bat izatea aurrean egoera berdin izango da

Zein t aldiunetan izango da $|\Psi(t)\rangle$ $|-+\rangle$? $\Rightarrow$ $\sin\left(\hbar\frac{Jt}{2}\right) = \pm 1$

denean eta $\cos\left(\hbar\frac{Jt}{2}\right) = 0$ denean $\Rightarrow$ $\hbar\frac{Jt}{2} = \frac{(2n+1)\pi}{2} \rightarrow t = \frac{(2n+1)}{J\hbar}$ $n \in \mathbb{N}$

• Berdinak diren $s = 1/2$ spina duten bi partikula dimentsio bakar batean mugitzen ari dira $\Rightarrow$ haien elkarrekintzaren lotura energia potentziala $\Rightarrow$ $V(x_1 - x_2) = \begin{cases} 0 & 0 \le |x_1 - x_2| \le a \\ \infty & |x_1 - x_2| > a \end{cases}$

↱ lineala → dimentsio bakarrean kasu honetan; ez da ezer momentu angeluarra

Bi partikulen momentu osoa zero delarik, spin osoa $\sqrt{2}\hbar$ duen

1. egoera kitzikatuan daude. $x_1 - x_2 = x \rightarrow V(x) = \begin{cases} 0 & -a \leq x \leq a \\ \infty & |x| \geq a \end{cases}$

$|S| = \sqrt{2}\hbar \rightarrow S = 1 \rightarrow$ simetrikoa /Datu honek ematen egoera espaziala antisimetrikoa izan behar dela jakiteko)

Partikulak berdintsuak dira eta fermioiak ⇒ uhin-funtzio osoa antisimetrikoa

[Oinarrizko egoeran ⇒ egoera espaziala simetrikoa da beti (egoera espazial berean daude) → Spin egoera $S=0$ denez (antisimetrikoa)]

Zein da bi partikulen arteko distantzia $a/4$ baino txikiagoa izateko probabilitatea? ($-a/4 \leq x \leq a/4$ izateko probabilitatea)

↳ egoera horretan egonik

* Lehendabizi ⇒ uhin-funtzio espaziala kalkulatu.

$$\hat{H}(x_1, x_2) = -\frac{\hbar^2}{2m}\frac{d^2}{dx_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dx_2^2} + V(x_1 - x_2)$$

↳ Aldagai aldaketa $\begin{cases} x = x_1 - x_2 \\ x_{MZ} = \frac{x_1 + x_2}{2} \\ \mu = \frac{m}{2} \quad , m_{MZ} = 2m \end{cases}$

$$\hat{H}(x_{MZ}, x) = -\frac{\hbar^2}{4m}\frac{d^2}{dx_{MZ}^2} - \frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V(x)$$

- $\Psi(x_{MZ}, x) = \phi(x_{MZ})\psi(x) \rightarrow -\frac{\hbar^2}{4m}\frac{d^2\phi}{dx_{MZ}^2} = E_{MZ}\,\phi(x_{MZ}) \longrightarrow \phi(x_{MZ}) = Ae^{iK_{MZ}x_{MZ}}$

$K = \frac{\sqrt{2mE_{MZ}}}{\hbar}$

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + V(x)\psi = E_\mu \psi \quad \text{(P. osin-infinitua)}$$

↳ $\psi_n = \sqrt{\frac{2}{2a}} \sin \frac{n\pi}{2a}(x-a) \qquad E_\mu^n = \frac{\hbar^2\pi^2 n^2}{8ma^2} \qquad n \in \mathbb{N}$

↗ $\vec{v}_{MZ} = \frac{\vec{v}_{osoa}}{2} \rightarrow \vec{p}_{MZ} = M_{MZ}\vec{v}_{MZ} = m\,\vec{v}_{osoa} = \vec{p}_{osoa}$ hasierako hipotesia

$K_{MZ} \rightarrow$ MZ-ren momentua = sistema osoaren momentua ⟶ MZ-ren momentua 0 ($K_{MZ} = 0$)

Hau erreferentzia-sistema masa zentroan jartzearen berdina da.

* Masa-zentroaren eltegena nulua da → $\Psi = \Psi(x) = \Psi(x_1, x_{MZ})$

1. egoera kitzikatuan daudenez eta uhin-funtzioak bikoitze elkartzearen
                                                                                                    → oinarrizkoa $n=1$

bidez eremanda daudenez bakarra behar dugu ⇒ $n=2$

$$\Psi(x) = \left(\sqrt{\frac{1}{a}} \sin \frac{\pi}{a}(x-a)\right) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi x}{a} - \pi\right) =$$

↘ espaziala soilik.

$$-\sqrt{\frac{1}{a}} \sin \frac{\pi x}{a} = -\sqrt{\frac{1}{a}} \sin \frac{\pi(x_1-x_2)}{a} \Rightarrow \text{Antisimetrikoa}$$

$$P(-a/4 \le x \le a/4) = \int_{-a/4}^{a/4} |\Psi(x)|^2 dx = \frac{1}{a}\int_{-a/4}^{a/4} \sin^2 \frac{\pi x}{a}\, dx =$$

$$\frac{1}{a}\left[\frac{(\pi-2)a}{4\pi}\right] = \frac{1}{4} - \frac{1}{2\pi} \simeq 0'1$$

- Zenbatekoa da a aldea duen kubo batean dauden 24 elektroi-ren oinarrizko energia?

* Kontsideratuko dugu independenteak direla ⇒ ez dute elkarrekintzarik.

* a aldeko kuboa ⇒ 3D-ko potentzial osin-infinitua.

- Partikula baten energia ⇒ $E_n = \frac{\hbar^2\pi^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2)$

  eta autofuntzioa ⇒ $\Psi_n = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\frac{\pi n_x x}{a} \sin\frac{\pi n_y y}{a} \sin\frac{\pi n_z z}{a}$

Paulinen esklusio printzipioa kontuan hartuz energia-mailak beteten joango gara 24 e^--rekin.

E

$\frac{12\hbar^2\pi^2}{2ma^2}$ ↑↓ $n_x=n_y=n_z=2$ $\Rightarrow$ 2 e^- kokatzea falta da → hauek kokatzeko dudan posible asko *

$\frac{11\pi^2\hbar^2}{2ma^2}$ ↑↓ $n_x=n_y=1, n_z=3$ ↑↓ $n_x=n_z=1, n_y=3$ ↑↓ $n_y=n_z=1, n_x=1$

$\frac{9\pi^2\hbar^2}{2ma^2}$ ↑↓ $n_x=n_y=2, n_z=1$ ↑↓ $n_x=n_z=2, n_y=1$ ↑↓ $n_y=n_z=2, n_x=1$

$\frac{6\hbar^2\pi^2}{2ma^2}$ ↑↓ $n_x=n_y=1, n_z=2$ ↑↓ $n_y=n_z=1, n_x=2$ ↑↓ $n_z=n_x=1, n_y=2$

$\frac{3\hbar^2\pi^2}{2ma^2}$ ↑↓ $n_x=n_y=n_z=1$

* $\frac{14\hbar^2\pi^2}{2ma^2}$ 123 132 213 231 321 312

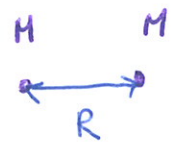
2 e^- hauek hemen kokatu behar ditugu.

$g = 4(5+4+3+2+1) = 60$; Energia osoa : $E_0 = \frac{\hbar^2\pi^2}{ma^2} 107$

MOLEKULAK.

- M masadun atomo berdinetako molekula diatomikoaren oinarrizko egoera elektronikoa $\Rightarrow$ $E_0(R) = D(1-e^{-\beta(R-\alpha)})^2$

↳ atomoen arteko distantzia



$D, \beta, \alpha > 0$ (Molekularen ezaugarrien parametro errealak)

Molekula oinarrizko egoeran dagoela suposatuz, zein da molekularen disoziazio energia? (Biraketa eta bibrazio akoplamenduak kontutan hartu)

$E_{disozio} = E_0(R\to\infty) - E_0(R=R_0) + \frac{\hbar\omega_0}{2}$ ($R_0 \equiv$ oreka distantzia → $E_0(R)$ minimizatzen duena)

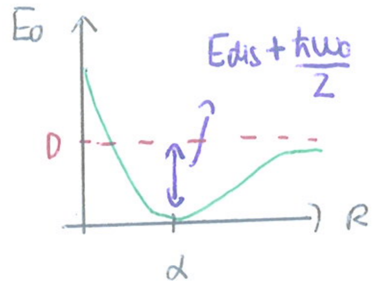
↳ oinarrizko egoeran $J=0 \rightarrow E_{errotazio} = 0$

* R_0? $\frac{dE_0(R)}{dR} = 2D(1-e^{-\beta(R-\alpha)}) \cdot \beta e^{-\beta(R-\alpha)} = 0 \Rightarrow$

$$e^{-\beta(R-\alpha)}\left(1-e^{-\beta(R-\alpha)}\right)=0 \to 1=e^{-\beta(R-\alpha)} \to \beta(R-\alpha)=0 \to R_0=\alpha$$

↳ $e^{-\beta(R-\alpha)} \neq 0 \quad (\leftrightarrow R \nrightarrow \infty)$

↳ oreka distantzia finitua da



$$* \quad \omega_0=\sqrt{\frac{K}{\mu}} \; ; \; K=\left.\frac{d^2E_0}{dR^2}\right|_{R=R_0} \; ; \; \mu=\frac{M}{2}$$

$$\frac{d^2E_0(R)}{dR^2}=2D\beta\left(-\beta e^{-\beta(R-\alpha)}\left(1-e^{-\beta(R-\alpha)}\right)+e^{-\beta(R-\alpha)}\cdot\beta e^{-\beta(R-\alpha)}\right) \Rightarrow R=R_0-n$$

ebaluatu $\Rightarrow \left.\frac{d^2E_0(R)}{dR^2}\right|_{R=R_0}=K=2D\beta(\beta)=2D\beta^2 \Rightarrow \omega_0=\sqrt{\frac{4D\beta^2}{M}}=2\beta\sqrt{\frac{D}{M}}$

$$\boxed{E_{disoziazio}}=D-0-\frac{2\hbar}{2}\beta\sqrt{\frac{D}{M}}=\boxed{D-\hbar\beta\sqrt{\frac{D}{M}}}$$

- Lotura ionikoa duen KBr molekulan osaketa urrutiko oso aldenduta dauden K eta Br atomo neutroekin hasiko gara. Lehenengo urratsean elektroi bat kenduko diogu K atomoari Br atomoari emanez. Horrela, oso aldenduta dauden K^+ eta Br^- ioiak izango ditugu. Ioi horiek hurbiltzean haien energia txikitzen joango da, haien energia potentzial Coulombiarra txikitzen joango delako. Bi ioiak (K^+ eta Br^-) osotuko energia oso urrun dauden K eta Br atomo neutroen energiaren berdina zein distantziatan izango da? Kontuan hartu ioien arteko potentzial Coulombiarra eta ioiak sortzeko energia.

afinitate elektronikoa

Datuak: $E_{ionizazio}(K) = 4'34\,eV$, $A(K) = -0'5\,eV$; $E_{ionizazio}(Br) = 11'8\,eV$

eta $A(Br) = -3'37\,eV$

K $\qquad$ Br

$\downarrow$ $E_{ionizazio}(K)$ $\qquad$ $\downarrow$ $A(Br)$

K^+ $\qquad$ e^- hori hartu $\qquad$ Br^-

⇒ Energian 0 maila hemen jarri ⇒ $E_1 = 0$

⇒ bi hauek hurbiltzean hauen energia txikitu

$$E_2^0 = E_{ion} + A = 0'97\,eV$$

distantzia honetan atomo neutroen energia bera

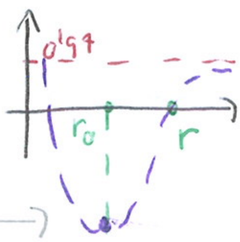
$$E_1 = E_2 = 0 = 0'97\,eV - \frac{e^2}{4\pi\varepsilon_0 r} \rightarrow \frac{e^2}{4\pi\varepsilon_0 r} = 0'97\,eV \rightarrow r = \frac{e^2}{4\pi\varepsilon_0 E_2^0} = 14\,Å$$

EZ DA OREKA DISTANTZIA

distantzia txikiagoa bada ioien energia atomo neutroena baino txikiagoa izango da ⇒ distantzia horretatik aurrera egonkorragoa dugu ioiek osatutako sistema atomo neutroena baino.

"Nahiago dute" hurbil daudenean ioi moduan egotea atomo neutro baino.

Distantzia txikitzean elektroien aldarapenak nabarmenak izango dira → energia handitu ⇒ Minimo bat egongo da:



$r_0 \simeq 2'82\,Å$

FISIKA KUANTIKOA

4. POTENTZIAL ZENTRALAK eta ELEKTROI BAKARREKO ATOMOAK

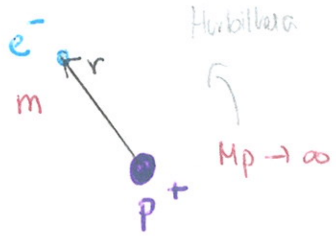
16-11-28

SARRERA: HIDROGENO - ATOMOA:

Hidrogeno-atomoari dagozkion autofuntzio eta autobalioak kalkulatuko ditugu, ezinbestekoa atomoak ulertzeko; atomorik sinpleena H atomoa delako.

Halaber, Schrödinger-ek aztertu zuen problema da bere ekuazioaren baliagarritasuna frogatzeko $\Rightarrow$ Bohr-ek bere ereduan lortu zituen autobalio berdinak lortu zituen

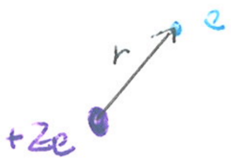
2 osagai: p^+ eta e^- ($e = 1'6 \cdot 10^{-19}$ C) ($M_p \approx 1836\, m_e$; $M_p >> m_e$)



Coulomb: $V = -\frac{1}{4\pi\varepsilon_0} \cdot \frac{e^2}{r}$

Hurbilketa $\Rightarrow$ $M_p >> m_e$ $\leftrightarrow$ $M_p \to \infty$: kontsideratu protoia ez dela mugitzen eta jatorria protoian kokatuz e^- bere inguruan mugitzen da. $\Rightarrow$ partikula bakarraren higidura (Hurbilketa hau ez da derrigorrezkoa).

Hidrogenoaz gain, atomo hidrogenoideak ditugu, e^- bakarra duten atomoak baina nukleoan Z protoi (karga ezberdina nukleoan) Ad: Li^{2+}



$V = -\frac{1}{4\pi\varepsilon_0} \frac{Ze^2}{r}$

Kasu orokorra aztertuko dugu atomo hidrogenoidearen problema ebatziz:

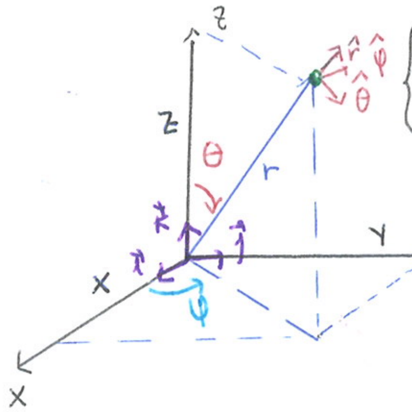
Schrödingeren ekuazioa: ($M_{nukleo} \to \infty$ hartu eta $\bar{e}$ baino ez dela mugitzen)

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r} \Rightarrow \hat{H}\psi(\vec{r}) = \varepsilon\,\psi(\vec{r})$$

Problemaren erroak, autobalio (ε) eta autofuntzioak ($\psi(\vec{r})$) kalkulatzea

KOORDENATU ESFERIKOAK:

Hidrogeno atomoaren problemak simetria esferikoa du beraz Schrödingeren ekuazioa ebazteko koordenatu esferikoak erabiliko ditugu:



$\theta \to$ angelu polarra, $\theta \in [0, \pi]$

$\varphi \to$ angelu azimutala, $\varphi \in [0, 2\pi]$

$$|\vec{r}| = r = \sqrt{x^2+y^2+z^2} \qquad x = r\sin\theta\cos\varphi$$

$$\theta = \operatorname{arctg}\sqrt{\frac{x^2+y^2}{z^2}} \quad \longleftrightarrow \quad y = r\sin\theta\sin\varphi$$

$$\varphi = \operatorname{arctg}\frac{y}{x} \qquad z = r\cos\theta$$

Bektore unitarioak:

$$\begin{cases} \hat{r} = \dfrac{\vec{r}}{r} = \sin\theta\cos\varphi\,\hat{\imath} + \sin\theta\sin\varphi\,\hat{\jmath} + \cos\theta\,\hat{k} \\ \hat{\theta} = \cos\theta\cos\varphi\,\hat{\imath} + \cos\theta\sin\varphi\,\hat{\jmath} - \sin\theta\,\hat{k} \\ \hat{\varphi} = -\sin\varphi\,\hat{\imath} + \cos\varphi\,\hat{\jmath} \end{cases}$$

$\vec{\nabla}$ eta $\vec{\nabla}^2$:

$$\begin{cases} \vec{\nabla} = \partial_r\,\hat{r} + \dfrac{1}{r}\partial_\theta\,\hat{\theta} + \dfrac{1}{r\sin\theta}\partial_\varphi\,\hat{\varphi} \\ \vec{\nabla}^2 = \dfrac{1}{r}\partial_r^2 r + \dfrac{1}{r^2}\left(\partial_{\theta^2}^2 + \dfrac{1}{\operatorname{tg}\theta}\partial_\theta + \dfrac{1}{\sin^2\theta}\partial_{\varphi^2}^2\right) \end{cases}$$

MOMENTU ANGELUARRA MEKANIKA KLASIKOAN:

$$\vec{L} = \vec{r}\wedge\vec{p} = m\vec{r}\wedge\vec{v} \quad ; \quad \vec{M} = \vec{r}\wedge\vec{F} = \dot{\vec{L}} = \frac{d\vec{L}}{dt}$$

Indarra zentrala bada $\vec{r} \parallel \vec{F} \leftrightarrow \vec{M} = 0 \Leftrightarrow \dot{\vec{L}} = 0 \leftrightarrow \vec{L} = kte$

(Indar elektrikoa, grabitazioa...)

Koordinatu kartesiarretan:

$$\vec{L} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

Baina koordinatu esferikoak erabiltzea komenigarria izan daiteke zenbait problematan (Hidrogenoaren probleman adibidez):

- $\vec{r} = r\hat{r}$, $\vec{v} = \frac{d\vec{r}}{dt} = \dot{r}\hat{r} + r\frac{d\hat{r}}{dt}$ $\quad$ ($\hat{r} = \sin\theta\cos\varphi\,\hat{i} + \sin\theta\sin\varphi\,\hat{j} + \cos\theta\,\hat{k}$, θ aldakorra)

* $\frac{d\hat{r}}{dt} = (\cos\theta\cos\varphi\,\dot{\theta} - \sin\theta\sin\varphi\,\dot{\varphi})\,\hat{i} + (\cos\theta\sin\varphi\,\dot{\theta} + \sin\theta\cos\varphi\,\dot{\varphi})\,\hat{j} - \sin\theta\cdot\dot{\theta}\,\hat{k} = \dot{\theta}\,(\cos\theta\cos\varphi\,\hat{i} + \cos\theta\sin\varphi\,\hat{j} - \sin\theta\,\hat{k}) + \sin\theta\,\dot{\varphi}(-\sin\varphi\,\hat{i} + \cos\varphi\,\hat{j}) = \dot{\theta}\,\hat{\theta} + \sin\theta\,\dot{\varphi}\,\hat{\varphi}$

Beraz, $\vec{r} = r\hat{r}$, $\vec{v} = \dot{r}\,\hat{r} + r\dot{\theta}\,\hat{\theta} + r\sin\theta\,\dot{\varphi}\,\hat{\varphi}$

- $$\vec{L} = m\begin{vmatrix} \hat{r} & \hat{\theta} & \hat{\varphi} \\ r & 0 & 0 \\ \dot{r} & r\dot{\theta} & r\dot{\varphi}\sin\theta \end{vmatrix} = m\,(r^2\dot{\theta}\,\hat{\varphi} - r^2\dot{\varphi}\sin\theta\,\hat{\theta}) \quad ; \quad \vec{L}^2 = m^2\,(r^4\dot{\theta}^2 + r^4\dot{\varphi}^2\sin^2\theta)$$

Koordinatu esferikoetan

- $H = T + V = \frac{1}{2}mv^2 + V(r,\theta,\varphi) = \frac{1}{2}m\,(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\varphi}^2\sin^2\theta) + V(r,\theta,\varphi) = \frac{1}{2}m\dot{r}^2 +$

Momentu linealaren eran idatzi daiteke

$\frac{L^2}{2}\cdot\frac{1}{mr^2} + V(r,\theta,\varphi) = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V(r,\theta,\varphi)$

MOMENTU ANGELUARRAREN ERAGILEA MEKANIKA KUANTIKOAN:

Klasikoki: $\vec{L} = \vec{r}\times\vec{p}$, beraz lehenengo saiakera kuantikoki gauza bera izatea izango litzateke. $\hat{\vec{r}} = \vec{r}$, $\hat{\vec{p}} = -i\hbar\vec{\nabla}$; $\hat{\vec{L}} = \hat{\vec{r}}\times\hat{\vec{p}}$

Baina era horretan definitutako eragilea hermitikoa da? Ikus dezagun osagai batean:

$\hat{L}_x = \hat{y}\hat{p}_z - \hat{p}_y\hat{z}$; $\hat{L}_x^+ = (\hat{y}\hat{p}_z)^+ - (\hat{p}_y\hat{z})^+ = \hat{p}_z^+\hat{y}^+ - \hat{z}^+\hat{p}_y^+ = \hat{p}_z\hat{y} - \hat{z}\hat{p}_y =$ trukakorrak direlako

$\hat{y}\hat{p}_z - \hat{p}_y\hat{z}$ $\Rightarrow$ Hermitikoa da.

$\frac{\partial}{\partial z}$-k ez du eragiten y-n

Beraz, $\hat{\vec{L}} = \hat{\vec{r}}\times\hat{\vec{p}}$ izango dugu momentu angeluarraren eragilea mekanika kuantikoan. Hauek dira $\hat{\vec{L}}$-ren osagaiak koordinatu kartesiarretan:

• $\hat L_x = -i\hbar(y\partial_z - z\partial_y)$ • $\hat L_y = -i\hbar(z\partial_x - x\partial_z)$ • $\hat L_z = -i\hbar(x\partial_y - y\partial_x)$

Koordenatu esferikoen funtzioan x, y eta z jarriz:

• $\hat L_x = -i\hbar\left(-\sin\varphi\,\partial_\theta - \frac{\cos\varphi}{tg\theta}\partial\varphi\right)$ • $\hat L_y = -i\hbar\left(\cos\varphi\,\partial_\theta - \frac{\sin\varphi}{tg\theta}\partial\varphi\right)$ • $\hat L_z = -i\hbar\partial\varphi$

Bestetik, $\hat L^2 = \hat L_x^2 + \hat L_y^2 + \hat L_z^2 = -\hbar^2\left(\partial_\theta^2 + \underbrace{\frac{1}{\sin^2\theta}\partial^2\varphi^2 + \frac{1}{tg\theta}\partial\theta}_{\text{bardina}}\right) \Rightarrow$ r-ren independentea

Hortaz, $\hat T = -\frac{\hbar^2}{2m}\underbrace{\nabla^2}_{\text{esferikoetan}} = -\frac{\hbar^2}{2m}\left[\frac{1}{r}\partial_{r^2}^2 r + \frac{1}{r^2}\left(\partial_{\theta^2}^2 + \frac{1}{tg\theta}\partial\theta + \frac{1}{\sin^2\theta}\partial^2\varphi^2\right)\right] = -\frac{\hbar^2}{2m}\left[\frac{1}{r}\partial_{r^2}^2 r - \frac{1}{r^2}\frac{\hat L^2}{\hbar^2}2m\right] =$

$-\frac{\hbar^2}{2m}\cdot\underbrace{\frac{1}{r}\partial_{r^2}^2 r}_{\text{energia zinetikoaren ekarpen erradiala}} + \frac{1}{r^2}\frac{\hat L^2}{2m} \Rightarrow$ Mekanika klasikoko adierazpena

MOMENTU-ANGELUARRAREN TRUKATZE-ERLAZIOAK:

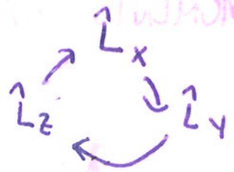
• Momentu-angeluarraren osagai ezberdinen trukatze-erlazioak:

* $[\hat L_x, \hat L_y] = [\hat y\hat p_z - \hat p_y\hat z, \hat z\hat p_x - \hat x\hat p_z] = [\hat y\hat p_z, \hat z\hat p_x] - \cancel{[\hat y\hat p_z, \hat x\hat p_z]}^{0} - \cancel{[\hat p_y\hat z, \hat z\hat p_x]}^{0} +$ (osagai guztiak ezberdinak)

$[\hat p_y\hat z, \hat x\hat p_z] = -i\hbar\hat y\hat p_x + i\hbar\hat p_y\hat x = -i\hbar(\hat y\hat p_x - \hat p_y\hat x) = i\hbar\hat L_z$

• $[\hat y\hat p_z, \hat z\hat p_x] = \hat y[\hat p_z, \hat z\hat p_x] + [\hat y, \hat z\hat p_x]\hat p_z = \hat y\{\hat z\cancel{[\hat p_z, \hat p_x]}^{0} + [\hat p_z, \hat z]\hat p_x\} + \{\hat z\cancel{[\hat y, \hat p_x]}^{0} +$
$\cancel{[\hat y, \hat z]}^{0}\hat p_x\}\hat p_z = -i\hbar\hat y\hat p_x$

• $[\hat p_y\hat z, \hat x\hat p_z] = \ldots = \hat p_y\hat x[\hat z, \hat p_z] = i\hbar\hat p_y\hat x$



* $[\hat L_y, \hat L_z] = i\hbar\hat L_x$ (Modu berean) ; * $[\hat L_z, \hat L_x] = i\hbar\hat L_y$

Beraz, momentu angeluarraren osagaiak zehaztasun osoz ezin izango dira aldi berean neurtu, ez dira trukakorrak ($\hat L_z \neq 0$ bada).

* $[\hat L^2, \hat L_x] = [\hat L_x^2 + \hat L_y^2 + \hat L_z^2, \hat L_x] = [\hat L_y^2, \hat L_x] + [\hat L_z^2, \hat L_x] + \cancel{[\hat L_x^2, \hat L_x]}^{0} =$

$\hat L_y[\hat L_y, \hat L_x] + [\hat L_y, \hat L_x]\hat L_y + \hat L_z[\hat L_z, \hat L_x] + [\hat L_z, \hat L_x]\hat L_z = \hat L_y(-i\hbar\hat L_z) +$

$(-i\hbar\hat L_z)\hat L_y + \hat L_z(i\hbar\hat L_y) + (i\hbar\hat L_y)\hat L_z = \cancel{-i\hbar\hat L_y\hat L_z} \cancel{-i\hbar\hat L_z\hat L_y} \cancel{+i\hbar\hat L_z\hat L_y} \cancel{+i\hbar\hat L_y\hat L_z} =$

0 Trukakorrak dira!

Beraz, aldi berean, zehaztasun osoz neurr ditzakegu osagairen bat ($\hat{L}_y$ eta $\hat{L}_z$-rako ondorio bera lortzen da) eta L-ren modulua. $[\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0$

Aurkitu dezakegu $\hat{L}^2$ eta osagai baten aldiberako autofuntzioen oinarri bat.

$$* \ [\hat{T}, \hat{L}^2] = \left[\frac{\hat{P}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2}, \hat{L}^2\right] = \left[\frac{\hat{P}_r^2}{2m}, \hat{L}^2\right] + \left[\frac{\hat{L}^2}{2mr^2}, \hat{L}^2\right] = 0$$

$\hat{L}^2$ r-ren independentea delako

Trukakorrak! osagaiak r-ren independenteak direlako

Ondorioz $\Rightarrow [\hat{T}, \hat{L}_x] = [\hat{T}, \hat{L}_y] = [\hat{T}, \hat{L}_z] = 0$

$* \ V(r) \to \vec{F} = -\frac{\partial V}{\partial r}\hat{r}$ (indar zentrala) $\Rightarrow$ Mekanika klasikoan $\vec{L} = kte$

Kuantikoan: $[V(r), \hat{L}^2] = 0$, baita $[V(r), \hat{\vec{L}}] = 0$

r-ren independenteak delako

Hortaz, baldin eta $V(r)$ bada, $[\hat{H}, \hat{L}^2] = 0$, baita $[\hat{H}, \hat{\vec{L}}] = 0$

Horrenbestez, ondoriozta dezakegu, $V(r)$ denean $\langle \hat{L}^2 \rangle = kte$ dela, denboran ez dela aldatzen. Gauza bera osagaiekin: $\langle \hat{L}_x \rangle$, $\langle \hat{L}_y \rangle$, $\langle \hat{L}_z \rangle$ kteak

Gainera, $\hat{L}^2$-ren eta $\hat{H}$-ren aldiberako autofuntzioen oinarri bat aurki dezakegu edo $\hat{L}$-ren osagaietariko baten eta $\hat{H}$-ren artekoa. (osagai guztien aldiberakoa ez)

Ondorio guzti hauek, besteak beste, Hidrogeno atomoaren kasuan aplika daitezke.

MOMENTU ANGELUARRAREN AUTOFUNTZIOAK eta AUTOBALIOAK:

$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$ denez, ez dugu aurkituko $\hat{L}$-ren edozein bi osagaien arteko aldiberako autofuntzioen oinarririk. Beraz ezin dugu aurkitu egoerarik non $\vec{L}$ bektorea guztiz zehaztuta dagoen (hau da, $\vec{L}$-ren osagai guztiak).

$[\hat{L}^2, \vec{L}] = 0$ da ordea, beraz aurki dezakegu $\vec{L}$-ren osagai baten eta $\hat{L}^2$-ren aldiberako autofuntzioen oinarri bat.

Beraz, alDibidez, koordenatu esferikoetan $\hat{L}_z$-ren adierazpena sinpleena denez eta

$[\hat{L}^2, \hat{L}_z]=0$ denez, horien aldiberako oinarria topatzen saiatuko gara: $\{\hat{L}^2, \hat{L}_z\}$

1 * $\hat{L}_z \Psi = l_z \Psi$

2 * $\hat{L}^2 \Psi = \lambda \Psi$

$\Rightarrow$ Bi aukera:

- Metodo diferentziala (ekuazio diferentziala ebatzi)
- Metodo aljebraikoa: $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

$\hat{L}_z$ kalkulatuko dugunez $\hat{L}_x^2 + \hat{L}_y^2$-ri dagokiona kalkulatu

$\hat{L}_+ = \hat{L}_x + i\hat{L}_y$ eta $\hat{L}_- = \hat{L}_x - i\hat{L}_y$ definitzeaz lagunduz

(osziladore harmonikoaren estrategiaren antzekoa)

L_z-REN AUTOFUNTZIOAK eta AUTOBALIOAK:

Gogoratu $\hat{L}^2$ eta $\hat{L}_z$ r-ren independenteak direla, beraz, koordenatu esferikoetan $\Psi(r,\theta,\varphi)$-k

r-rekiko edozein menpekotasun izango du $\Rightarrow$ $\Psi(r,\theta,\varphi) = f(r)\, Y(\theta,\varphi)$

Beraz, $f(r)$ edozein izan daitekeenez gelan arduratuko gaituena $Y(\theta,\varphi)$ izango da,

eta bi angelu horien menpekotasuna aztertzen zentratuko gara.

horren ze θ-ren menpekotasuna edozein izango da

$\hat{L}_z \cdot \Psi = l_z \Psi$; $\hat{L}_z Y(\theta,\varphi) = l_z Y(\theta,\varphi) \leftrightarrow -i\hbar\partial_\varphi Y(\theta,\varphi) = l_z Y(\theta,\varphi)$

φ-rekiko menpekotasuna aztertu soilik

$$\frac{dY}{d\varphi} = \frac{il_z}{\hbar} Y \leftrightarrow \frac{dY}{Y} = +\frac{il_z}{\hbar} d\varphi \leftrightarrow \ln Y = \frac{il_z}{\hbar} d\varphi + C(\theta) \rightarrow$$

$Y(\theta,\varphi) = F(\theta)\, e^{i\frac{l_z}{\hbar}\varphi}$ $\Rightarrow$ Periodikoa izan behar du: $Y(\theta,\varphi) = Y(\theta, \varphi + 2\pi)$;

$$F(\theta)\, e^{i\frac{l_z}{\hbar}\varphi} = F(\theta)\, e^{i\frac{l_z}{\hbar}(\varphi+2\pi)} \Rightarrow e^{i\frac{l_z}{\hbar}\cdot 2\pi} = 1 \leftrightarrow \frac{l_z}{\hbar}\cdot 2\pi = m\cdot 2\pi \quad m \in \mathbb{Z}$$

Hortaz, $l_z = \hbar m$ (ezin da edozein izan) $m \in \mathbb{Z}$

Orduan $\Rightarrow$ $\Psi(r,\theta,\varphi) = f(r)\, F(\theta)\, e^{im\varphi}$

* Geroago ikusiko dugu zein den $F(\theta)$ $\hat{L}^2$-ren autofuntzioa izateko ere.

$\hat{L}^2$ eta $\hat{L}_z$-ren ALDIBEREKO AUTOFUNTZIOAK (METODO DIFERENTZIALA)

$\hat{L}_z$-renak kalkulatu ditugu, beraz $\hat{L}^2$-renak aztertzea baino ez zaigu falta:

r-ren independentzia

$$\hat{L}_z \Psi = l_z \Psi \; ; \; \hat{L}_z Y(\theta,\varphi) = l_z Y(\theta,\varphi) \implies \hat{L}^2 Y_\lambda^m(\theta,\varphi) = \underset{\hbar^2 \tilde{\lambda}}{\lambda} Y_\lambda^m(\theta,\varphi)$$

(izen berria)

L_z-ren autofuntzioak izan behar direnez, φ-ren menpekotasuna ezagutzen dugu $\Rightarrow$

$e^{im\varphi}$. Beraz $\Rightarrow Y_\lambda^m(\theta,\varphi) = e^{im\varphi} F_\lambda^m(\theta)$

Koordenatu esferikoetan: $\hat{L}^2 = -\hbar^2 \left(\partial^2_{\theta^2} + \frac{1}{\sin^2\theta}\partial^2_{\varphi^2} + \frac{1}{\operatorname{tg}\theta}\partial_\theta\right) \implies \hat{L}^2 Y_\lambda^m(\theta,\varphi) = \lambda Y_\lambda^m(\theta,\varphi)$

$$-\cancel{\hbar^2}\left(\cancel{e^{im\varphi}}\frac{d^2F_\lambda^m}{d\theta^2} - \frac{m^2F_\lambda^m \cancel{e^{im\varphi}}}{\sin^2\theta} + \frac{1}{\operatorname{tg}\theta}\cancel{e^{im\varphi}}\frac{dF_\lambda^m}{d\theta}\right) = \lambda \cancel{e^{im\varphi}} F_\lambda^m(\theta) = \cancel{\hbar^2}\tilde{\lambda}\cancel{e^{im\varphi}} F_\lambda^m(\theta)$$

Aldagai aldaketa: $x = \cos\theta$, $dx = -\sin\theta \cdot d\theta$, $y = F_\lambda^m$

$$(1-x^2)y'' - 2xy' + \left(\tilde{\lambda} - \frac{m^2}{1-x^2}\right)y = 0$$ Legendreren ekuazio elkartua

Bi zatitan aztertu, $m=0$ (→ l_z-ren menpekoa ($l_z = \hbar m$)) deneko kasua (Legendreren ekuazioa $\Rightarrow$ soluzioak Legendreren polinomioak) eta $m \neq 0$ denekoa (soluzioa $\Rightarrow$ Legendreren polinomio elkartuak)

LEGENDREREN EKUAZIOA eta LEGENDREREN POLINOMIOAK:

$$(1-x^2)y'' - 2xy' + \left(\tilde{\lambda} - \frac{m^2}{1-x^2}\right)y = 0$$ Legendreren ekuazio elkartua

Kasu partikularra: $m=0 \Rightarrow$ Legendreren ekuazioa $\Rightarrow (1-x^2)y'' - 2xy' + \tilde{\lambda}y = 0$

Polinomioen metodoa: $y = \sum_{n=0}^\infty c_n x^n \; ; \; y' = \sum_{n=1}^\infty n c_n x^{n-1} \; ; \; y'' = \sum_{n=2}^\infty n(n-1)c_n x^{n-2}$

indizeak berrindatu

$$(1-x^2)\sum_{n=2}^\infty n(n-1)c_n x^{n-2} - 2x\sum_{n=1}^\infty n c_n x^{n-1} + \tilde{\lambda}\sum_{n=0}^\infty c_n x^n = \sum_{n=0}^\infty \left[c_{n+2}(n+2)(n+1) - c_n(n-1)n + \right.$$

$$\left. -2c_n n + \tilde{\lambda}c_n\right]x^n = 0 \iff c_{n+2}(n+2)(n+1) - c_n n(n-1) + \tilde{\lambda}c_n - 2nc_n = 0 \iff$$

- $c_{n+2} = \dfrac{n(n+1)-\tilde{\lambda}}{(n+1)(n+2)} c_n$; c_0 eta c_1 finkatuz beste guztiak kalkula daitezke

(c_0-rekin bikoitiak eta c_1-ekin bakoitiak $\Rightarrow$ zehaztugabeko 2 konstante ; 2. ordenako ekuazio diferentziala)

- Seriea zein neurritan konbergentea den aztertzeko $n \to \infty$ limitea aztertuko dugu:

$n \gg$ $\quad c_{n+2} = \dfrac{n}{n+2} c_n \simeq c_n$ Ez dira txikitzen, konstante mantendu $\Rightarrow$ Dibergentea!

Beraz, dibergentea denez ez da fisikoki esanguratsuak izango $\Rightarrow$ Y bornatua izan behar da, orduan koefiziente horietako bat nulua izan behar da: $\tilde{\lambda} = l(l+1)$

$l \in \mathbb{N}$

Beraz $n = l$ horretarako $c_{n+2} = 0$ eta hortik aurrera guztientzat.

koefiziente bakoitiak geratu bakarrik

Bi aukera:

- $l =$ bakoitia $\Rightarrow$ $c_{l+2} = 0$ eta gainontzeko koefiziente bakoitiak ere, baina bikoitiak ez. Beraz, bornatua izateko $c_0 = 0$ izan behar da. $Y(x) = -Y(-x)$

- $l =$ bikoitia $\Rightarrow$ $c_{l+2} = 0$ eta gainontzeko koefiziente bikoitiak ere, baina bakoitiak ez. Beraz, Y bornatua izateko $c_1 = 0$ izan behar da. $Y(x) = Y(-x)$

- Soluzioak: Legendreren polinomioak $\Rightarrow P_l(x)$

Ad: $P_0 = 1$, $P_1 = x$, $P_2 = \frac{1}{2}(3x^2-1)$ ...

Rodrigues-en formula:

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2-1)^l$$

aurreko bi jakinda bestea lor daiteke

Errepikapen erlazioa:

$$(l+1) P_{l+1} = (2l+1) x P_l - l P_{l-1}$$

- $\tilde{\lambda}$ diskretua $\Rightarrow \tilde{\lambda} = l(l+1) \Leftrightarrow \lambda = \hbar^2 \tilde{\lambda} = \hbar^2 l(l+1)$

$\hat{L}^2$-ren autobalioak diskretuak dira

$\hbar^2 l(l+1)$ $\quad l \in \mathbb{N}$

ez da betetzen baina egia diskretua dela

(Bohr-en hipotesian L kuantizatuta zegoela iruditzen zen $\Rightarrow L = \hbar n$)

LEGENDREREN EKUAZIO ELKARTUA: $(1-x^2) Y'' - 2xY' + (\tilde{\lambda} - \frac{m^2}{1-x^2}) Y = 0$

Ez dugu ekuazioa zehaztasunez ebatziko zuzenean aztertuko dugu lortzen diren soluzioak.

Legendreren polinomio elkartuak: $\tilde{\lambda} = l(l+1)$ $\quad l \in \mathbb{N}$ orokorra da kasu guztietarako, m-ren independentea da. m l_z $\hat{L}_z$-ren autobalioarekin lotuta dago ($l_z = m\hbar$);

$l \geq |m|$ izan behar da, $m \in \mathbb{Z}$. Legendreren polinomio elkartuak:

Legendreren polinomioak

$m \geq 0$ $\begin{cases} * \; P_l^m(x) = (-1)^m (1-x^2)^{m/2} \dfrac{d^m}{dx^m}(P_l(x)) & \Rightarrow \text{Rodrigues-en formula} \Rightarrow \\ * \; P_l^m(x) = \dfrac{(-1)^m}{2^l \cdot l!} (1-x^2)^{m/2} \dfrac{d^{l+m}}{dx^{l+m}} (x^2-1) \end{cases}$

$m < 0$ * $P_l^{-m}(x) = (-1)^m \dfrac{(l-m)!}{(l+m)!} P_l^m(x)$ $\left(\text{Ad. } P_2^{-1} = (-1) \dfrac{(2-1)!}{3!} P_2^1\right)$

Beraz, hau ezaguta $Y(\theta,\varphi)$, $\hat{L}^2$ eta L_z-ren autofuntzioak ezagutzen ditugu $\Rightarrow$

Harmoniko esferikoak.

HARMONIKO ESFERIKOAK:

l_z-ren zenbaki kuantikoa $\rightarrow$ $\hat{L}_z$-ren autobalioak $\rightarrow l_z = m\hbar$ $m \in \mathbb{Z}$; $(l \geq |m|)$

- $Y_l^m(\theta,\varphi) \Rightarrow$ $\hat{L}_z$ eta $\hat{L}^2$-ren autofuntzioak $\Rightarrow$ Harmoniko esferikoak

zenbaki kuantikoa $\rightarrow$ $\hat{L}^2$-ren autobalioak $\hbar^2 l(l+1)$ $l \in \mathbb{N}$

- $Y_l^m(\theta,\varphi) = P_l^m(\cos\theta)\, e^{im\varphi} \cdot \left[\dfrac{2l+1}{4\pi} \dfrac{(l-m)!}{(l+m)!}\right]^{1/2}$

Normalizazio ktea

Legendreren polinomio elkartuak

$\hat{L}_z$ autofuntzioen eskema

Oinarri ortonormala!

$(Y_{l_1}^{m_1}, Y_{l_2}^{m_2}) = \delta_{l_1,l_2}\delta_{m_1,m_2}$

* $(Y_{l_1}^{m_1}, Y_{l_2}^{m_2}) = \int_0^\pi \int_0^{2\pi} (Y_{l_1}^{m_1})^* \, Y_{l_2}^{m_2} \sin\theta \, d\theta \, d\varphi = \delta_{l_1 l_2}\delta_{m_1,m_2}$

r-rekiko menpekotasuna falta delako $\Rightarrow$ angeluarreko integrala soilik.

Ad: $\int_0^\pi P_{l_1}^m(\cos\theta) P_{l_2}^m(\cos\theta) \sin\theta \, d\theta = \dfrac{2}{(2l_1+1)} \dfrac{(l_1+m)!}{(l_1-m)!} \delta_{l_1,l_2}$

- Adibideak: (Gogoratu $l \geq |m|$) $\Rightarrow$ $l=0, m=0 \Leftrightarrow Y_0^0 = \sqrt{\frac{1}{4\pi}}$

$l=1, m=0 \Leftrightarrow Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$; $l=1, m=\pm1 \Leftrightarrow Y_1^{\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\varphi}$

$l=2, m=0 \Leftrightarrow Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$; $l=2, m=\pm1 \Leftrightarrow Y_2^{\pm1} = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\varphi}$

$l=2, m=\pm2 \Leftrightarrow Y_2^{\pm2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\varphi}$ ...

HARMONIKO ESFERIKOEN PROPIETATE BATZUK:

1.) Simetria: simetrikoak edo antisimetrikoak dira (bai $\vec{L}$ eta $\vec{L}^2$ inbertsio eragilearekin trukakorrak dira $\Rightarrow [\hat{I}, \vec{L}] = 0$; aurkitu ditzakegu $\hat{I}$ eta $\hat{L}_z, \hat{L}_x, \hat{L}_y$ eta $\vec{L}^2$-ren aldiberako autofuntzioak (simetrikoak eta antisimetrikoak))

-$\vec{r}$-n ebaluatu — normalizazio utea

- $\hat{I} Y_l^m(\theta,\varphi) = Y_l^m(\pi-\theta, \pi+\varphi) = A_l^m P_l^m(\cos(\pi-\theta)) e^{im(\pi+\varphi)} = A_l^m P_l^m(-\cos\theta) e^{im(\pi+\varphi)} =$

(-$\vec{r}$-ri dagozkion angeluak $\Rightarrow \theta \Rightarrow \pi-\theta, \quad \varphi \Rightarrow \varphi+\pi$ ) $(-1)^m A_l^m (-1)^{l+m} P_l^m(\cos\theta) e^{im\varphi} =$

$(-1)^l P_l^m(\cos\theta) e^{im\varphi}$

$*$ l bakoitia $\Rightarrow Y_l^m$ bakoitia

$*$ l bikoitia $\Rightarrow Y_l^m$ bikoitia

2.) Itxidura - erlazioa: $\sum_{l,m} Y_l^m(\theta,\varphi) Y_l^m(\theta',\varphi') = \delta(\cos\theta - \cos\theta')\,\delta(\varphi-\varphi')$ $\Rightarrow$ edozein funtzio harmoniko esferikoen konbinazio lineal moduan jar daiteke

3.) Erlazio erabilgarriak: $x = r\sin\theta\cos\varphi$; $y = r\sin\theta\sin\varphi$; $z = r\cos\theta$

$*$ $x = r\sqrt{\frac{2\pi}{3}}(Y_1^{-1} - Y_1^{1})$ $\quad$ $*$ $y = ri\sqrt{\frac{2\pi}{3}}(Y_1^{-1} + Y_1^{1})$ $\quad$ $*$ $z = r\sqrt{\frac{4\pi}{3}}\, Y_1^{0}$

4.) Konplexu konjokatua: $\left(Y_l^m(\theta,\varphi)\right)^* = (-1)^m Y_l^{-m}(\theta,\varphi)$

HARMONIKO ESFERIKOEN ADIERAZPEN GRAFIKOA:

- $Y_l^m(\theta,\varphi) = \left[\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta)\, e^{im\varphi}$

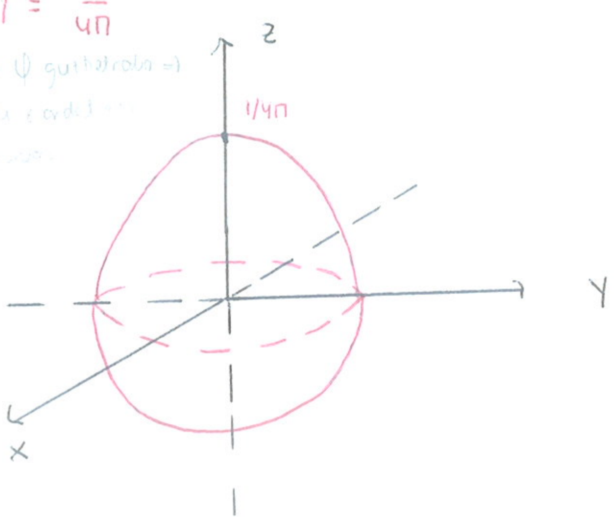
- Harmoniko esferikoa $\Rightarrow$ konplexua $\Rightarrow$ zaila irudikatzeko $\Rightarrow \|\Psi_l^m(\theta,\varphi)\|^2$ irudikatu

$$|\Psi_l^m(\theta,\varphi)|^2 = \frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}\left(P_l^m(\cos\theta)\right)^2$$

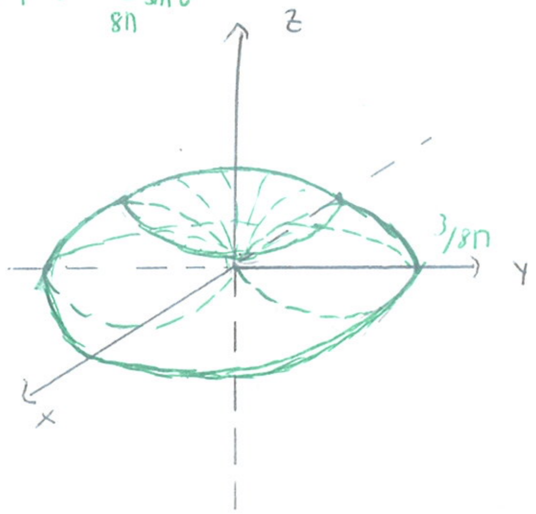
Koordenatu esferikoak erabili irudikatzeko $\Rightarrow |\vec{r}| = (Y_l^m(\theta,\varphi))^2$ hartu

- $(Y_0^0)^2 = \frac{1}{4\pi}$

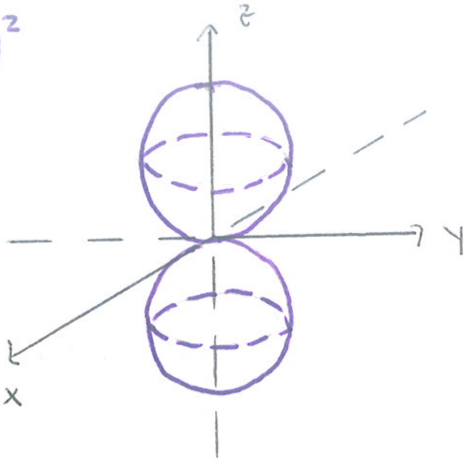
Berdina φ guztietarako ⇒



- $(Y_1^{-1})^2 = \frac{3}{8\pi}\sin^2\theta$



- $(Y_1^0)^2$



L_+ eta L_- ERAGILEAK:

$\{\hat{L}^2, \hat{L}_z\}$-ren autofuntzioak $\{Y_\lambda^m(\theta,\varphi)\}$ ⇒ $Y_\lambda^m(\theta,\varphi) = F_\lambda^m(\theta)\, e^{im\varphi}$ ⇒

m: $\hat{L}_z$-rekin lotuta; λ: $\hat{L}^2$-rekin lotuta; $F_\lambda^m(\theta)$: $\hat{L}^2$-ren autofuntzioa izateko bete behar den funtzioa; $e^{im\varphi}$: L_z-ren autof.

- $\hat{L}_z Y_\lambda^m = m\hbar\, Y_\lambda^m \quad m \in \mathbb{Z}$ (autobalioak)

- $\hat{L}^2 Y_\lambda^m = \lambda Y_\lambda^m$ ⇒ zeintzuk dira λ eta $F_\lambda^m(\theta)$?

Beste modu batean kalkulatu, ekuazio diferentziala ebatzi gabe ⇒ beste eragile batzuk definitu: $\hat{L}^2 = \underbrace{\hat{L}_x^2 + \hat{L}_y^2}_{\text{ekarpen hauen edozein}} + \hat{L}_z^2$ → honen autofuntzioak baditugu

λ bada $\hat{L}^2$-ren autobalioa $L_x^2 + L_y^2 \geq 0$ denez λ $\hat{L}_z^2$-ren ekarpena baino handiagoa izan behar da: $\lambda \geq m^2\hbar^2$

Bi eragile berri definitu: $\hat{L}_+ = \hat{L}_x + i\hat{L}_y$ (ez da hermitikoa) eta

$$\hat{L}_- = \hat{L}_+^{\dagger} = L_x - i\hat{L}_y \qquad \begin{cases} \hat{L}_x = \dfrac{\hat{L}_+ + \hat{L}_-}{2} \\ \hat{L}_y = \dfrac{\hat{L}_+ - \hat{L}_-}{2i} \end{cases} \qquad [\hat{L}_+, \hat{L}_-] = -i[\hat{L}_x, \hat{L}_y] + i[\hat{L}_y, \hat{L}_x] = 2\hbar \hat{L}_z$$

∘ Trukatze erlazioak:

$$* \; [\hat{L}^2, \hat{L}_\pm] = [\hat{L}^2, \hat{L}_x]^{0} \pm i [\hat{L}^2, \hat{L}_y]^{0} = 0 \Rightarrow$$ aldiberako autofuntzioak izan daitezke

$$* \; [\hat{L}_z, \hat{L}_\pm] = [\hat{L}_z, \hat{L}_x \pm i\hat{L}_y] = [\hat{L}_z, \hat{L}_x] \pm i [\hat{L}_z, \hat{L}_y] = i\hbar \hat{L}_y \pm i(-i\hbar \hat{L}_x) =$$

$$\hbar(i\hat{L}_y \pm \hat{L}_x) = \pm\hbar(\hat{L}_x \pm i\hat{L}_y) = \pm\hbar\hat{L}_\pm$$ (ez dira trukakorrak ⇒ ez dugu aldiberako autofuntzioak aurkituko)

∘ $\hat{L}^2$ eta $\hat{L}_\pm$-ren aldiberako autofuntzioak aurki daitezkenez, $\hat{L}_\pm Y_\lambda^m$?

$*$ $\hat{L}^2(\hat{L}_+ Y_\lambda^m)$ kalkulatuko dugu honetarako ⇒ trukakorrak direnez $\hat{L}^2 \hat{L}_+ = \hat{L}_+ \hat{L}^2$ ⇒

$$\hat{L}_+(\hat{L}^2 Y_\lambda^m) = \hat{L}^2(\hat{L}_+ Y_\lambda^m) = \hat{L}_+(\lambda Y_\lambda^m) = \lambda \hat{L}_+ Y_\lambda^m \Leftrightarrow \hat{L}_+ Y_\lambda^m \quad \hat{L}^2\text{-ren}$$

edozein m ⇒ λ berdina baina m ez dakigu

autofuntzioa da ⇒ $Y_\lambda^{m'}$-ren proportzionala izan beharko da: $\hat{L}_+ Y_\lambda^m \propto Y_\lambda^{m'}$

↳ Bestez $\sum\limits_m C_m Y_\lambda^m$ (endekatua dalako m-n)

$$* \; \hat{L}_z(\hat{L}_+ Y_\lambda^m) = \hat{L}_z \hat{L}_+ Y_\lambda^m = (\hbar\hat{L}_+ + \hat{L}_+\hat{L}_z) Y_\lambda^m = \hat{L}_+ \hat{L}_z Y_\lambda^m + \hbar \hat{L}_+ Y_\lambda^m =$$

$$\hat{L}_+ m\hbar Y_\lambda^m + \hbar \hat{L}_+ Y_\lambda^m = (m\hbar + \hbar)\hat{L}_+ Y_\lambda^m = \hbar(m+1)\hat{L}_+ Y_\lambda^m \Leftrightarrow \hat{L}_+ Y_\lambda^m$$

$\hat{L}_z$-ren autofuntzio bat da, baina autobalioa $(m+1)\hbar$ da ⇔

λ edozein izan daiteke printzipioz, $\hat{L}_+ Y_\lambda^m \propto Y_{\lambda'}^{m+1}$

Bi ondorioak batuz, badakigu λ konstante mantenduko dela eta m bakarrik

igoko da: $\hat{L}_+ Y_\lambda^m \propto Y_\lambda^{m+1} \Leftrightarrow \boxed{\hat{L}_+ Y_\lambda^m = A_\lambda^m Y_\lambda^{m+1}}$

$*$ $\hat{L}_-$-ekin ondorio bera ⇒ $\hat{L}_- Y_\lambda^m \propto Y_\lambda^{m-1} \Leftrightarrow \boxed{\hat{L}_- Y_\lambda^m = A'^m_\lambda Y_\lambda^{m-1}}$

Halaber, badakigu $\lambda \geq m^2\hbar^2$ izan behar dela. Beraz, $\hat{L}_+ Y_\lambda^m = A_\lambda^m Y_\lambda^{m+1}$

egiteraluon limite bat izango dugu, m maximo bat egongo baita. Orduan.

m_{max} duen uhin-funtzioa aplikatzerakoan $\boxed{\hat{L}_+ Y_\lambda^{m_{max}} = 0}$ izan behar da.

Bestalde, m-k balio minimo bat izango du ere. Ondorioz,

m_{min} duen uhin-funtzioari $\hat{L}_-$ aplikatzerakoan $\boxed{\hat{L}_- Y_\lambda^{m_{min}} = 0}$ izan behar da.

$\hat{L}^2$-ren AUTOBALIOAK L_+ eta L_- ERAGILEAK ERABILIZ:

$\{Y_\lambda^m\}$ autofuntzioak ditugu. Badakigu $m \in \mathbb{Z}$ dela baina λ? Hauxe

izango da gure helburua, L_+ eta L_- eragileen laguntzaz.

* Badakigu $L_+ Y_\lambda^{m_{max}} = 0$ dela eta $L_- Y_\lambda^{m_{min}} = 0$.

m_{max} eta m_{min} hartuko ditugu:

- $\hat{L}^2 Y_\lambda^{m_{max}} = \lambda Y_\lambda^{m_{max}}$; $\hat{L}^2 Y_\lambda^{m_{max}} = (\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2) Y_\lambda^{m_{max}} =$

$\left(\left(\frac{\hat{L}_+ + \hat{L}_-}{2}\right)^2 + \left(\frac{\hat{L}_+ - \hat{L}_-}{2i}\right)^2 + \hat{L}_z^2 \right) Y_\lambda^{m_{max}} = \left(\frac{1}{2}\left(\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+ \right) + \hat{L}_z^2 \right) Y_\lambda^{m_{max}} \overset{*'}{=}$

$\left(*' \; [\hat{L}_+, \hat{L}_-] = \hat{L}_+\hat{L}_- - \hat{L}_-\hat{L}_+ = 2\hbar \hat{L}_z \right)$ $\quad \left[\frac{1}{2}\left(2\hat{L}_-\hat{L}_+ + 2\hbar\hat{L}_z \right) + \hat{L}_z^2 \right] Y_\lambda^{m_{max}} =$

$\left[\hat{L}_-\hat{L}_+ + \hbar \hat{L}_z + \hat{L}_z^2 \right] Y_\lambda^{m_{max}} = \hbar\, m_{max} \hbar\, Y_\lambda^{m_{max}} + \hbar^2 m_{max}^2 Y_\lambda^{m_{max}} =$

$\hbar^2 m_{max}(1 + m_{max}) Y_\lambda^{m_{max}} = \lambda Y_\lambda^{m_{max}} \longleftrightarrow \lambda = \hbar^2 m_{max}(1 + m_{max}) \quad m_{max} \in \mathbb{Z}$

- $\hat{L}^2 Y_\lambda^{m_{min}} = \lambda Y_\lambda^{m_{min}}$; $\hat{L}^2 Y_\lambda^{m_{min}} = \left[\hat{L}_+\hat{L}_- - \hbar \hat{L}_z + \hat{L}_z^2 \right] Y_\lambda^{m_{min}} =$

$- \hbar \hat{L}_z Y_\lambda^{m_{min}} + \hat{L}_z^2 Y_\lambda^{m_{min}} = (-\hbar \cdot \hbar m_{min} + \hbar^2 m_{min}^2) Y_\lambda^{m_{min}} = \hbar^2 m_{min}(m_{min} - 1) Y_\lambda^{m_{min}}$

$\longleftrightarrow \lambda = \hbar^2 m_{min}(m_{min} - 1) \quad m_{min} \in \mathbb{Z}$

- $\hbar^2 m_{min}(m_{min} - 1) = \hbar^2 m_{max}(1 + m_{max}) \longleftrightarrow m_{max} = -m_{min} = l$

Beraz, $\lambda = \hbar^2 l(1+l) = -l(-l-1)\hbar^2$ izango da, non $l \in \mathbb{N}$ den ($m_{max} \in \mathbb{Z}$ eta ≥ 0 delako) Balio diskretuak!

$\hat{L}^2$-ren AUTOFUNTZIOAK (HARMONIKO ESFERIKOAK) L_+ eta L_- ERAGILEAK ERABILIZ:

- $\{Y_\lambda^m\} \Rightarrow$ autofuntzioen oinarria ; $m \in \mathbb{Z}$ eta $\lambda = \hbar^2 l(l+1)$ $l \in \mathbb{N}$ $\Rightarrow$

  Zenbaki kuantikoak l eta m izango dira $\Rightarrow \{Y_l^m\}$ $|m| \leq l$

- Y_l^m-ren adierazpena kalkulatuko dugu ekuazio diferentziala ebatzi gabe, L_+ eta L_- eragileekin:

$$\begin{cases} \hat{L}_+ Y_l^l = 0 \\ \hat{L}_- Y_l^{-l} = 0 \end{cases} \qquad Y_l^l\,?$$

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y \underset{\text{esferikoetan}}{=} -i\hbar\left(-\sin\varphi\, \partial_\theta - \frac{\cos\varphi}{\mathrm{tg}\theta}\partial_\varphi\right) \pm \hbar\left(\cos\varphi\, \partial_\theta - \frac{\sin\varphi}{\mathrm{tg}\theta}\partial_\varphi\right) =$$

$$\hbar e^{\pm i\varphi}\left[\pm\partial_\theta + i\,\mathrm{cotg}\theta\, \partial_\varphi\right]$$

$*$ $\hat{L}_+ Y_l^l = 0 \iff Y_l^l(\theta,\varphi) = F_l^l(\theta) e^{il\varphi} \iff \hat{L}_+ F_l^l(\theta) e^{il\varphi} = \hbar e^{i\varphi}[\partial_\theta + i\,\mathrm{cotg}\theta\, \partial_\varphi]\cdot$

$$F_l^l(\theta)e^{il\varphi} = \cancel{\hbar e^{i\varphi}}\cdot \cancel{e^{il\varphi}} \frac{dF_l^l}{d\theta} + \cancel{\hbar e^{i\varphi}} \cdot F_l^l(\theta)\, i\, \mathrm{cotg}\theta\, il\, \cancel{e^{il\varphi}} = 0 \iff$$

$$\frac{dF_l^l}{d\theta} - l\,\mathrm{cotg}\theta\, F_l^l = 0 \iff \frac{dF_l^l}{F_l^l} = l\,\mathrm{cotg}\theta\, d\theta \Rightarrow \ln F_l^l = l \ln \sin\theta + K$$

$$\ln F_l^l = \ln(\sin^l\theta \cdot C) \iff F_l^l(\theta) = C\cdot \sin^l\theta$$

m max duen harmoniko esferikoaren adierazpena

Beraz, $Y_l^l(\theta,\varphi) = C\cdot \sin^l\theta\, e^{il\varphi}$

$*$ $\hat{L}_- Y_l^m \propto Y_l^{m-1} \Rightarrow$ hau aplikatuz Y_l^{l-1} lortu: $\hat{L}_- Y_l^l = \underset{\text{normalizatu}}{C}\, Y_l^{l-1}$

eta horrela jarraituz gainerantzekoak (gogoratu $|m| \leq l$)

normalizazio ktea

$$C Y_l^m = \underbrace{\hat{L}_- \hat{L}_- \ldots}_{l-m} Y_l^l \quad \text{edozein } Y_l^m \text{ kalkulatzeko}$$

L_+ eta L_- ERAGILEAK HARMONIKO ESFERIKOEN GAINEAN:

$\hat{L}^2$ eta $\hat{L}_z$-ren autofuntzioak: $\{Y_\ell^m\}$ $(\lambda = \hbar^2 \ell(\ell+1)$ $\ell \in \mathbb{N}$, $l_z = m\hbar$ $m \in \mathbb{Z})$

- $\hat{L}_+ Y_\ell^m = A_\ell^m Y_\ell^{m+1}$
- $\hat{L}_- Y_\ell^m = B_\ell^m Y_\ell^{m-1}$ $\Rightarrow A_\ell^m, B_\ell^m$?

$\Rightarrow A_\ell^m$: $(\hat{L}_+ Y_\ell^m, \hat{L}_+ Y_\ell^m) = |A_\ell^m|^2 = (Y_\ell^m, \hat{L}_- \hat{L}_+ Y_\ell^m) \overset{\hat{L}_-\hat{L}_+ = \hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z}{=} (Y_\ell^m, \hat{L}^2 Y_\ell^m) +$

$- (Y_\ell^m, \hat{L}_z^2 Y_\ell^m) - \hbar (Y_\ell^m, \hat{L}_z Y_\ell^m) = (Y_\ell^m, \hbar^2 \ell(\ell+1) Y_\ell^m) - (Y_\ell^m, m^2\hbar^2 Y_\ell^m) +$

$- \hbar (Y_\ell^m, m\hbar Y_\ell^m) = \hbar^2 \ell(\ell+1) - m^2\hbar^2 - m\hbar^2 = \hbar^2(\ell(\ell+1) - m(m+1))$

- $|A_\ell^m| = \hbar\sqrt{\ell(\ell+1) - m(m+1)}$ $\Rightarrow A_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m+1)}\, e^{i\alpha}$ $\alpha \in \mathbb{R}$

α edozein izan daiteke (esanahi fisikoa ez da aldatzen) $\Rightarrow \alpha = 0$ hartu

$$A_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m+1)}$$

$\Rightarrow B_\ell^m$: $(\hat{L}_- Y_\ell^m, \hat{L}_- Y_\ell^m) = |B_\ell^m|^2 = (Y_\ell^m, \hat{L}_+ \hat{L}_- Y_\ell^m) \overset{\hat{L}_+\hat{L}_- = \hat{L}^2 - \hat{L}_z^2 + \hbar \hat{L}_z}{=} (Y_\ell^m, \hat{L}^2 Y_\ell^m) +$

$- (Y_\ell^m, \hat{L}_z^2 Y_\ell^m) + \hbar (Y_\ell^m, \hat{L}_z Y_\ell^m) = (Y_\ell^m, \hbar^2 \ell(\ell+1) Y_\ell^m) - (Y_\ell^m, m^2\hbar^2 Y_\ell^m) +$

$\hbar^2 (Y_\ell^m, m\hbar Y_\ell^m) = \hbar^2(\ell(\ell+1) - m(m-1))$

- $|B_\ell^m| = \hbar\sqrt{\ell(\ell+1) - m(m-1)}$ $\Rightarrow B_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m-1)}\, e^{i\alpha}$ $\alpha \in \mathbb{R}$

$\alpha = 0$ aukeratu: $B_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m-1)}$

Beraz, $\hat{L}_\pm Y_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}\, Y_\ell^{m\pm 1}$

L_+ eta L_- ERAGILEEN APLIKAZIO BATZUK:

Oso eragile erabilgarriak zenbait kalkulu egiteko. Adibidez:

- $\psi = Y_1^0 + Y_1^1$ uhin-funtzioa $\Rightarrow \langle \hat{L}_x \rangle_\psi$? Bi aukera, zuzenean egin (espezifikoetan) edo L_+ eta L_- erabili

Normalizatu lehenengo: $\psi = \frac{1}{\sqrt{2}} (Y_1^0 + Y_1^1)$

$* \ (\psi, \psi) = (Y_1^0 + Y_1^1, Y_1^0 + Y_1^1) = 2$

$\hat{L}_+$ eta $\hat{L}_-$ erabiliz: $\hat{L}_x = \frac{\hat{L}_+ + \hat{L}_-}{2}$

$$* \ (\psi, \hat{L}_x \psi) = \frac{1}{2} (\psi, \hat{L}_+ \psi) + \frac{1}{2} (\psi, \hat{L}_- \psi) = \frac{1}{4} \Big[(Y_1^0 + Y_1^1, \hat{L}_+ (Y_1^0 + Y_1^1)) +$$

$$(Y_1^0 + Y_1^1, \hat{L}_- (Y_1^0 + Y_1^1)) \Big] = \frac{1}{4} \Big[\underbrace{(Y_1^0 + Y_1^1, \hbar\sqrt{2}\, Y_1^1 + 0)}_{\hbar\sqrt{2}} + (Y_1^0 + \cancel{Y_1^1 \hbar\sqrt{2}\, Y_1^{-1}}) +$$

$$\underbrace{(Y_1^0 + Y_1^1, \sqrt{2}\hbar\, Y_1^0)}_{\sqrt{2}\hbar} \Big] = \frac{1}{4} \cdot 2\sqrt{2}\,\hbar = \frac{\hbar}{\sqrt{2}}$$

- Adierazpen matriziala: Matrizeen dimentsioa infinitua da (infinitu autofuntzio) $\Rightarrow$

$$\hat{L}_x \Rightarrow (Y_l^m, \hat{L}_x Y_{l'}^{m'}) = \frac{1}{2} (Y_l^m, (\hat{L}_+ + \hat{L}_-) Y_{l'}^{m'})$$

Blokeka: $L_x = $

$$\begin{pmatrix} \begin{smallmatrix} l=0 \\ 1\times1 \end{smallmatrix} & & & 0 \\ & \begin{smallmatrix} l=1 \\ 3\times3 \end{smallmatrix} & & \\ & & \begin{smallmatrix} l=2 \\ 5\times5 \end{smallmatrix} & \\ 0 & & & \ddots \end{pmatrix}$$

$m = -l, \dots, 0, \dots, l$

Blokeka har daiteke. Ad: $l = 1 \Rightarrow \{Y_1^1, Y_1^0, Y_1^{-1}\}$ izango litzateke oinarria:

$(\hat{L}_x)_{11} = (Y_1^1, \hat{L}_x Y_1^1) = 0$, $(\hat{L}_x)_{12} = (Y_1^1, \hat{L}_x Y_1^0) = \frac{1}{2}(Y_1^1, \hat{L}_+ Y_1^0) = \frac{\hbar}{\sqrt{2}}$

✓ diagonaleko 0

$(\hat{L}_x)_{13} = (Y_1^1, \hat{L}_x Y_1^{-1}) = 0$, ...

$$\begin{pmatrix} 0 & \frac{\hbar}{\sqrt{2}} & 0 \\ \frac{\hbar}{\sqrt{2}} & 0 & \cdot \\ 0 & \cdot & 0 \end{pmatrix} = \hat{L}_x$$

Hemendik kalkulatu autofuntzioak, autobalioak.

POTENTZIAL ZENTRALPEKO PARTIKULAREN SCHRÖDINGER-EN EKUAZIOAREN EBAZPENA:

Potentzial zentrala $\Leftrightarrow V = V(r) \Rightarrow \{\hat{H}, \hat{L}_z, \hat{L}^2\}$ trukakorrak dira.

Hiruren aldiberako autofuntzioak aurkitu daitezke:

$\hat{L}^2$ eta $\hat{L}_z$-renak: $Y_l^m(\theta,\varphi)$ — $\hat{H}$-k zehazten du autofuntzioen r-rekiko menpekotasuna

$\hat{H}$-renak: $\Psi_{n,l,m}(r,\theta,\varphi) = R_{n,l,m}(r)\, Y_l^m(\theta,\varphi)$

3 zenbaki kuantiko

- $\hat{H} = -\dfrac{\hbar^2}{2m}\cdot\dfrac{1}{r}\,\partial_{r^2}^2 r + \dfrac{\hat{L}^2}{2mr^2} + V(r) \Rightarrow \hat{H}\Psi_{n,l,m} = \varepsilon_{n,l,m}\Psi_{n,l,m} \Rightarrow$

$$-\frac{\hbar^2}{2m}\cdot\frac{1}{r}\,\cancel{Y_l^m(\theta,\varphi)}\,\partial_{r^2}^2\left(r R_{n,l,m}(r)\right) + \frac{R_{n,l,m}(r)}{2mr^2}\,\hbar^2 l(l+1)\,\cancel{Y_l^m(\theta,\varphi)} + V(r)\,R_{n,l,m}\cancel{Y_l^m}(\theta,\varphi) =$$

$$\varepsilon_{n,l,m}\cdot R_{n,l,m}(r)\,\cancel{Y_l^m(\theta,\varphi)} \overset{\cdot r}{\Longleftrightarrow} -\frac{\hbar^2}{2m}\,\partial_{r^2}^2\left(r R_{n,l,m}\right) + \frac{R_{n,l,m}}{2mr}\,\hbar^2 l(l+1) + V(r)\, r R_{n,l,m} =$$

$r\,\varepsilon_{n,l,m}\cdot R_{n,l,m}$ ($rR_{n,l,m} = U_{n,l,m}$ deitu) $+$ m ez da agertzen $\Rightarrow$ $\hat{H}$-ren autofuntzioak m-ren independenteak dira $\Rightarrow$ $-\dfrac{\hbar^2}{2m}\dfrac{d^2U_{n,l}}{dr^2} + \dfrac{\hbar^2 l(l+1)}{2mr}U_{n,l} + V(r)\,U_{n,l} =$

$\varepsilon_{n,l}\cdot U_{n,l}$ (dimentsio bakarreko ekuazioa)

$$* \quad \frac{\hbar^2 l(l+1)}{2mr} + V(r) = V_{ef}(r) \quad \text{(potentzial efektiboa)}$$

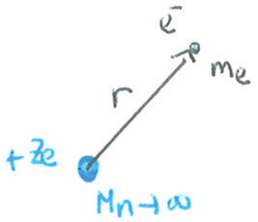
$\Rightarrow$ hau ordezkatuz dimentsio bakarreko

Schrödingeren ekuazioa daukagu, baina ezberdintasun batzuekin: $r \in [0,\infty)$

eta $U_{n,l}(r=0) = 0$ izan behar da. ($R_{n,l}(r) = \dfrac{U_{n,l}}{r}$)

↳ Mugalde baldintza!

ATOMO HIDROGENOIDEAREN ENERGIA MAILAK eta AUTOFUNTZIOAK:



(Gorputz bakarreko problema)

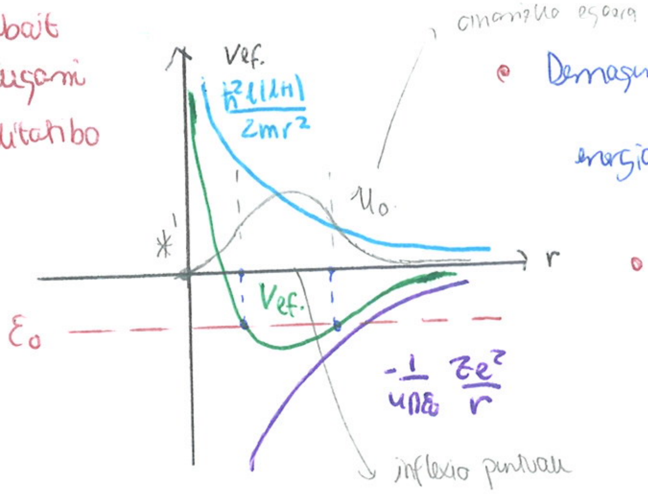
- $V(r) = -\dfrac{1}{4\pi\varepsilon_0}\dfrac{Ze^2}{r}$; $\Psi_{n,l,m}(r,\theta,\varphi) = R_{n,l}(r)\,Y_l^m(\theta,\varphi)$

↳ $U_{n,l} = r R_{n,l}$

Schrödinger:

- $$-\frac{\hbar^2}{2m}\frac{d^2U_{n,l}}{dr^2} + \underbrace{\left[\frac{\hbar^2 l(l+1)}{2mr^2} - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r}\right]}_{V_{ef}(r)} U_{n,l} = \varepsilon_{n,l}\,U_{n,l}$$

Zenbait ezaugarri kualitatibo



- Demagun egoera lotu bat dugula, eta oinarrizkoa den energiaren balioa $\mathcal{E}_0$ dela.
- $u_{n,l}(r=0) = 0 \quad *'$

- Hurbilketa: ikusi $r \to 0$ eta $r \to \infty$ limiteetan Schrödingeren ekuazioak duen itxura:

$\mathcal{E}_{n,l} < 0$

$$* \; r \to \infty: \quad \frac{d^2 u_{n,l}}{dr^2} + \underbrace{\frac{2m\mathcal{E}_{n,l}}{\hbar^2}}_{-k^2} u_{n,l} = 0 \qquad u_{n,l} = Ae^{-kr} + \cancel{Be^{kr}} = Ae^{-\sqrt{\frac{2m\mathcal{E}_{n,l}}{\hbar}}\,r}$$

$(V_{ef} \to 0)$ $\qquad (u_{n,l}(r\to\infty) \to 0)$

$$r \to 0 \quad \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r} \simeq \frac{\hbar^2 l(l+1)}{2mr^2}$$

$$* \; r \to 0: \quad -\frac{d^2 u_{n,l}}{dr^2} + \frac{l(l+1)}{r^2} u_{n,l} = 0 \qquad u_{n,l} \propto r^s \text{ saiatu} \Rightarrow$$

$$-s(s-1)r^{s-2} + \frac{l(l+1)}{r^2} r^s = \left(l(l+1) - s(s-1)\right) r^{s-2} = 0 \iff s(s-1) = l(l+1) \quad \begin{matrix} \nearrow s_1 = l+1 \\ \searrow s_2 = -l \end{matrix}$$

$s_1 \Rightarrow \quad u_{n,l} = C r^{l+1} \quad ; \quad s_2 \Rightarrow u_{n,l} = D r^{-l}$ Ezinezkoa! ez du $u_{n,l}(0) = 0$ baldintza betetzen!

Beraz, $\quad u_{n,l} = Cr^{l+1} \iff R_{n,l}(r) = C r^l$

- Azterketa zehatza: Emaitza: (Laguerreren ekuazio diferentziala)

Egoera lotuak: $\quad \mathcal{E}_{n,l} = \dfrac{-m Z^2 e^4}{2(4\pi\varepsilon_0)^2 \hbar^2 n^2}$ (Bohr-en berdina) $\quad n > l \;, n \in \mathbb{N} - \{0\}$

Laguerre-en polinomio elkartuak

$$R_{n,l}(r) = N_{n,l} \left(\frac{a_0}{Z}\right)^{3/2} \left(\frac{2Zr}{na_0}\right)^l e^{-\frac{Zr}{na_0}} L^{2l+1}_{n-l-1}\left(\frac{2Zr}{na_0}\right)$$

$a_0 \Rightarrow$ Bohr-en erradioa $\Rightarrow \quad a_0 = \dfrac{4\pi\varepsilon_0 \hbar^2}{m e^2} = 0'529\,\text{Å}$

ATOMO HIDROGENOIDEAREN AUTOFUNTZIOEN AZTERPENA:

ellorpen erradiala

$$* \quad R_{n,l}(r) = N_{nl}\left(\frac{a_0}{Z}\right)^{-3/2} \underbrace{\left(\frac{2Zr}{na_0}\right)^{l}}_{③} \underbrace{e^{-\frac{Z\cdot r}{na_0}}}_{②} \underbrace{L_{n-l-1}^{2l+1}\left(\frac{2Zr}{na_0}\right)}_{\text{Laguerre-ren polinomio elkartuak. ①}} \qquad \begin{cases} n > l \\ n \in \mathbb{N}-\{0\} \\ l \in \mathbb{N} \end{cases}$$

Normalizazio baldintza

polinomioaren maila ⇒ nodo kopurua

n-k l-ren balioa mugatzen

$$\left(a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}\right)$$

① $L_{n-l-1}^{2l+1}(x) = \dfrac{e^{x}e^{-2l+1}}{(n+l)!}\dfrac{d^{n+l}}{dx^{n+l}}\left(e^{-x}x^{n+3l+1}\right)$

② $r\to\infty$; esponentzial negatiboa ⇒ Schrödingeren ekuazioan $\lim\limits_{r\to\infty}$ egitean lortutakoa

n zenbat eta handiagoa izan beherapena gero eta txikiagoa da, gero eta astiroago doa zerorantz. (E zenbat eta handiagoa izan ez dago hain lotua). Z zenbat eta handiagoa izan gero eta lokalizatuago dago eta gero eta arinago doa 0-rantz r handitzean (Z zenbat eta handiagoa izan erakarpena gero eta handiagoa da ⇒ gehiago lotu)

③ $r\to 0$ denean garrantzitsua den terminoa ⇒ $R_{n,l} \propto r^{l}$ ⇒ (Schrödingeren ekuazioan $r\to 0$ limitea egitean lortu genuena)

l zenbat eta handiagoa izan, nukleotik hurbil duen ellorpena ($r\to 0$) gero eta txikiagoa da.

Adibideak:

polinomioaren gradua 0

$*^1$ $R_{10} = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$; $R_{21} = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$ $*^2$

$R_{20} = 2\left(\frac{Z}{2a_0}\right)^{3/2}\left(1-\frac{Zr}{2a_0}\right)e^{-Zr/2a_0}$; $R_{32} = \frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Z}{3a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$

$R_{31} = \frac{4\sqrt{2}}{3}\left(\frac{Z}{3a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)\left(1-\frac{Zr}{6a_0}\right)e^{-Z\cdot r/3a_0}$; $R_{30} = 2\left(\frac{Z}{3a_0}\right)^{3/2}\left(1-\frac{2Zr}{3a_0}+\frac{2(Zr)^2}{27a_0^2}\right)e^{-Zr/3a_0}$

$*^1$ $n=1,\ l=0$ izan daitezke bakarrik ; gradua: $n-l-1=0$ (kte bat dugu)

$*^2$ $n=2,\ l=1,0\ \ldots$

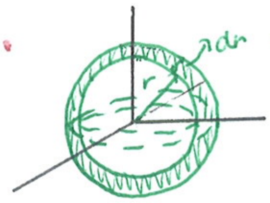
ATOMO HIDROGENOIDEOAREN AUTOFUNTZIOEN ADIERAZPEN GRAFIKOA:

Dentsitate probabilitate erradiala indikatu: $P(r) = r^2 |R_{nl}(r)|^2 = P_{n,l}(r)$

- $\Psi_{n,l,m}$ ⇒ normalizatu ⇒ $(\Psi_{n,l,m}, \Psi_{n,l,m}) = 1 \longleftrightarrow \iiint R_{n,l}^* Y_l^{m*} R_{n,l} Y_l^m r^2 dr \sin\theta d\theta d\varphi = 1$

Y_l^m-ak normalizatuta ⇒ $\underbrace{\int_0^\infty R_{nl}^2 r^2 dr}$ $= 1$

$P(r) = P_{n,l}(r) = |R_{n,l}|^2 r^2$ $[r, r+dr]$ ↗ $(r, r+dr)$ tartean egoteko probabilitatea

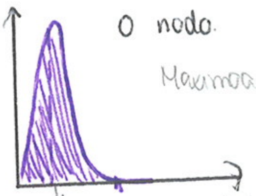
- 

⇒ hemen egoteko probabilitatea.

$P_{n,l}(r) = \underbrace{\cancel{4\pi} r^2 dr}_{dV} |R_{nl}|^2 = r^2 dr |R_{nl}|^2$

normalizazioa dela eta enulatu

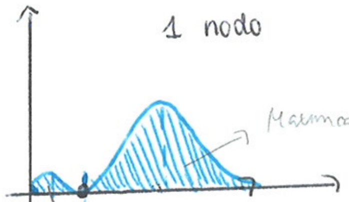
n=1, l=0



Maximoa lokalizatuagoa

a_0 ↘ Maximoa Bohr-en aurresandako erradioa

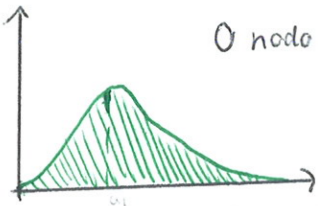
n=2, l=0



Maximoa gehiago urrundu

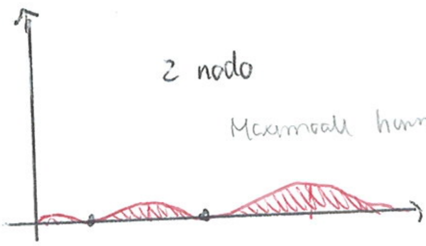
↳ l zenbat eta txikiagoa izan nukleotik hurbil egoteko probabilitatea handiagoa da.

n=2, l=1



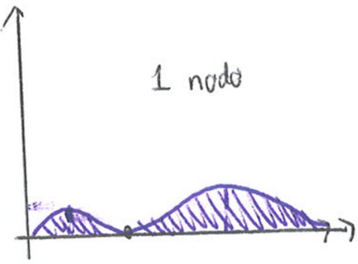
*

n=3, l=0

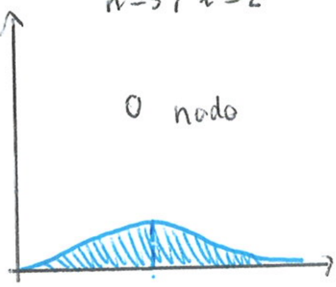


Maximoak hurrunago

n=3, l=1



n=3, l=2



n zenbat eta handiagoa izan $P_{n,l}(r)$-ren maximoa hurrunago agertzen da

* Nodoak energia zinetiko erradialarekin lotuta daude eta zenbat eta handiagoa izan nodo kopurua energia zinetiko erradiala handiagoa da. ⇒ l=0 energia zinetiko orbitalak 0 da → energia zinetiko erradiala altuagoa izango da. (nukleotik hurbil egoteko energia gehiago)

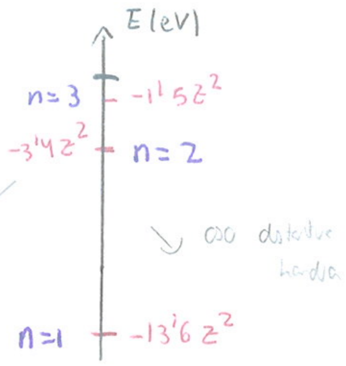
ZENBAKI KUANTIKOAK eta ENDAKAPENA:

$$\{\hat{H}, \hat{L}^2, \hat{L}_z\} \equiv \Psi_{n,l,m} = R_{nl}(r)\, Y_l^m(\theta,\varphi)$$

$$E_n = -\frac{m Z^2 e^4}{(4\pi\varepsilon_0)^2 \cdot 2\hbar^2 n^2} = -\frac{Z^2 \cdot 13'6\,eV}{n^2}$$

$$L^2 = \hbar^2 l(l+1)$$

$$L_z = m\hbar$$



Hanbat egoera energia berdinekin

- Mailak endakatuta daude ⇒ energia berdina l eta m-ren balio ezberdinentzat

$$n > l \quad (n \in \mathbb{N}-\{0\},\ l \in \mathbb{N}) \quad \text{eta} \quad |m| \le l \quad (m \in \mathbb{Z})$$

$\underbrace{l = 0, 1, \dots, n-1}_{n \text{ balio posible}}$ (n finkatuta badago)

$\underbrace{m = -l, -l+1, \dots, 0, \dots, l+1}_{2l+1 \text{ balio posible}}$

- Ad: • $n=1$, $l=0$ da bakarrik eta ondorioz $m=0$ ere ($g=1$ endakapena)
  • $n=2$, $l=0,1$ da eta $m=-1,0,1$ ⇒ $g=4$ endakapena $\left\{ (0,0);\ (1,-1);\ (1,1);\ (1,0) \right.$

  m-k 2l+1 aukera posible l bakoitzeko

- Maila bakoitzari dagokion endakapena: $g = \sum_{l=0}^{n-1}(2l+1) = 2\sum_{l=0}^{n-1} l + \sum_{l=0}^{n-1} 1 = n + 2\sum_{l=0}^{n-1} l \overset{*}{=}$

$$n + n(n-1) = n(1+n-1) = n^2$$

Espina kontuan hartu gabe! (Bestela bikoitza ⇒ $g' = 2n^2$)

$$* \left.\begin{aligned} \sum_{l=0}^{n-1} l &= \overbrace{0+1+2+\dots+(n-1)}^{n \text{ elementu}} \\ &\ (n-1)+(n-2)+\dots+0 = \sum_{l=0}^{n-1} l \end{aligned}\right\} \ 2\sum_{l=0}^{n-1} l = (n-1)\cdot n$$

- Egoera-geldikorrak: (n finkoa duen egoera)

  l eta m edozein izan daiteke.

$$\Phi_n = \sum_{l=0}^{n-1} \sum_{m=-l}^{l} c_{lm} \Psi_{nlm}(\vec{r})$$

n berdina duten uhin-funtzioen edozein konbinazio lineal

ORBITAL ATOMIKOAK:

- Espazioko zonaldeak non elektroi bat aurkitzeko probabilitatea handia den.

Mekanika klasikoan ⇒ orbitak ; mekanika kuantikoan ⇒ orbital ⇒ e^--ri dagokion uhin-funtzioarekin erlazionatuta (energia maila batean dagoen e^--aren uhin funtzioa):

$$\Psi_{n,l,m} = R_{n,l}(r)\, \underbrace{Y_l^m(\theta,\varphi)}_{= N_l^m P_l^m(\cos\theta)\, e^{im\varphi} \;*^1}$$

*¹ Harmoniko esferikoa konplexua da $e^{im\varphi}$ esponentziala duelako ; izan ere $\hat{L}_z$ ragilea konplexua da beraz autofuntzioak ere, autofuntzio honi dagokion autobalioa 0 ez bada ⇒

Hala ere, $\hat{L}^2$ erreala denez, printzipioz erreala den $\hat{L}^2$ autofuntzioak aukera genitzazke (orduan ez dira $\hat{L}_z$-ren autofuntzioak) ⇒ erreala izateko (kimikan aukeratzen dira) ⇒

m = bikoiti ⇒ $\dfrac{Y_l^m + Y_l^{-m}}{\sqrt{2}}$, $\dfrac{Y_l^m - Y_l^{-m}}{\sqrt{2}i}$ $\quad\left(Y_l^{m\,*} = (-1)^m Y_l^{-m} \right)$

m = bakoiti ⇒ $\dfrac{Y_l^m + Y_l^{-m}}{\sqrt{2}i}$, $\dfrac{Y_l^m - Y_l^{-m}}{\sqrt{2}}$

Ad: $l=1$ $\{Y_1^0, Y_1^1, Y_1^{-1}\}$ oinarria ez da erreala baina; erreala aukera dezakegu: $\left\{ Y_1^0 ,\ \dfrac{Y_1^1 + Y_1^{-1}}{\sqrt{2}i} ,\ \dfrac{Y_1^1 - Y_1^{-1}}{\sqrt{2}} \right\}$

Y_1^0 ∝ z ($\hat{L}_z$-ren autof.)

$\dfrac{Y_1^1 + Y_1^{-1}}{\sqrt{2}i}$ ∝ y ($\hat{L}_y$-ren autof.)

$\dfrac{Y_1^1 - Y_1^{-1}}{\sqrt{2}}$ ∝ x ($\hat{L}_x$-ren autof.)

m-ren balio ezberdinen konbinazioa ⇒ ez dira $\hat{L}_z$-ren autofuntzioa

Desabantaila ⇒ orduan ez dakigu $\hat{L}$-ren zein osagaiaren autofuntzioak diren

Abantaila ⇒ errealak dira

- Orbitala ⇒ espazioko zonaldea non elektroi bat aurkitzeko probabilitatea %90 den. (orbitalaren itxura egoeraren menpekoa: n, l, m)

- Notazio espektroskopikoa: l zenbaki kuantikoen ordez letrak erabiltzen dira: → hemendik aurrera alfabetikoki jarraitu

$l=0 \Rightarrow s$; $l=1 \Rightarrow p$; $l=2 \Rightarrow d$; $l=3 \Rightarrow f$ ...

sharp, principal, diffuse, fundamental

n handitzerakoan nodo kopurua handitu. $l=0$ (s)

Uhin errealak hartuz: $l=1 \Rightarrow$ uhin-funtzioak: p_z , p_x , p_y ($m=0$, $m=1$, $m=-1$) $p \to l=1$ delako

αz → z norabidean luzatuta; αx → x norabidean luzatuta; αy → y norabidean luzatuta

$l=2$ (d) $\Rightarrow$ uhin-funtzioak: d_{z^2} , d_{xz} , d_{yz} , d_{xy} , $d_{x^2y^2}$ ($m=0$; $m=\pm1$; $m=\pm2$)

αz^2 αxz αyz αxy αx^2y^2

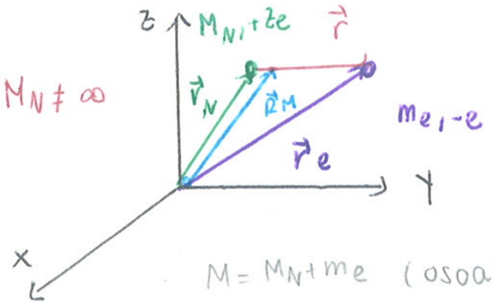
ATOMO HIDROGENOIDEOA: BI GORPUTZEN PROBLEMA

Zer gertatzen da nukleoaren masa infinitutzat hartzen ez dugunean? ($M_N \neq \infty$) $\Rightarrow$

Bi gorputzen problema.

↗ uhin-funtzioa bi posizio bektoreen menpekoa

$$\Psi(\vec{r}_N, \vec{r}_e, t) \Rightarrow \hat{H} = -\frac{\hbar^2}{2M_N}\vec{\nabla}_N^2 - \frac{\hbar^2}{2m_e}\vec{\nabla}_m^2 + V(|\vec{r}_e - \vec{r}_N|)$$



Aldagai aldaketa: $\vec{R}_M = \dfrac{m_e\vec{r}_e + M_N\vec{r}_N}{m_e + M_N}$; $\vec{r} = \vec{r}_e - \vec{r}_N$

masa zentroaren posizioa; posizio erlatiboa

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla^2_{MZ} - \frac{\hbar^2}{2\mu}\nabla_r^2 + V(r)$$

$M = M_N + m_e$ (osoa)

$\mu = \dfrac{m_e M_N}{m_e + M_N}$ (masa laburbildua)

Hamiltondarraren autofuntzioek bete behar duten adierazpena: $\hat{H}\Psi_\varepsilon(\vec{R}_{MZ}, \vec{r}) = E\Psi_\varepsilon(\vec{R}_{MZ}, \vec{r})$

Banangarria (MZari dagokiona alde batetik eta besteetik posizio erlatiboari dagokiona):

aldagaien banantzea $\Rightarrow$ $\Psi_\varepsilon(\vec{R}_{MZ}, \vec{r}) = \phi_M(\vec{R}_{MZ})\,\psi_\mu(\vec{r})$:

↗ ekarpen hori dagokion energia

$$\begin{cases} -\dfrac{\hbar^2}{2m}\vec{\nabla}_{MZ}^2\,\phi_M(\vec{R}_{MZ}) = E_{MZ}\,\phi_M & \to \text{partikula askeari dagokiona (MZ aske desplazatzen da)} \\ -\dfrac{\hbar^2}{2m}\vec{\nabla}_r^2\,\psi_\mu(\vec{r}) + V(r)\,\psi_\mu(\vec{r}) = E_\mu\,\psi_\mu(\vec{r}) & \to \text{potentzial zentralari dagokion Schrödingeren ekuazioa (me ordez } \mu) \end{cases}$$

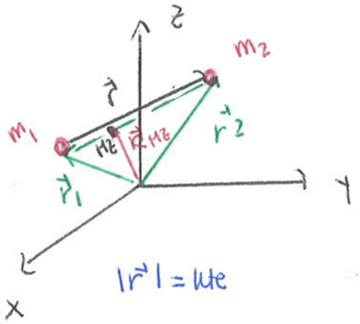
$E = E_{MZ} + E_{\mu}$ → e-ren ordezkatu graduatu lortuko

• $(E_{\mu})_n = -\dfrac{\mu z^2 e^4}{(4\pi\varepsilon_0)^2 2\hbar^2 n^2}$ → $\Psi_{\mu}(\vec{r})$ ere ezaguna (Laguerren polinomioak) Barne uhin-funtzioak → $m_e \leftrightarrow \mu$

• $a_0' = \dfrac{m_e}{\mu} a_0$
"Bohr"-en erradioa

✳ Jatorria MZ-n jarriz ⇒ $\phi_M(\vec{R}_{MZ})$ ellerpena ez genuke izango, ezta E_{MZ} ellerpena

HIRU DIMENTSIOKO ERROTORE-ZURRUNA:



$|\vec{r}| = kte$

• $\{\vec{r}_1, \vec{r}_2\} \to \{\vec{R}_{MZ}, \vec{r}\}$ $|\vec{r}|=kte$ denez aldagaiak $\{\vec{R}_{MZ}, r\}$ hartu

$$\vec{R}_{MZ} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2}, \quad \vec{r} = \vec{r}_2 - \vec{r}_1$$

masa osoa — masa laburbildua

• Hamiltondarraren adierazpena: $\hat{H} = -\dfrac{\hbar^2}{2M}\nabla_{MZ}^2 - \dfrac{\hbar^2}{2\mu}\nabla_r^2 =$

$$-\frac{\hbar^2}{2M}\nabla_{MZ}^2 - \cancel{\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r} + \frac{\hat{L}^2}{2\mu r^2} \to \mu r^2 = I$$

↳ $|\vec{r}| = kte$ (ez dugu energia zinetiko erradiala)

• Bera, errotore zurrunean ($|\vec{r}|=kte$): $\hat{H} = -\dfrac{\hbar^2}{2M}\nabla_{MZ}^2 + \dfrac{\hat{L}^2}{2I}$ (Banangarria) ⇒

$$\Psi = \phi_{MZ}(\vec{R}_{MZ})\,\Psi(\vec{r})$$

m-k ez du eragiten energian

$$\Psi_{\vec{K},l,m} = e^{i\vec{K}\cdot\vec{R}_{MZ}}\, Y_l^m(\theta,\phi) \Rightarrow E_{\vec{K},l} = \frac{\hbar^2 \vec{K}^2}{2M} + \frac{\hbar^2 l(l+1)}{2I}$$

MZri dagokiona — biraketari dagokiona.

PARTIKULA ASKEA HIRU DIMENTSIOTAN (KOORDENATU ESFERIKOETAN):

$\{\hat{H}, \hat{\vec{p}}\}$ ⇒ trukakorrak ⇒ aldi berako autofuntzioak: $e^{i\vec{K}\cdot\vec{r}}$ ⇒ $\{\hat{H}, \hat{L}^2, \hat{L}_z\}$ partikula askean!

trukakorrak ere, hauen aldiberako autofuntzioak aurkitu daitezke (beste batzuk):

$R_{nl}(r)\,Y_l^m(\theta,\phi)$ ⇒ $\hat{H}$-n sartuz ⇒ $R_{nl}(r)$ lortu (Hidrogeno atomoan egindakoa baina $V=0$)

hidrogeno atomoaren ezberdina

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(rR_{nl})+\frac{\hbar^2 l(l+1)}{2mr^2}R_{nl}=ER_{nl}$$

$$l=0 \Rightarrow -\frac{\hbar^2}{2m}\cancel{\frac{1}{r}}\frac{d^2}{dr^2}\underbrace{(rR_{n0})}_{u_{n0}}=\underbrace{ER_{n0}r}_{u_{n0}} \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u_{n0}=Eu_{n0}$$

$$\frac{2mE}{\hbar^2}=k^2 \quad (E>0) \Rightarrow u_{n0}=A\sin kr+B\cos kr = rR_{n0} \quad \leftrightarrow$$

$l \geq |m| \quad l=0 \leftrightarrow m=0$

$$u_{n0}(0)=0=B \Rightarrow u_{n0}=A\sin kr \Rightarrow \psi_{n00}=\frac{A\sin kr}{r}$$

$$l\neq 0 \Rightarrow k=\sqrt{\frac{2mE}{\hbar^2}}=\frac{\sqrt{2mE}}{\hbar} \quad \text{eta} \quad \rho=kr \quad \text{definitu:}$$

E k-ren lokia

$$\rho^2\frac{d^2R_{kl}}{d\rho^2}+2\rho\frac{dR_{kl}}{d\rho}+[\rho^2-l(l-1)]R_{kl}=0$$ Besselen ekuazioak $\Rightarrow$

Besselen funtzio esferikoak

$$R_{kl}=R_{kl}(\rho)=A\,j_l(\rho)+B\,\eta_l(\rho)$$ Neumann-en funtzio esferikoak

- $j_l(\rho)=(-\rho)^l\left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l\frac{\sin\rho}{\rho}$; $\eta_l(\rho)=-(-\rho)^l\left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l\frac{\cos\rho}{\rho}$

* $l=0 \Rightarrow j_0(\rho)=\frac{\sin\rho}{\rho}$ (kalkulatutakoa) , $\eta_0(\rho)=\frac{\cos\rho}{\rho}$

* $l=1 \rightarrow j_1(\rho)=\frac{\sin\rho}{\rho^2}-\frac{\cos\rho}{\rho}$, $\eta_1(\rho)=-\frac{\cos\rho}{\rho^2}-\frac{\sin\rho}{\rho}$

Uhin-funtzioa finitua izan dadin tarte osoan eta jatorrian ere $B=0$ izan behar da $\Rightarrow$ Fisikoki onargarriak Besselen funtzioak soilik:

$$\psi_{k,l,m}=j_l(kr)\,Y_l^m(\theta,\varphi)$$

Lehen genituen uhin lauak, $e^{i\vec{k}\cdot\vec{r}}$, oinarri honetan adierazi daitezke; $\vec{k}$ ekoztuta badago $\Rightarrow$ $\vec{k}\parallel OZ$ aukeratuz;
$$e^{i\vec{k}\cdot\vec{r}}=e^{ikr\cos\theta}=4\pi\sum_l i^l\left(\frac{2l+1}{4\pi}\right)^{1/2}j_l(kr)\,Y_l^0(\theta,\varphi)$$

Biak dira partikula askean kasuan hamiltondarraren autofuntzioak adierazteko era bat.

HIRU DIMENTSIOKO POTENTZIAL-OSIN INFINITU ESFERIKOA:

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

Simetria esferikoa dela eta koordenatu esferikoak aukeratuko ditugu:

$$\Psi_{nlm} = R_{nl} Y_l^m(\theta, \varphi)$$

Denigarez $R_{kl}(r) = 0$

$r>a \Rightarrow \Psi = 0$ eta $r<a$ denean partikula-askeak betetzen duen uhin-ekuazioa bera:

$$\Psi = \begin{cases} 0 & r \geq a \\ j_l(Kr)\, Y_l^m(\theta,\varphi) & r<a \end{cases}$$

Muga baldintzak: $\Psi|_{r=a} = 0 = j_l(Ka) \cdot Y_l^m(\theta,\varphi) \rightarrow j_l(Ka) = 0 \rightarrow$

$K = \sqrt{\frac{2mE}{\hbar^2}}$ denez hemendik $E = \frac{\hbar^2 K^2}{2m}$-ren balioak lortu (diskretuak)

* $l=0$ denean adibidez: $j_0(Ka) = \frac{\sin Ka}{Ka} = 0 \Rightarrow Ka = n\pi \rightarrow K = \frac{n\pi}{a}$

(dimentsio bakarrean lortutako ondorio bera) $\Rightarrow E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2}$ $(l=0)$

↓ energia orokorra aldaraziko ez dugu
↓
dimentsio bakarreko higidura

Beraz, $\Psi_{klm} = \begin{cases} j_l(Kr)\, Y_l^m & r<a \\ 0 & r>a \end{cases}$ non K, $j_l(Ka) = 0$ baldintza betetzen duena den.

Potentzial osina finitua bada, kanpoan $\Psi \neq 0$:

$$\Psi_{Klm} = \begin{cases} C j_l(K_1 r)\, Y_l^m & r<a \\ [A g_l(K_2 r) + B \eta_l(K_2 r)]\, Y_l^m(\theta,\varphi) & r>a \end{cases}$$

Muga baldintzak aplikatuz konstanteak lortu.

$K_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

Normalizazioa (K-ren balioa aztertzen)

HIRU DIMENTSIOKO OSZILATZAILE HARMONIKOA:

- $V = \frac{1}{2}\underbrace{m\omega^2}_{K} r^2 \Rightarrow$ isotropoa $\leftrightarrow$ zentrala da potentziala $\Rightarrow$ $\{\hat{H}, \hat{L}^2, \hat{L}_z\}$-ren aldiberako autofuntzioak aurki daitezke; hau da, endakapena badago ez da zertan hau bete baina aurkitu ditzakegu.

- $\Psi_{nlm} = R_{n,l}(r) Y_l^m(\theta,\varphi)$ $\Rightarrow$ denboraren independentea den Schrödingeren ekuazioa $\Rightarrow$

  $\hookrightarrow$ $\hat{L}$ eta $\hat{L}_z$-ren autofuntzioak

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(rR) + \frac{\hbar^2 l(l+1)}{2mr^2}R + \frac{1}{2}m\omega^2 r^2 R = E\cdot R$$

Ald. aldaketa: $\rho = r\sqrt{\frac{m\omega}{\hbar}}$ $\Rightarrow$ $-\frac{1}{\rho}\frac{d^2}{d\rho^2}(\rho R) + \frac{l(l+1)}{\rho^2}R + \rho^2 R = \varepsilon R$; $\varepsilon = \frac{E}{\frac{1}{2}\hbar\omega}$

* $\rho \to \infty$ $\quad -\frac{d^2R}{d\rho^2} + \rho^2 R = 0$ (1D-ko ekuazioa) ; $R \sim e^{-\rho^2/2}$

Banandu: $R = e^{-\rho^2/2}\cdot f(\rho)$ $\quad(\rho\to\infty \quad f(\rho)\to 1)$:

$$\rho^2 f'' + 2\rho f' - l(l+1)f = 2\rho^3 f' + (3-\varepsilon)\rho^2 f$$

Serieen garapena: $f = \sum_p c_p \rho^p$: (garatuz) $\Rightarrow$

$$[p(p+1) - l(l+1)]c_p = [2(p-2)+3-\varepsilon]\,c_{p-2}$$

(koefiziente bikoiti bat finkatuz koefiziente bikoitiak finkatuk egongo dira, eta bakoiti bat finkatuz gauza bera)

- $p_{min} = l$; $\cancel{-l}-1$ $\rightarrow$ bestela f dibergentea

- $2p_{max} + 3 - \varepsilon \Rightarrow \varepsilon = 2p_{max}+3 \Rightarrow E = \frac{\hbar\omega}{2}(2p_{max}+3) \overset{p_{max}=n}{=} \hbar\omega(n+3/2)$

  $n \geq l$

$f_{nl} = c_l r^l + c_{l+2} r^{l+2} + \ldots + c_n r^n$ (koefiziente bakoitiak eta bikoitiak banandurik daude)

* l eta n bakoitiak edo bikoitiak!

- $E_n = \hbar\omega\left(\frac{3}{2}+n\right)$; $\psi_{n,l,m} = \underbrace{e^{-\rho^2/2} f_{nl}(r)}_{R_{nl}(r)} Y_l^m(\theta,\varphi)$ $\quad\left(\rho = r\sqrt{\frac{m\omega}{\hbar}}\right)$

  * $n \geq l$ (biak bakoitiak edo bikoitiak) eta $l \geq |m|$; $n \in \mathbb{N}$

* $E_0 = \frac{3}{2}\hbar\omega$; $\psi_{000} \propto e^{-\rho^2/2} \, \overset{\text{kte bat}}{Y_0^0} \leftrightarrow \psi_{000} \propto e^{-\rho^2/2}$; Endekapenik ez. $g=1$

* $E_1 = \frac{5}{2}\hbar\omega$; $\psi_{11m} \propto e^{-\rho^2/2} \rho \, Y_1^m$ $\quad m=-1,0,1$; $g=3$

* $E_2 = \frac{7}{2}\hbar\omega$; $\psi_{200} \propto e^{-\rho^2/2}(a+br^2) Y_0^0$ $\quad m=-2,-1,0,1,2$

  $\psi_{22m} \propto e^{-\rho^2/2} \rho^2 Y_2^m$; $g=6$

  ⋮

- Kartesiarretan lortutako autofuntzioen konbinazioak egitez hemen lor daitezke ⇒ hauen esberdintasuna: $\hat{L}_z$ eta $\hat{L}^2$-ren autofuntzioak dira

KONTROLA: (Pikarke)

1.) $s = \frac{1}{2}$ spin-eko partikula-sorta, OY ardatzaren norabidean higitzen ari delarik, Stern-Gerlach gailu bat pasoratzen da. Gailu hori OZ norabidean lerrokatuta dago. Stern-Gerlach gailua zeharkatu beraien $|+\rangle$ egoeran lasterak aterazten den partikula-sortak bigarren Stern-Gerlach gailu bat pasoratzen du. Bigarren gailu hori $\hat{u} = \sin\theta\,\hat{\imath} + \cos\theta\,\hat{k}$ norabidean lerrokatuta dago.

a) S_u matrizea.

$$S_u = \vec{S}\cdot\vec{u} = (S_x u_x + S_y u_y + S_z u_z) \Rightarrow [S_x]\sin\theta + [S_z]\cos\theta = \sin\theta\,\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} +$$

$$\frac{\hbar}{2}\cos\theta\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}\cos\theta & \sin\theta\\ \sin\theta & -\cos\theta\end{pmatrix} = [S_u] \quad (\{|+\rangle, |-\rangle\}\text{ oinarrian})$$

b) S_u behagarriaren autobalioak eta autobektoreak (normalizatuta).

$$|S_u - \lambda \mathbb{1}| = \frac{\hbar}{2}\begin{vmatrix}\cos\theta - \frac{2\lambda}{\hbar} & \sin\theta\\ \sin\theta & -\cos\theta - \frac{2\lambda}{\hbar}\end{vmatrix} \underset{\lambda = \frac{\tilde{\lambda}\hbar}{2}}{=} \frac{\hbar}{2}\begin{vmatrix}\cos\theta - \tilde{\lambda} & \sin\theta\\ \sin\theta & -\cos\theta - \tilde{\lambda}\end{vmatrix} = 0 \rightarrow$$

$$-(\cos\theta - \tilde{\lambda})(\cos\theta + \tilde{\lambda}) - \sin^2\theta = (\tilde{\lambda} - \cos\theta)(\tilde{\lambda} + \cos\theta) - \sin^2\theta = \tilde{\lambda}^2 \underbrace{-\cos^2\theta - \sin^2\theta}_{-1} = 0 \rightarrow$$

$$\tilde{\lambda}^2 = 1 \rightarrow \tilde{\lambda} = \pm 1 \rightarrow \quad \lambda = \pm\hbar/2$$

$*$ $\lambda = \hbar/2 \Rightarrow$

$$\begin{pmatrix}\cos\theta - 1 & \sin\theta\\ \sin\theta & -(\cos\theta + 1)\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \begin{pmatrix}a(\cos\theta - 1) + b\sin\theta\\ a\sin\theta - (\cos\theta + 1)b\end{pmatrix} = \begin{pmatrix}0\\ 0\end{pmatrix} \rightarrow$$

$$a\sin\theta = b(\cos\theta + 1) \rightarrow a = b\,\frac{(\cos\theta + 1)}{\sin\theta} = b\left(\cot g\,\theta + \frac{1}{\sin\theta}\right)$$

Normalizatu $\Rightarrow$ $$b^2\left[1 + \frac{(\cos\theta + 1)^2}{\sin^2\theta}\right] = b^2\left[\frac{\sin^2\theta + \cos^2\theta + 1 + 2\cos\theta}{\sin^2\theta}\right] = b^2\,\frac{[2 + 2\cos\theta]}{\sin^2\theta} =$$

$$b^2 \, 2 \, \frac{[1+\cos\theta]}{\sin^2\theta} = \frac{2b^2 \cdot 2\cos^2\theta/2}{\sin^2\theta} = \frac{4b^2\cos^2\theta/2}{\sin^2\theta} = 1 \rightarrow b = \frac{\sin\theta}{2\cos\theta/2} = \frac{2\sin\theta/2\cancel{\cos\theta/2}}{2\cancel{\cos\theta/2}} =$$

$$\sin\theta/2 \rightarrow \quad a = \sin\theta/2 \, \frac{(\cos\theta+1)}{\sin\theta} = \cancel{\sin\theta/2} \, \frac{2\cos^2\theta/2}{2\cancel{\sin\theta/2}\cos\theta/2} = \cos\theta/2$$

$$|\psi_1\rangle = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle = |+\rangle_u$$

$* \; \lambda = -\hbar/2 \Rightarrow$

$$\begin{pmatrix} \cos\theta+1 & \sin\theta \\ \sin\theta & 1-\cos\theta \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a(\cos\theta+1)+b\sin\theta \\ \sin\theta \, a + b(1-\cos\theta) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow$$

$$a = -b\,\frac{(1-\cos\theta)}{\sin\theta} = -b\,\frac{2\sin^2\theta/2}{2\sin\theta/2\cos\theta/2} = -b\,\mathrm{tg}\,\theta/2$$

Normalizatu $\Rightarrow$ $b^2(1+\mathrm{tg}^2\theta/2) = b^2\frac{1}{\cos^2\theta/2} = 1 \rightarrow b = \cos\theta/2$

$$|\psi_2\rangle = \sin\frac{\theta}{2}|+\rangle - \cos\frac{\theta}{2}|-\rangle = |-\rangle_u$$

c) Lor bedi Stern-Gerlach gailutik ateratzen diren partikulen intentsitateen ratioa, $\frac{\theta}{2}$ angeluaren funtzioan. (1. gailutik $S_z = \hbar/2$ balioarekin atera dira)

Bigarren gailutik pasatzean $S_u = \pm\hbar/2$ izan dezake $\rightarrow$ $|+\rangle_u$ edo $|-\rangle_u$ egoerekin ateratzeko da elektroia.

$$P_{\hbar/2} = |{}_u\langle +|+\rangle|^2 = \cos^2\frac{\theta}{2} \quad , \quad P_{-\hbar/2} = |{}_u\langle -|+\rangle|^2 = \sin^2\frac{\theta}{2}$$

2) Izan bedi $s=1/2$ spin-eko 2 partikulez osatutako sistema. Partikula horien aldagai orbitalak (posizioa eta momentua) arbuiatzen dira. Partikula sistema horren
↳ H_s espazioa
hamiltondarra hauxe da: $\hat{H} = \omega_1 \hat{S}_{1z} + \omega_2 \hat{S}_{2z}$ $(\omega_1, \omega_2 \in \mathbb{R})$. Partikula sistemaren hasierako aldiuneko spin-egoera $|1,0\rangle$ da $(S=0 \, ; m_s=0)$. t aldiunean S^2

$|S^2 = |\vec{S}_1 + \vec{S}_2|^2 = S_1^2 + S_2^2 + 2\vec{S}_1 \cdot \vec{S}_2$) neurtzen badugu zeintzuk dira lor daitezkeen emaitzak eta haien probabilitateak?

- $S^2 = (\vec{S}_1 + \vec{S}_2)^2 = S_1^2 + S_2^2 + 2\vec{S}_1 \cdot \vec{S}_2 = S_1^2 + S_2^2 + 2(S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}) =$

$S_1^2 + S_2^2 + 2S_{1z}S_{2z} + (S_{1+}S_{2-} + S_{1-}S_{2+})$

- $\hat{H} = \omega_1 \hat{S}_{1z} + \omega_2 \hat{S}_{2z} \Rightarrow$ H-ren autobektoreak $|m_1, m_2\rangle$ dira eta autobalioak $\hbar[\omega_1 m_1 + \omega_2 m_2]$ $(m_1, m_2 = \pm 1/2)$

Gogoratzeko denboran hasieratako egoera, $\{|m_1, m_2\rangle\}$ oinarrian gorde behako dugu:

$S_1, S_2 = 1/2 \rightarrow m_1, m_2 = \pm 1/2 \rightarrow m = \begin{cases} 1 \\ 0 \\ -1 \end{cases} \rightarrow j = 1, 0$

* $|1,1\rangle = |m_1 = 1/2, m_2 = 1/2\rangle$

* $|1,0\rangle = \frac{1}{\hbar\sqrt{2}} J_- |1,1\rangle = \frac{1}{\hbar\sqrt{2}}(J_{1-} + J_{2-})|m_1 = 1/2, m_2 = 1/2\rangle =$

$\frac{1}{\hbar\sqrt{2}}(\hbar|m_1 = -1/2, m_2 = 1/2\rangle + \hbar|m_1 = 1/2, m_2 = -1/2\rangle) = \frac{1}{\sqrt{2}}(|+,-\rangle + |-,+\rangle)$

$|\psi(0)\rangle = |1,0\rangle = \frac{1}{\sqrt{2}}|+,-\rangle + \frac{1}{\sqrt{2}}|-,+\rangle \xrightarrow{t} |\psi(t)\rangle = \frac{1}{\sqrt{2}}|+,-\rangle e^{-i(\omega_1-\omega_2)t/2} +$

$\frac{1}{\sqrt{2}}|-,+\rangle e^{i(\omega_1-\omega_2)t/2} = \frac{1}{\sqrt{2}}\left[e^{-i(\omega_1-\omega_2)t/2}|+,-\rangle + e^{i(\omega_1-\omega_2)t/2}|-,+\rangle\right]$

S^2 neurtu ditzakegun balioak jakiteko $|+,-\rangle$ eta $|-,+\rangle$ kalkulatu behar ditugu.

$|0,0\rangle = \alpha|+,-\rangle + \beta|-,+\rangle \rightarrow \langle 0,0|1,0\rangle = \frac{\alpha}{\sqrt{2}} + \frac{\beta}{\sqrt{2}} = 0 \rightarrow \alpha = -\beta$

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

$$\begin{cases} |+,-\rangle = \frac{1}{\sqrt{2}}\left(|1,0\rangle + |0,0\rangle\right) \\ |-,+\rangle = \frac{1}{\sqrt{2}}\left(|1,0\rangle - |0,0\rangle\right) \end{cases}$$

$$|\psi(t)\rangle = \frac{1}{2} e^{-i(\omega_1-\omega_2)t/2}\left(|1,0\rangle + |0,0\rangle\right) + \frac{1}{2} e^{i(\omega_1-\omega_2)t/2}\left(|1,0\rangle - |0,0\rangle\right) =$$

$$\frac{1}{2}\left[|1,0\rangle\left(e^{-i(\omega_1-\omega_2)t/2} + e^{i(\omega_1-\omega_2)t/2}\right) + |0,0\rangle\left(e^{-i(\omega_1-\omega_2)t/2} + \right.\right.$$

$$\left.\left. - e^{i(\omega_1-\omega_2)t/2}\right)\right] = |1,0\rangle \cos\left(\frac{(\omega_1-\omega_2)t}{2}\right) - i \sin\left(\frac{(\omega_1-\omega_2)t}{2}\right)|0,0\rangle$$

Lor daitezken S^2-ren balioak: $s = 1, 0$

$$P_{s=1} = \sum_{m=-1}^{1} |\langle 1,m|\psi(t)\rangle|^2 = \cos^2\left(\frac{(\omega_1-\omega_2)t}{2}\right)$$

$$P_{s=0} = |\langle 0,0|\psi(t)\rangle|^2 = \sin^2\left(\frac{(\omega_1-\omega_2)t}{2}\right)$$

3) Kontsidera bedi atomo hidrogenoideoaren hamiltondarraren Darwin-en ekarpena: $W_D = \frac{1}{8}\lambda_C \Delta V(r)$ non $\lambda_C \equiv$ Compton-en uhin-luzera den.

Kontsidera bitez, halaber,

i) $\{H_0, L^2, S^2, I^2, L_z, S_z, I_z\}$ behagarri trukakorren aldibereko autobektore normalizatuek osatutako oinarria $\Rightarrow \{|n,l,s,i,m_l,m_s,m_i\rangle\}$

ii) $\{H_0, L^2, S^2, I^2, J^2, F^2, F_z\}$ behagarri trukakorren aldibereko autobektore normalizatuek osatutako oinarria $\Rightarrow \{|n,l,s,i,j,f,m_f\rangle\}$

$\vec{F} = \vec{S} + \vec{I}$ non I eta S nukleoaren eta elektroiaren spin momentu

momentu angeluarrak diren)

$$\lambda_C = \frac{\hbar}{m_e c} = a_0 \alpha$$

Kalkulatu:

a) W_D behagarria 2 oinarri horietan diagonala al da? Zergatik?

$$W_D = \frac{1}{8} \lambda_C \Delta V(r) = \frac{-1}{8} \lambda_C \frac{Ze^2}{4\pi\varepsilon_0} \Delta\left(\frac{1}{r}\right) = -\frac{Ze^2 \lambda_C}{32\pi\varepsilon_0} \delta(\vec{r}) \propto r$$

W_D-k osagai erradialetan bakarrik eragiten du eta $L^2, S^2, I^2, L_z, S_z, I_z, J^2, F^2, F_B$ r-ren independenteak dira → beraz guztiz horiekin trukakorra izango da.

H_0-rekin bestalde, ez da trukakorra: $H_0 = -\frac{\hbar}{2m} \nabla^2_r + \frac{L^2}{2mr^2} - \frac{Ze^2}{4\pi\varepsilon_0 r}$

$[H_0, W_D] \neq 0 \Rightarrow$ printzipioz W_D 2 oinarri horietan ez da diagonala izango bakarrik n zehatzean, $\mathcal{E}_n$ azpiespazio bakoitzean bai.

(azpitiko eragileekin trukakorra delako)

↳ hauek ez dute sistema osoa osatzen, n behar dute beltzera endekapenak adierazteko

b) Lor bitez, 2 oinarri horietan, W_D matrizearen elementu diagonalak, hidrogeno-atomoaren ionizazio-energiaren eta egitura-meheko konstantearen funtzioan.

$\langle W_D \rangle_{n\,l\,s\,i\,m_s\,m_l\,m_i}$? eta $\langle W_D \rangle_{n\,l\,s\,i\,j\,J\,m_J}$?

FISIKA KUANTIKOA Kontrola

2017ko martxoak 24

1.)

$\{|+\rangle, |-\rangle\}$ baita

Bi dimentsioko bektore-espazioa $\Rightarrow \{|1\rangle, |2\rangle\}$ oinarri ortonormala

Bektore espazio horretako Pauli-ren σ_y matrizea $\Rightarrow \sigma_y = i\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

a) σ_y hermitikoa den ikusteko hori ze betetzen den edo ez ikusiko dugu.

A matrizea hermitikoa baita $(A^t)^* = A$

Orduan $\Rightarrow$ $\sigma_y{}^t = i\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \Rightarrow (\sigma_y{}^t)^* = -i\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \sigma_y$

<u>Hermitikoa da</u> ($\Rightarrow$ bere autobalioak errealak dira)

b) σ_y-ren autobektoreetara proiektatzen duten proiektoreen matrizeak:

Lehenengo σ_y-ren autobektoreak kalkulatuko ditugu:

$$|\sigma_y - \lambda \mathbb{1}| = \begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} = \lambda^2 - 1 = 0 \rightarrow \lambda = \pm 1$$

• $\lambda_1 = 1 \Rightarrow$ $\begin{pmatrix} -1 & -i \\ i & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -a-ib \\ ia-b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \rightarrow b = ia \Rightarrow$

$$|\varphi_1\rangle = \frac{1}{\sqrt{2}}[|1\rangle + i|2\rangle]$$

• $\lambda_2 = -1 \Rightarrow$ $\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a-ib \\ ia+b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \rightarrow a = ib \rightarrow ia = -b$

$$|\varphi_2\rangle = \frac{1}{\sqrt{2}}[|1\rangle - i|2\rangle]$$

* $\lambda_1 = 1 \Rightarrow$ $\hat{P}_1 = |\varphi_1\rangle\langle\varphi_1| \rightarrow$ Matrizea $\{|\varphi_1\rangle, |\varphi_2\rangle\}$ oinarrian garatuko dugu eta gero oinarri aldaketa baten bidez $\{|1\rangle, |2\rangle\}$ oinarrian garatuko dugu.

- $\langle \varphi_1 | \hat{P}_1 | \varphi_1 \rangle = \langle \varphi_1 | \varphi_1 \rangle \langle \varphi_1 | \varphi_1 \rangle = 1$ (Normalizatuta)
- $\langle \varphi_1 | \hat{P}_1 | \varphi_2 \rangle = \langle \varphi_1 | \varphi_1 \rangle \langle \varphi_1 | \varphi_2 \rangle = 0$ (ortonormalak)
- $\langle \varphi_2 | \hat{P}_1 | \varphi_1 \rangle = \langle \varphi_2 | \varphi_1 \rangle \langle \varphi_1 | \varphi_1 \rangle = 0$
- $\langle \varphi_2 | \hat{P}_1 | \varphi_2 \rangle = \langle \varphi_2 | \varphi_1 \rangle \langle \varphi_1 | \varphi_2 \rangle = 0$

$\{|\varphi_1\rangle, |\varphi_2\rangle\}$ oinarria

$$\Rightarrow \hat{P}_1' = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$|2\rangle$-ren koefizienteak $\{|\varphi_1\rangle, |\varphi_2\rangle\}$-n

oinarri aldaketa $\Rightarrow$ $P_1 = T^{-1} P_1' T \Rightarrow T = \begin{pmatrix} | & | \\ | & | \end{pmatrix}$ *[1]

$|1\rangle$-en koefizienteak $\{|\varphi_1\rangle, |\varphi_2\rangle\}$-n

*[1]

- $|1\rangle = \alpha|\varphi_1\rangle + \beta|\varphi_2\rangle = \frac{\alpha}{\sqrt{2}}\{|1\rangle + i|2\rangle\} + \frac{\beta}{\sqrt{2}}\{|1\rangle - i|2\rangle\} \Rightarrow \alpha = \beta = \frac{1}{\sqrt{2}}$

$$|1\rangle = \frac{1}{\sqrt{2}}|\varphi_1\rangle + \frac{1}{\sqrt{2}}|\varphi_2\rangle$$

- $|2\rangle = \alpha|\varphi_1\rangle + \beta|\varphi_2\rangle = \frac{\alpha}{\sqrt{2}}\{|1\rangle + i|2\rangle\} + \frac{\beta}{\sqrt{2}}\{|1\rangle - i|2\rangle\} \Rightarrow \alpha = -\beta = \frac{-i}{\sqrt{2}}$

$$|2\rangle = \frac{i}{\sqrt{2}}\{|\varphi_2\rangle - |\varphi_1\rangle\} \Rightarrow T = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \rightarrow T^{-1} = \frac{(\mathrm{adj}T)^t}{|T|}$$

$$\mathrm{adj}\, T = \begin{pmatrix} \frac{1}{\sqrt{2}}i & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}}i & \frac{1}{\sqrt{2}} \end{pmatrix}, \quad |T| = \begin{vmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{vmatrix} = \frac{i}{2} + \frac{i}{2} = i$$

$$T^{-1} = -i \begin{pmatrix} \frac{1}{\sqrt{2}}i & \frac{1}{\sqrt{2}}i \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$$

$$\Rightarrow P_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$$

* $\lambda_2 = -1 \Rightarrow \hat{P}_2 = |\varphi_2\rangle\langle\varphi_2|$

- $\langle 1|\hat{P}_2|1\rangle = \langle 1|\varphi_2\rangle\langle\varphi_2|1\rangle = |\langle 1|\varphi_2\rangle|^2 = \frac{1}{2}$

- $\langle 1|\hat{P}_2|2\rangle = \langle 1|\varphi_2\rangle\langle\varphi_2|2\rangle = \frac{1}{\sqrt{2}}\,\langle 2|\varphi_2\rangle^* = \frac{1}{\sqrt{2}}\left(\frac{-i}{\sqrt{2}}\right)^* = \frac{i}{2}$

- $\langle 2|\hat{P}_2|1\rangle = \langle 2|\varphi_2\rangle\langle\varphi_2|1\rangle = \langle 2|\varphi_2\rangle\langle 1|\varphi_2\rangle^* = \frac{-i}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}} = \frac{-i}{2}$

- $\langle 2|\hat{P}_2|2\rangle = \langle 2|\varphi_2\rangle\langle\varphi_2|2\rangle = |\langle 2|\varphi_2\rangle|^2 = \frac{1}{2}$

$$\Rightarrow \quad P_2 = \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$$

- Frogatu proiektoreak ortogonalak direla $\Rightarrow$ $P_1 P_2 = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}\frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} =$

$$\frac{1}{4}\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$ ortogonalak

- Itxitura erlazioa: $\sum_n \hat{P}_n = \mathbb{1}$

$$\sum_{n=1}^{2} \hat{P}_n = \hat{P}_1 + \hat{P}_2 = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} = \frac{1}{2}\left[\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}\right] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

c) Kontsideratu orain 3 dimentsioko bektore-espazio baten $\{|1\rangle, |2\rangle, |3\rangle\}$ oinarri ortonormala. $\Rightarrow$ J_y matrizea

$$\begin{matrix} |1\rangle & |2\rangle & |3\rangle \\ \downarrow & \downarrow & \downarrow \\ 1 & 0 & -1 \end{matrix} \quad \text{autobal.}$$

$$J_y = \frac{\hbar i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \Rightarrow \text{Hermitiarra den jakiteko: } J_y \overset{?}{=} (J_y^t)^*$$

$$J_y^t = \frac{\hbar i}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \rightarrow (J_y^t)^* = -\frac{\hbar i}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} = \frac{\hbar i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} = J_y$$

Hermitikoa da

* J_y-ren osagaiak kalkulatzeko: $\hat{J}_y = \frac{\hat{J}_+ - \hat{J}_-}{2i}$ eta $\langle i|\hat{J}_y|j\rangle$ kalkulatu.

$$\Rightarrow J_y = \frac{\hbar i}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \rightarrow \quad |J_y - \lambda I| = \begin{vmatrix} -\lambda & -\hbar i/\sqrt{2} & 0 \\ \hbar i/\sqrt{2} & -\lambda & -\hbar i/\sqrt{2} \\ 0 & \hbar i/\sqrt{2} & -\lambda \end{vmatrix} =$$

$$-\lambda^3 + \frac{\lambda \hbar^2}{2} \cdot 2 = -\lambda^3 + \lambda\hbar^2 = 0 \rightarrow \lambda(\hbar^2 - \lambda^2) = 0 \rightarrow \lambda_1 = 0,\ \lambda_2 = \hbar,\ \lambda_3 = -\hbar$$

$$\bullet\ \lambda_1 = 0 \Rightarrow \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} -b \\ a-c \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow a = c,\ b = 0 \quad |\varphi_1\rangle = \frac{1}{\sqrt{2}}[|1\rangle + |3\rangle]$$

$$\bullet\ \lambda_2 = \hbar \Rightarrow \begin{pmatrix} -\hbar & -\hbar i/\sqrt{2} & 0 \\ \hbar i/\sqrt{2} & -\hbar & -\hbar i/\sqrt{2} \\ 0 & \hbar i/\sqrt{2} & -\hbar \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \hbar \begin{pmatrix} -1 & -i/\sqrt{2} & 0 \\ i/\sqrt{2} & -1 & -i/\sqrt{2} \\ 0 & i/\sqrt{2} & -1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} =$$

$$\hbar \begin{pmatrix} -a - ib/\sqrt{2} \\ ai/\sqrt{2} - b - ic/\sqrt{2} \\ ib/\sqrt{2} - c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow \begin{array}{l} -a = ib/\sqrt{2} \rightarrow a = -ib/\sqrt{2} \\ c = ib/\sqrt{2} \rightarrow a = -c \end{array}$$

$$|\varphi_2\rangle = \frac{1}{2}[|1\rangle + \sqrt{2}i|2\rangle - |3\rangle]$$

$$\bullet\ \lambda_3 = -\hbar \Rightarrow \begin{pmatrix} \hbar & -\hbar i/\sqrt{2} & 0 \\ \hbar i/\sqrt{2} & \hbar & -\hbar i/\sqrt{2} \\ 0 & \hbar i/\sqrt{2} & \hbar \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \hbar \begin{pmatrix} +1 & -i/\sqrt{2} & 0 \\ i/\sqrt{2} & 1 & -i/\sqrt{2} \\ 0 & i/\sqrt{2} & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} =$$

$$\hbar \begin{pmatrix} a - ib/\sqrt{2} \\ ia/\sqrt{2} + b - ic/\sqrt{2} \\ bi/\sqrt{2} + c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{array}{l} a = ib/\sqrt{2} \rightarrow b = -i\sqrt{2}a \\ \qquad \rightarrow a = -c \Rightarrow |\varphi_3\rangle = \frac{1}{2}[|1\rangle - \sqrt{2}i|2\rangle - |3\rangle] \\ c = -ib/\sqrt{2} \\ \quad \hookrightarrow b = ic\sqrt{2} \end{array}$$

itxaitura erlazioa + normalizazioa edozeinetan bete behar da

d) $\lambda_1 \Rightarrow \hat{P}_1 = |\varphi_1\rangle\langle\varphi_1| \Rightarrow \{|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle\}$ oinarrian.

$$\langle\varphi_1|\hat{P}_1|\varphi_1\rangle = 1 \ ; \ \langle\varphi_i|\hat{P}_1|\varphi_j\rangle = \langle\varphi_i|\varphi_1\rangle\langle\varphi_1|\varphi_j\rangle = \delta_{i1}\delta_{1j}$$

Orduan $[\hat{P}_1] = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ $\{|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle\}$ oinarrian

$\lambda_2 \Rightarrow \hat{P}_2 = |\psi_2\rangle\langle\psi_2| \Rightarrow \quad \langle\psi_i|\hat{P}_2|\psi_j\rangle = \delta_{i2}\delta_{2j} \Rightarrow [\hat{P}_2] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

$\lambda_3 \Rightarrow \hat{P}_3 = |\psi_3\rangle\langle\psi_3| \Rightarrow \quad \langle\psi_i|\hat{P}_3|\psi_j\rangle = \delta_{i3}\delta_{3j} \Rightarrow [\hat{P}_3] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

* $\{|1\rangle, |2\rangle, |3\rangle\}$ oinarrian idazteko oinarri aldaketa egin beharko dugu.

$U' = T^{-1} U T \rightarrow T \rightarrow$ $\{|1\rangle, |2\rangle, |3\rangle\}$ autobektoreen koefizienteak $\{|\psi_i\rangle\}_{i=1}^{3}$

oinarrian zutabetan.

$*^1$ $|1\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle + \gamma|\psi_3\rangle = \frac{\alpha}{\sqrt{2}}\{|1\rangle + |3\rangle\} + \frac{\beta}{2}\{|1\rangle + \sqrt{2}i|2\rangle - |3\rangle\} +$

$\frac{\gamma}{2}\{|1\rangle - \sqrt{2}i|2\rangle - |3\rangle\} \rightarrow \quad \frac{\alpha}{\sqrt{2}} - \frac{\beta}{2} - \frac{\gamma}{2} = 0 \rightarrow \alpha = \frac{\beta+\gamma}{\sqrt{2}}, \quad \frac{\beta\sqrt{2}i}{2} - \frac{\gamma\sqrt{2}i}{2} = 0 \rightarrow \gamma = \beta$

$\Rightarrow |1\rangle = \frac{1}{2}\{\sqrt{2}|\psi_1\rangle + |\psi_2\rangle + |\psi_3\rangle\}$

$*^2$ $|2\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle + \gamma|\psi_3\rangle \rightarrow \quad \frac{\alpha}{\sqrt{2}} + \frac{\beta}{2} + \frac{\gamma}{2} = 0 \rightarrow \alpha = -\frac{(\beta+\gamma)}{\sqrt{2}}, \quad -\frac{\beta}{2} + \frac{\alpha}{\sqrt{2}} - \frac{\gamma}{2} = 0 \Rightarrow$

$\alpha = 0, \quad \beta = -\gamma = \frac{1}{\sqrt{2}i} = \frac{-i}{\sqrt{2}} \Rightarrow |2\rangle = \frac{-i}{\sqrt{2}}\{|\psi_2\rangle - |\psi_3\rangle\}$

$*^3$ $|3\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle + \gamma|\psi_3\rangle \rightarrow \quad \frac{\alpha}{\sqrt{2}} + \frac{\beta}{2} + \frac{\gamma}{2} = 0 \rightarrow \alpha = -\frac{(\beta+\gamma)}{\sqrt{2}} \quad / \quad \frac{\sqrt{2}i\beta}{2} - \frac{\gamma\sqrt{2}i}{2} = 0 \rightarrow$

$\gamma = \beta \rightarrow \quad \alpha = -\sqrt{2}\beta \quad \Rightarrow |3\rangle = \frac{1}{2}\{\sqrt{2}\psi_1 - |\psi_2\rangle - |\psi_3\rangle\}$

$$\Rightarrow T = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 1/\sqrt{2} \\ 1/2 & -i/\sqrt{2} & -1/2 \\ 1/2 & i/\sqrt{2} & -1/2 \end{pmatrix} \rightarrow |T| = \frac{i}{4} + \frac{i}{4} + \frac{i}{4} + \frac{i}{4} = i$$

$$(\mathrm{adj}\,T) = \begin{pmatrix} i/\sqrt{2} & 0 & i/\sqrt{2} \\ i/2 & -i/\sqrt{2} & -i/2 \\ i/2 & 1/\sqrt{2} & -i/2 \end{pmatrix} \Rightarrow T^{-1} = \frac{(\mathrm{adj}\,T)^{t}}{|T|} = -i\begin{pmatrix} i/\sqrt{2} & i/2 & i/2 \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} \\ i/\sqrt{2} & -i/2 & -i/2 \end{pmatrix} =$$

$$\begin{pmatrix} 1/\sqrt{2} & 1/2 & 1/2 \\ 0 & i/\sqrt{2} & -i/\sqrt{2} \\ 1/\sqrt{2} & -1/2 & -1/2 \end{pmatrix} \Rightarrow [\hat{P}_1] = \begin{pmatrix} 1/\sqrt{2} & 1/2 & 1/2 \\ 0 & i/\sqrt{2} & -i/\sqrt{2} \\ 1/\sqrt{2} & -1/2 & -1/2 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/2 & -i/\sqrt{2} & -1/2 \\ 1/2 & +i/\sqrt{2} & -1/2 \end{pmatrix} =$$

$\{|\psi_i\rangle\}_{i=1}^{3}$ -ren koordenatuak $\{|1\rangle, |2\rangle, |3\rangle\}$ oinarrian

$$\begin{pmatrix} 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \\ 1/\sqrt{2} & 0 & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/2 & -i/\sqrt{2} & -1/2 \\ 1/2 & i/\sqrt{2} & -1/2 \end{pmatrix} = \begin{pmatrix} 1/2 & 0 & 1/2 \\ 0 & 0 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

$$\Rightarrow [\hat{P}_2] = \begin{pmatrix} 1/\sqrt{2} & 1/2 & 1/2 \\ 0 & i/\sqrt{2} & -i/\sqrt{2} \\ 1/\sqrt{2} & -1/2 & -1/2 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/2 & -i/\sqrt{2} & -1/2 \\ 1/2 & i/\sqrt{2} & -1/2 \end{pmatrix} = \begin{pmatrix} 0 & 1/2 & 0 \\ 0 & i/\sqrt{2} & 0 \\ 0 & -1/2 & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/2 & -i/\sqrt{2} & -1/2 \\ 1/2 & i/\sqrt{2} & -1/2 \end{pmatrix} =$$

$$\begin{pmatrix} 1/4 & -i/2\sqrt{2} & -1/4 \\ i/2\sqrt{2} & 1/2 & -i/2\sqrt{2} \\ -1/4 & i/2\sqrt{2} & 1/4 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1/2 & -i/\sqrt{2} & -1/2 \\ +i/\sqrt{2} & 1 & -i/\sqrt{2} \\ -1/2 & i/\sqrt{2} & 1/2 \end{pmatrix}$$

$$\Rightarrow [\hat{P}_3] = \begin{pmatrix} 1/\sqrt{2} & 1/2 & 1/2 \\ 0 & i/\sqrt{2} & -i/\sqrt{2} \\ 1/\sqrt{2} & -1/2 & -1/2 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/2 & -i/\sqrt{2} & -1/2 \\ 1/2 & i/\sqrt{2} & -1/2 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1/2 \\ 0 & 0 & -i/\sqrt{2} \\ 0 & 0 & -1/2 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/2 & -i/\sqrt{2} & -1/2 \\ 1/2 & i/\sqrt{2} & -1/2 \end{pmatrix} =$$

$$\begin{pmatrix} 1/4 & i/2\sqrt{2} & -1/4 \\ -i/2\sqrt{2} & 1/2 & i/2\sqrt{2} \\ -1/4 & -i/2\sqrt{2} & 1/4 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1/2 & i/\sqrt{2} & -1/2 \\ -i/\sqrt{2} & 1 & i/\sqrt{2} \\ -1/2 & -i/\sqrt{2} & 1/2 \end{pmatrix}$$

Ortogonalak direla frogatuko dugu aurreko oinarriaren adierazpenean:

$$[\hat{P}_1][\hat{P}_2] = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad [\hat{P}_1][\hat{P}_3] = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$[\hat{P}_2][\hat{P}_3] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Itxitura baldintza $\Rightarrow$ $\sum_i \hat{P}_i = \mathbb{1} = \hat{P}_1 + \hat{P}_2 + \hat{P}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} =$

$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ (* Beste oinarrian ere egin daiteke baina errazagoa da horrela)

Zeeman bortitza
+
Stark efektua ↳ perturbazioak

2)

a) $E, B \rightarrow$ eremu estatiko eta uniformeak (B handia eta E txikia)

Hidrogeno-atomoa (spin momentu angeluarra kontsideratu + espin-orbita arbuiatu) $\Rightarrow n=2$ energiak eta egoera geldikorrak aztertu.

* B eta E paraleloak $\Rightarrow$ z norabidean jarriko dugu

$$\hat{H} = \hat{H}_0 - \vec{M}\cdot\vec{B} + e\vec{E}\cdot\vec{r} = \hat{H}_0 - (\vec{M}_L + \vec{M}_S)\cdot\vec{B} + eEz = \hat{H}_0 + \frac{\mu_B}{\hbar}(\vec{L}+2\vec{S})\cdot\vec{B} +$$

$$eEz = \underbrace{\hat{H}_0 + \frac{\mu_B}{\hbar}(L_z+2S_z)B}_{\hat{H}_1} + \underbrace{eEz}_{\hat{W}}$$

$\Rightarrow$ Perturbazioki aztertuko dugu eremuaren eragina.

↳ elektrikoa soilik

$\hat{H}_1 \Rightarrow |n\, l\, s\, m_l\, m_s\rangle = |\varphi_n^0\rangle \Rightarrow E_n^0 = -\frac{E_I}{n^2} + \mu_B B(m_l + 2m_s)$

$n=2$ energiak $\rightarrow$ $l=0,1 \rightarrow m_l = \begin{cases} -1 \\ 0 \\ 1 \end{cases}$ $(g=2)$ $\rightarrow m_s = \pm 1/2$ $(s=1/2$ finkoa$)$

- $l=0,\ m_s=1/2,\ m_l=0 \rightarrow E_1^0 = -\frac{E_I}{4} + \mu_B B\cdot\frac{2}{2} = \mu_B B - \frac{E_I}{4}$ $(g=2)$

- $l=0,\ m_l=0,\ m_s=-1/2 \rightarrow E_2^0 = -\frac{E_I}{4} + \mu_B B\, 2\left(-\frac{1}{2}\right) = -\frac{E_I}{4} - \mu_B B$ $(g=2)$

- $l=1,\ m_l=-1,\ m_s=1/2 \rightarrow E_3^0 = -\frac{E_I}{4} + \mu_B B\cdot 0 = -\frac{E_I}{4}$ $(g=2)$

- $l=1,\ m_l=-1,\ m_s=-1/2 \rightarrow E_4^0 = -\frac{E_I}{4} + \mu_B B(-2) = -2\mu_B B - \frac{E_I}{4}$

- $l=1,\ m_l=0,\ m_s=1/2 \rightarrow \cancel{E_5}^0 = -\frac{E_I}{4} + \mu_B B\cdot\frac{2}{2} = \mu_B B - \frac{E_I}{4} = E_1^0$

- $l=1,\ m_l=0,\ m_s=-1/2 \rightarrow E_2^0 = -\frac{E_I}{4} - \mu_B B$

- $l=1,\ m_l=1,\ m_s=1/2 \rightarrow E_5^0 = -\frac{E_I}{4} + 2\mu_B B$

• $l=1$, $m_l=1$, $m_s=-1/2 \rightarrow$ $\cancel{E_6^0} = -\frac{E_I}{4} + \mu_B B \cdot 0 = -\frac{E_I}{4} = E_3^0$

✱ Perturbazioa aztertu.

1. $E_4^0 = -2\mu_B B - \frac{E_I}{4}$ $(g=1) \rightarrow$ $|\psi_4^0\rangle = |2\ 1\ -1\ -1/2\rangle$

$E_4(\lambda) = \mathcal{E}_0 + \lambda\mathcal{E}_1 + O(\lambda^2)$; $\mathcal{E}_0 = E_4^0$, $|0\rangle = |\psi_4^0\rangle$

$|\psi_4(\lambda)\rangle = |0\rangle + \lambda|1\rangle + O(\lambda^2)$

• $\mathcal{E}_1 = \langle\psi_4^0|\tilde{W}|\psi_4^0\rangle = \langle 2\ 1\ -1\ -1/2\ |eEz|\ 2\ 1\ -1\ -1/2\rangle =$

$z = rY_1^0\sqrt{\frac{4\pi}{3}}$

$eE\langle 2\,1\,-1\,-1/2\,|z|\,2\,1\,-1\,-1/2\rangle = eE\int |R_{21}(r)|^2\ z\,|Y_1^{-1}(\theta,\phi)|^2 d^3r =$

$\sqrt{\frac{4\pi}{3}}\, eE\int_0^\infty |R_{21}(r)|^2 r^3 dr \int |Y_1^{-1}(\theta,\phi)|^2\ Y_1^0(\theta,\phi)\, d\Omega = 0$ → bakoitia

✱ Perpendikularrak badira → $\vec{E} = E\hat{x} \rightarrow W = eEx$

$\mathcal{E}_1 = \langle\psi_4^0|\tilde{W}|\psi_4^0\rangle = \langle 2\,1\,-1\,-1/2\,|eEx|\,2\,1\,-1\,-1/2\rangle = eE\langle 2\,1\,-1\,-1/2|x|2\,1\,-1\,-1/2\rangle =$

$x = r\sqrt{\frac{2\pi}{3}}(Y_1^{-1} - Y_1^{1})$ → $m=-1$

$eE\int |R_{21}(r)|^2 x\,|Y_1^{-1}(\theta,\phi)|^2 d^3r = eE\sqrt{\frac{2\pi}{3}}\int_0^\infty |R_{21}(r)|^2 r^3 dr \int (Y_1^{-1} - Y_1^{1})|Y_1^{-1}(\theta,\phi)|^2 d\Omega \overset{?}{=}$

$eE\sqrt{\frac{2\pi}{3}}\int_0^\infty |R_{21}(r)|^2 r^3 dr \int \underbrace{(Y_1^1(\theta,\phi) - Y_1^{-1}(\theta,\phi))|Y_1^{-1}(\theta,\phi)|^2}_{\text{Bakoitia}} d\Omega = 0$ (Paritatea)

$|1\rangle = \sum_n\sum_{m_l}\sum_{m_s}\sum_i^g \frac{|\langle n\,l\,m_l\,m_s|\tilde{W}|2\,1\,-1\,-1/2\rangle|}{E_4^0 - E_{n,m_l,m_s}}|n\,l\,m_l\,m_s\rangle$ (E_7 dugu kalkulatzeko)

Berdt perpendikular zein paralelo izanda lehen ordenako zuzenketarik ez dago.

2. $E_5^0 = -\frac{E_I}{4} + 2\mu_B B \rightarrow$ $|\psi_5^0\rangle = |2\ 1\ 1\ 1/2\rangle$

$E_5(\lambda) = \mathcal{E}_0 + \lambda\mathcal{E}_1 + O(\lambda^2)$, $|\psi_5(\lambda)\rangle = |0\rangle + O(\lambda)$

$$eE\frac{\sqrt{3}}{4\pi}\int_0^\infty R_{20}^*(r)R_{21}(r)r^3dr\int_0^\pi 2\pi\sin\theta\cos^2\theta\,d\theta = \frac{eE\sqrt{3}}{2}\int_0^\infty R_{20}^*(r)R_{21}(r)r^3dr.$$

$$-\frac{\cos^3\theta}{3}\Big]_0^\pi = \frac{eE\sqrt{3}}{\cancel{2}}\int_0^\infty R_{20}^*(r)R_{21}(r)r^3dr\cdot\frac{1}{3}\left(+\cancel{1+1}\right) =$$

$$\frac{eE}{\sqrt{3}}\int_0^\infty 2\left(\frac{Z}{2a_0}\right)^{3/2}\left(1-\frac{Zr}{2a_0}\right)e^{-Zr/2a_0}\cdot\frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)e^{-Zr/2a_0}r^3dr =$$

$$\frac{Z}{a_0}\frac{\cancel{2}eE}{3}\frac{1}{2^{\cancel{3}}}\left(\frac{Z}{a_0}\right)^3\int_0^\infty e^{-Zr/a_0}\left(r^3-\frac{Zr^4}{2a_0}\right)r\,dr = \left(\frac{Z}{a_0}\right)^4\frac{eE}{6}\cdot$$

Hermitikoa (eta erreala)

$$\int_0^\infty e^{-Zr/a_0}\left(r^4-\frac{Zr^5}{a_0}\right)dr = \langle 2\,1\,0\,1/2\,|\,W\,|\,2\,0\,0\,1/2\rangle = W_1$$

Hau egiten badugu $\Rightarrow W^{(2)} = \begin{pmatrix} 0 & W_1 \\ W_1 & 0 \end{pmatrix} \Rightarrow |W^{(2)}-\lambda\mathbb{1}| = \begin{vmatrix} -\lambda & W_1 \\ W_1 & -\lambda \end{vmatrix} =$

$\lambda^2 - W_1^2 = 0 \to \lambda = \pm W_1 \to \varepsilon_1$ zuzenketak $\Rightarrow$ balioztatzeko $|0\rangle$ bat

lortu

* Gauza bera egin $\vec{E} = E\hat{x}$ denean eta E_2^0, E_3^0 energiekin.

b) B eremu magnetiko estatiko eta uniformean kokaturiko hidrogeno atomoa (B handia). Efektu elastikoak (egitura mehea) perturbazio bezala hartuz zeintzuk dira ordena txikieneko autobalioak?

edo $|n\,l\,j\,m_s\rangle$

$\hookrightarrow$ W-ren autobalioak (endekapena desagertu)

$$\underbrace{H = H_0 + \frac{\mu_B}{\hbar}(L_z+2S_z)B}_{H_1} + W \qquad W \to W_{mv}+W_p+W_{so}$$

ordena txikiena $|0\rangle = |n\,l\,s\,m_l\,m_s\rangle$

$H_1 \Rightarrow |n,l,s,m_l,m_s\rangle \to E_{n,m_l,m_s} = -\frac{E_I}{n^2}+\mu_B B(m_l+2m_s)$

• $\mathcal{E}_0 = E_S^0 = -\frac{E_I}{4} + 2\mu_B B \qquad |0\rangle = |2\ 1\ 1\ 1/2\rangle = |\psi_S^0\rangle$

$z = r Y_1^0 \sqrt{\frac{4\pi}{3}}$

$\mathcal{E}_1 = \langle \psi_S^0 | \tilde{W} | \psi_S^0 \rangle = \langle 2\ 1\ 1\ 1/2 | eEz | 2\ 1\ 1\ 1/2 \rangle =$

$eE \langle 2\ 1\ 1\ 1/2 | z | 2\ 1\ 1\ 1/2 \rangle = eE \int |R_{21}(r)|^2 z |Y_1^1(\theta,\phi)|^2 d\Omega =$

$\sqrt{\frac{4\pi}{3}} \cdot eE \int_0^\infty |R_{21}(r)|^2 r^3 dr \int \underbrace{Y_1^0 |Y_1^1|^2}_{\text{bakoitia}} d\Omega = 0$

* Perpendikularrak badira $\Rightarrow \vec{E} = E\hat{x}, \quad W = eEx$

$\mathcal{E}_1 = \langle \psi_S^0 | \tilde{W} | \psi_S^0 \rangle = \langle 2\ 1\ 1\ 1/2 | eEx | 2\ 1\ 1\ 1/2 \rangle \overset{\text{paritatea}}{=} 0$

Beraz $\perp$ zein $\parallel$ izanda ez dago lehen ordenako zuzenketarik.

3. $E_1^0 = -\frac{E_I}{4} + \mu_B B \Rightarrow g = 2$ endakapena

$W^{(1)}$ (W-ren murriztketa E_1^0-en azpiespazioan) diagonalizatu behar dugu.

$W = eEz \Rightarrow E_1^0$ energia duten egoerak $\begin{cases} |\psi_{1,1}^0\rangle = |2, 0, 0, 1/2\rangle \\ |\psi_{1,2}^0\rangle = |2, 1, 0, 1/2\rangle \end{cases}$

$W^{(1)} \Rightarrow$ 2x2-koa : • $\langle \psi_{1,1}^0 | W | \psi_{1,1}^0 \rangle = \langle 2\ 0\ 0\ 1/2 | eEz | 2\ 0\ 0\ 1/2 \rangle =$

$eE \langle 2\ 0\ 0\ 1/2 | z | 2\ 0\ 0\ 1/2 \rangle \overset{\text{paritatea}}{=} 0 = \langle \psi_{1,2}^0 | W | \psi_{1,2}^0 \rangle$

Hermitikoa

• $\langle \psi_{1,1}^0 | W | \psi_{1,2}^0 \rangle = \langle 2\ 0\ 0\ 1/2 | eEz | 2\ 1\ 0\ 1/2 \rangle = eE \langle 2\ 0\ 0\ 1/2 | z | 2\ 1\ 0\ 1/2 \rangle =$

$z = r Y_1^0 \sqrt{\frac{4\pi}{3}}$

$eE \int R_{20}^*(r) R_{21}(r) Y_0^{0*}(\theta,\phi) z Y_1^0(\theta,\phi) d^3r = eE \int_0^\infty R_{20}^*(r) R_{21}(r) r^3 dr \left[\sqrt{\frac{4\pi}{3}} \int Y_1^{0\,2}(\theta,\phi) \cdot \right.$

$\left. Y_0^0(\theta,\phi) d\Omega \right] = eE \int_0^\infty R_{20}^*(r) R_{21}(r) r^3 dr \sqrt{\frac{4\pi}{3}} \int \frac{1}{4} \cdot \frac{3}{\pi} \cdot \frac{1}{2} \frac{1}{\sqrt{\pi}} \cos^2\theta \, d\Omega =$

FISIKA KUANTIKOA:

16-09-20

1. TEORIA KUANTIKOAREN SARRERA: (pasaden urteko bideoak)

• UHIN-FUNTZIOEN ARTEKO BIDERKADURA ESKALARRA:

Ezinbestekoa uhin-funtzioek osatuko duten espazio bektoriala zehazteko → uhin-funtzioak konplexuak direnez espazio bektorial berezia sortu → Hilbert-en espazioa

$\Psi(x,t)$, $\varphi(x,t)$ bi uhin funtzio → bien arteko biderkadura eskalarra

$$\boxed{* \ (\Psi, \varphi) = \int_{-\infty}^{\infty} \Psi^* \varphi \, dx}$$

↳ x-ren menpekoa baino ez delako, hiru dimentsiotan izango bagenu hiru dimentsioko integrala izango litzateke (dx, dy, dz)

Biderkadura eskalarraren propietateak:

a) Ez da trukakorra → $(\Psi, \varphi) = (\varphi, \Psi)^*$ $\quad ((\Psi, \varphi) \neq (\varphi, \Psi))$

b) $\lambda \in \mathbb{C}$, $(\lambda\Psi, \varphi) = \lambda^*(\Psi, \varphi)$; $(\Psi, \lambda\varphi) = \lambda(\Psi, \varphi)$

Ez da elkarkorra

c) Banakorra da → $(\Psi + \xi, \varphi) = (\Psi, \varphi) + (\xi, \varphi)$; integrala lineala delako

d) $(\Psi, \varphi) = 0$ → ortogonalak dira Ψ, φ

e) $(\Psi, \Psi) = 1$ → normalizatuta dago uhin-funtzioa

• MOMENTUEN ERAGILEA

$\Psi(x,t)$ uhin funtzioa ezagututa erraz kalkulatu posizioaren batez-bestekoa:

$$* \ \bar{x} = \int_{-\infty}^{\infty} x \underbrace{\Psi^*(x,t)\,\Psi(x,t)}_{|\Psi(x,t)|^2 = P(x,t)} dx = (\Psi, x\Psi)$$

Honetaz gain desbideraketa estandarra eta bestelako magnitude estatistikoak kalkula daitezke. → bidekadura eskalararen definizioaz baliatu gaitezke

- Momentuaren batez-bestekoa → $A(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,t)\, e^{-ikx}\, dx$ Fourieren transformatua →

$|A(k,t)|^2 = P(k,t)$ k-ren dentsitate probabilitatea → $\bar{p} = \int_{-\infty}^{\infty} \hbar k \underbrace{|A(k,t)|^2}_{P(k,t)} dk$

Baina bitarteko pausua behar da, Fourieren transformatua kalkulatu → errazago → bidekadura eskalararen definizioaz baliatu:

$$\boxed{* \quad \bar{p} = \left(\Psi, -i\hbar \frac{\partial \Psi}{\partial x} \right)}$$

Froga:

$$\bar{p} = \int_{-\infty}^{\infty} \hbar k\, |A(k,t)|^2 dk \overset{\text{hipotesia}}{=} \left(\Psi, -i\hbar \frac{\partial \Psi}{\partial x} \right) = \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{\partial \Psi}{\partial x} \right) dx =$$

k' deitu integralak bereizteko

$$-i\hbar \int_{-\infty}^{\infty} \underbrace{\left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A^*(k,t)\, e^{-ikx}\, dk \right]}_{\Psi^*} \frac{\partial}{\partial x} \underbrace{\left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k',t)\, e^{ik'x}\, dk' \right]}_{\Psi} dx =$$

$$\frac{-i\hbar}{2\pi} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} A^*(k,t)\, e^{-ikx}\, dk \right] i \left[\int_{-\infty}^{\infty} A(k',t)\, e^{ik'x}\, k'\, dk' \right] dx =$$

$$\frac{\hbar}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A^*(k,t)\, e^{-ikx} A(k',t)\, k'\, e^{ik'x}\, dx\, dk'\, dk =$$

$$\frac{\hbar}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A^*(k,t)\, A(k',t)\, k'\, e^{i(k'-k)x}\, dx\, dk'\, dk =$$

$$= \delta(k'-k)$$

$$\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A^*(k,t)\, A(k',t)\, k'\, \delta(k'-k)\, dk'\, dk = \hbar \int_{-\infty}^{\infty} A^*(k,t)\, A(k,t)\, k\, dk =$$

$$\int_{-\infty}^{\infty} \hbar k\, |A(k,t)|^2 dk = \bar{p}$$ ✓ → $\Psi \in \mathbb{R}$ bada $\bar{p} = 0$, bestela irudikaria izango litzatekeelako −i bat dagoelako aurrean

Eragilea, p-rekin lotutakoa → $\hat{p} = -i\hbar \frac{\partial}{\partial x}$

• ERAGILEAK ETA BEHAGARRIAK: POSIZIOA, MOMENTUA, ENERGIA ZINETIKOA...

$\Psi(x,t)$ sistema baten uhin-funtzioa → horrekin → $\begin{cases} \bar{x} = (\Psi, x\Psi) \\ \bar{p} = (\Psi, -i\hbar \frac{\partial \Psi}{\partial x}) \end{cases}$

* Momentuarekin lotutako eragilea: $\hat{p} = -i\hbar \frac{\partial}{\partial x}$
* Posizioarekin lotutako eragilea: $\hat{x} = x$ (goiko argudio bera jarraituz)

Horrela beste magnitude fisikoekin lotutako eragileak aurkitu daitezke:

* $V(x,t)$ energia potentziala → $\bar{V}(x,t) = (\Psi, V\Psi) \leftrightarrow \hat{V} = V(x,t)$
  ↳ x eta t-rekin baino ez delako aldatzen

* $T = \frac{p^2}{2m}$ energia zinetikoa → $\bar{T} = \frac{\overline{p^2}}{2m} = \frac{\hbar^2 \overline{k^2}}{2m} = \int_{-\infty}^{\infty} \frac{\hbar^2 k^2}{2m} \underbrace{|A(k,t)|^2}_{*} dk$

  * $A(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,t) e^{-ikx} dx$ → nola kalkulatu uhin funtziotik abiatuta zuzenean? → $\bar{T} = (\Psi, -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2})$ (Goraino gauza bera)

  Beraz $\hat{T}(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = \frac{\hat{p} \cdot \hat{p}}{2m} = \frac{(-i\hbar \frac{\partial}{\partial x})(-i\hbar \frac{\partial}{\partial x})}{2m} = \frac{\hat{p}^2}{2m}$

  lehengo bat aplikatu gero bestea, jarraian

* Hamiltondarra → $H = T + V$ → $\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t)$

  (Schrödingerren ekuazioan agertzen dena)

* Beraz hainbat magnitude fisikorekin lotuta dauden eragileak daude ⇒ Behagarriak

  Baina edozein eragile ez da magnitude fisiko baten behagarria, eta baldintza batzuk bete behar ditu (hermitikoa, ...)

• ERAGILE ADJUNTOAK:

Demagun $\hat{A}$ eragilea → beti definitu dezakegu bere eragile adjuntua; $\hat{A}^+$

* Bien arteko erlazioa → $(\Psi, \hat{A}\varphi) = (\hat{A}^+\Psi, \varphi)$

  (ψ uhin funtzioa izanda)

$$\int_{-\infty}^{\infty} \Psi^* (\hat{A}\varphi)\, dx = \int_{-\infty}^{\infty} (\hat{A}^+\Psi)^* \varphi \, dx$$

- Adjuntoren, $\hat{A}^+$, propietateak:

a) $\hat{A}$ eta $\hat{B}$ bi eragile badira $\rightarrow$ $(\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+$ aldearantzikatu

b) $\hat{A}$ eta $\hat{B}$ bi eragile badira $\rightarrow$ $(\hat{A}+\hat{B})^+ = \hat{A}^+ + \hat{B}^+$

c) $\lambda \in \mathbb{C}$ bada $(\lambda\hat{A})^+ = \lambda^*\hat{A}^+$

d) $(\hat{A}^+)^+ = \hat{A}$

Froga: $(\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+$ Frogatu beharrekoa

lehenengo $\hat{B}$ gero $\hat{A}$

$\hookrightarrow (\Psi, \hat{A}(\hat{B}\varphi)) = ((\hat{A}\hat{B})^+\Psi, \varphi) = (\hat{B}^+\hat{A}^+\Psi, \varphi) \Longrightarrow$

adjuntuaren definizioz

$(\Psi, \hat{A}(\hat{B}\varphi)) = (\hat{A}^+\Psi, \hat{B}\varphi) = (\hat{B}^+\hat{A}^+\Psi, \varphi)$ ✓ $\leftrightarrow (\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+$

- ERAGILE HERMITIKOAK:

* Eragile hermitikoak eragile adjuntuen kasu partikularra: $\hat{A}$ eta $\hat{A}^+$ badira $\hat{A} = \hat{A}^+$ direnean $\rightarrow$ orduan hermitikoak edo autoadjuntoak

* Kasu partikular honek mekanika kuantikoan ezinbestekoak $\rightarrow$ magnitude fisiko guztiei dagozkien eragileak hermitikoak dira ($\hat{p} = \hat{p}^+, \ldots$)

Izan ere magnitude fisiko bat neurtzean emaitza beti izan behar da erreala, beraz batez bestekoak ere errealak:

- Demagun sistema $\Psi(x,t)$ egoera batean dagoela eta A magnitude fisikoa dela $\rightarrow$

hermitikoa definizioz

$\langle A \rangle = (\Psi, \hat{A}\Psi) = (\hat{A}\Psi, \Psi) = (\Psi, \hat{A}\Psi)^* \in \mathbb{R}$ (Konjokatuaren berdina delako)

Beraz ezinbestekoa $\hat{A} = \hat{A}^+$ izatea erreala izateko;

$(\Psi, \hat{A}\Psi) = (\Psi, \hat{A}\Psi)^*$ izateko

Adibidez: $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ eragilea konplexua izanda nola lortu $\hat{p} \in \mathbb{R}$ izatea?

Frogatuko dugu $(\Psi, \hat{p}\varphi) = (\hat{p}\Psi, \varphi)$ dela $\Leftrightarrow$ $(\Psi, \hat{p}\varphi) = (\Psi, -i\hbar\frac{\partial\varphi}{\partial x}) =$

$(-i\hbar\frac{\partial\Psi}{\partial x}, \varphi) \Rightarrow \int_{-\infty}^{\infty}\Psi^*\left[-i\hbar\frac{\partial\varphi}{\partial x}\right]dx = \int_{-\infty}^{\infty}\left[-i\hbar\frac{\partial\Psi}{\partial x}\right]^*\varphi\, dx \Rightarrow$

$$-i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \varphi}{\partial x}\, dx = i\hbar \int_{-\infty}^{\infty} \frac{\partial \psi}{\partial x}^* \varphi\, dx \Rightarrow \cancel{\varphi \psi^*}\Big]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \psi^* \frac{\partial \varphi}{\partial x}\, dx =$$

Zatikako metodoa aplikatu:

$$\begin{cases} \frac{\partial \psi^*}{\partial x} dx = dv & v = \psi^* \\ \varphi = u & \frac{\partial \varphi}{\partial x} = \frac{du}{dx} \end{cases}$$

$$- \int_{-\infty}^{\infty} \psi^* \frac{\partial \varphi}{\partial x}\, dx \quad * \quad \checkmark$$

* Baina φ, ψ uhin funtzioak normalizagarriak izateko ∞ eta $-\infty$-n anulatu behar dira $\Rightarrow$ $\varphi\psi^*\Big]_{-\infty}^{\infty} = 0$ Beraz frogatuta da $\hat{p}$ hermitiarra dela

16-09-25

• ERAGILE ADJUNTOEN KALKULUA:

* Badakigu $\hat{x}$ eta $\hat{p}$ hermitikoak direla (autoadjuntoak): $\begin{cases} \hat{x}^+ = x \\ \hat{p}^+ = -i\hbar \frac{\partial}{\partial x} \end{cases} \Rightarrow$

eragile hauekin beste eragile batzuk eraikiko ditugu adjuntuen propietateak erabiliz

a) $\hat{A} = x^2$ eragilea (Hermitikoa da), $\hat{A}^+$? $\Rightarrow \hat{A}^+ = (x^2)^+ = (x \cdot x)^+ = x^+ \cdot x^+ = x \cdot x = x^2 = \hat{A}$

$(\hat{A}\cdot\hat{B})^+ = \hat{B}^+\hat{A}^+$

$x^+ = x$

b) $\hat{B} = \frac{\partial}{\partial x}$ eragilea, $\hat{B}^+$? $\Rightarrow \hat{B}^+ = \left(\frac{\hat{p}}{(-i\hbar)}\right)^+ = \left(\frac{1}{-i\hbar}\right)^+ \hat{p}^+ = \frac{1}{i\hbar}\hat{p} = -\frac{\partial}{\partial x} = -\hat{B}$

$(\lambda \hat{A})^+ = \lambda^* \hat{A}^+$

$\hat{p} = \hat{p}^+$

(Ez da hermitikoa) $\rightarrow$ ez dago magnitude fisiko batekin lotuta

c) $\hat{C} = x\frac{\partial}{\partial x}$ eragilea, $\hat{C}^+$? $\Rightarrow \hat{C}^+ = \left(x\frac{\partial}{\partial x}\right)^+ = \left(\frac{\partial}{\partial x}\right)^+ x^+ = \hat{B}^+ x = -\hat{B}x = -\frac{\partial}{\partial x}x$

(Ez da hermitikoa) $\rightarrow$ ez dago magnitude fisiko batekin lotuta

$\hookrightarrow$ ψ aplikatzerakoan $\hat{C}^+\psi = -\frac{\partial}{\partial x}(x\psi) = -\psi - x\frac{\partial \psi}{\partial x}$

• ERAGILE HERMITIKOEN AUTOFUNTZIO ETA AUTOBALIOEN PROPIETATEAK:

Demagun $\hat{A}$ eragile hermitikoa dugula $\Rightarrow (\hat{A} = \hat{A}^+) \Rightarrow$ eta demagun eragile horren autofuntzioak ezagutzen ditugula; $\hat{A}\psi_n = a_n \psi_n$, betetzen duten ψ_n-ak.

autobalioak

autofuntzioak

Suposa dezagun ψ_n-ak normalizaturik daudela $\Rightarrow (\psi_n, \psi_n) = 1$

Propietateak:

1. $a_n \in \mathbb{R}$ (autobalioak errealak dira) $\Rightarrow$ Froga $(\Psi_n, \hat{A}\Psi_n) \overset{\text{autofuntzioaren def}}{=} (\Psi_n, a_n\Psi_n) \overset{\text{biderk. eskalarraren propietateak}}{=} a_n(\Psi_n,\Psi_n) \overset{\text{normal}}{=}$

$a_n \overset{\hat{A} \text{ hermitikoa}}{=} (\hat{A}\Psi_n, \Psi_n) = (a_n\Psi_n, \Psi_n) = a_n^*(\Psi_n,\Psi_n) = a_n^* \Leftrightarrow a_n^* = a_n \Leftrightarrow a_n \in \mathbb{R}$

2. $a_n \neq a_m$ $m\neq n$ (sistema ez-endakatua) $\Rightarrow$ $(\Psi_n, \Psi_m) = 0$ (ortogonalak dira)
$\hookrightarrow m \neq n$

Sistema endakatua bada ezin da aurresan ortogonalak diren edo ez baina beti eraiki daitezke ortogonalak direnak. $\Rightarrow$ *

Froga: * $(\Psi_n, \hat{A}\Psi_m) = (\Psi_n, a_m\Psi_m) = a_m(\Psi_n,\Psi_m) \overset{\hat{A} \text{ autoadjuntoa da}}{=} (\hat{A}\Psi_n, \Psi_m) =$

$(a_n\Psi_n, \Psi_m) = a_n^*(\Psi_n,\Psi_m) = a_n(\Psi_n,\Psi_m) \Rightarrow a_n \neq a_m \Leftrightarrow$

$(\Psi_n,\Psi_m) = 0$

(ORTOGONALAK)

$\hookrightarrow$ autofuntzio horiek oinarri ortogonala sortu $\rightarrow$ beste funtzioak oinarri honetan garatu.

3. Demagun sistema endakatua dugula, $a_n = a_m = a \Leftrightarrow \hat{A}\Psi_n = a_n\Psi_n = a\Psi_n$ eta $\hat{A}\Psi_m = a_m\Psi_m = a\Psi_m$; ezin dugu aurresan Ψ_n eta Ψ_m ortogonalak direnik.

Baina autofuntzio horiek ez dira bakarrak $\rightarrow$ defini dezakegu $\Psi_m' = \alpha\Psi_n + \beta\Psi_m$, edozein, eta honek ere autobalioen ekuazioa beteko du $\Rightarrow \hat{A}\Psi_m' = a\Psi_m'$ *

* $\hat{A}\Psi_m' = \hat{A}(\alpha\Psi_n + \beta\Psi_m) \overset{\text{eragile lineala}}{=} \alpha\hat{A}\Psi_n + \beta\hat{A}\Psi_m = \alpha a\Psi_n + \beta a\Psi_m =$

$a(\beta\Psi_m + \alpha\Psi_n) = a\Psi_m'$

Beraz, eraiki ditzakegu ortogonalak diren bi autofuntzio beti:

* $\Psi_n' = \Psi_n$, $\Psi_m' = \Psi_n + \beta\Psi_m$ definitu, $\Rightarrow$ β? $(\Psi_n', \Psi_m') = 0$?

Beti existitzen da β bat $(\Psi_n', \Psi_m') = 0$ izateko?

Hauxe da kalkulatuko duguna

Bete beharreko ekuazioa $\rightarrow 0 = (\Psi_n', \Psi_m') = (\Psi_n, \Psi_n + \beta\Psi_m) = (\Psi_n, \Psi_n) +$

$(\Psi_n, \beta\Psi_m) = (\Psi_n, \Psi_n) + \beta(\Psi_n, \Psi_m) = 1 + \beta(\Psi_n, \Psi_m) \rightarrow \beta = -\frac{1}{(\Psi_n, \Psi_m)}$

* $(\Psi_n, \Psi_m) = 0$ balitz ez genuke kalkulu hau egin beharko, aldez aurretik bi autofuntzio ortogonal izango genituzkelako.

Beraz, oinarri berria $\Rightarrow$ $\Psi_n' = \Psi_n$, $\Psi_m' = \Psi_m - \frac{1}{(\Psi_n, \Psi_m)}\Psi_m$

normalizatu gabe!

$(\Psi_n', \Psi_m') = 0$

Beraz $\Rightarrow$ sistema endakatua bada ere eta bi autofuntzio ortogonal ez baditugu aurkitzen beti eraiki daitezke bi ortogonalak izateko (Gram-Smith-en metodoa)

- HAMILTONDARRAREN AUTOFUNTZIOAK ETA AUTOBALIOAK:

* $\hat{H}\Psi_n = \mathcal{E}_n\Psi_n$ $\Rightarrow$ ezinbestekoak Schrödingerren ekuazioa garatzeko eta uhin-funtzioen denboraren garapena aztertzeko.

1. Hamiltondarraren eragilea $\rightarrow$ hermitikoa $\leftrightarrow$ $\mathcal{E}_n \in \mathbb{R}$ (Gainera energiak direnez ezinbesteen errealak izan behar dira)

2. $(\Psi_n, \Psi_m) = 0 \leftrightarrow n \neq m$ eta $\mathcal{E}_n \neq \mathcal{E}_m$ (bestela ere beti aurki ditzakegu ortogonalak diren bi autofuntzio)

3. Eragilea erreala da $\rightarrow (\hat{H}\Psi_n = \mathcal{E}_n\Psi_n)^* = \hat{H}^*\Psi_n^* = \hat{H}\Psi_n^* = \mathcal{E}_n^*\Psi_n^* = \mathcal{E}_n\Psi_n^* \Rightarrow$

beraz Ψ_n^* autofuntzioa da ere eta autobalio bera dagokio, $\mathcal{E}_n$

$\leftrightarrow$ sistema endakatua da $\rightarrow$ bien arteko konbinazio lineala den autofuntzioa aukera daiteke eta hau ere autofuntzioa izango da.

Ad: $\Psi_n' = \frac{\Psi_n + \Psi_n^*}{2}$, $\hat{H}\Psi_n' = \mathcal{E}_n\Psi_n'$

$\Psi_n' \in \mathbb{R}$ $\Rightarrow$ Beti aukera daitezke errealak diren autofuntzioak, $\Psi_n \in \mathbb{R}$ izan daitezke

* (Azkenengo ezaugarri hau eragilea erreala denean betetzen da)

- SCHRÖDINGER-EN EKUAZIOAREN EBAZPEN FORMALA:

Schrödingeren ekuazioa: $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$

- Bigarren ordeneko deribatu partzialetako ekuazioa
- Ekuazio lineala

* V kontserbakorra denean $\Leftrightarrow$ denboraren independentea denean (Hidrogenoaren atomoaren kasuan) $\Rightarrow$ x eta t aldagaiak banandu daitezke, desakoplatuta agertzen dira $\Rightarrow$ Aldagaien banantzea aplikatu

letra larria · letra xehea

$$V \neq V(t) \Rightarrow \Psi(x,t) = \psi(x)\varphi(t) \Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi = i\hbar\frac{\partial\Psi}{\partial t} \Rightarrow$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}(\psi(x)\varphi(t)) + V(\psi(x)\varphi(t)) = -\frac{\hbar^2}{2m}\varphi\frac{d^2\psi}{dx^2} + V\psi\varphi = i\hbar\frac{\partial}{\partial t}(\psi\varphi) =$$

$V \neq V(t)$

$\cdot \frac{1}{\psi\varphi} = \frac{1}{\Psi}$

$$i\hbar\psi\frac{d\varphi}{dt} \Rightarrow \underbrace{-\frac{\hbar^2}{2m}\cdot\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V}_{\text{x-ren menpekoa soilik}} = \underbrace{i\hbar\cdot\frac{1}{\varphi}\frac{d\varphi}{dt}}_{\text{t-ren menpekoa soilik}} = E \text{ (kte bat)}$$

energia (dimentsioengatik)

$$\hookrightarrow (1) \quad -\frac{\hbar^2}{2m}\cdot\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E \rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \leftrightarrow \hat{H}\psi = E\psi$$

$\frac{d^2}{dx^2} = \hat{p}^2$ · infinitu

Hamiltondarraren autofuntzio eta autobalioen problema $\Rightarrow \{\psi_n\} \rightarrow \{E_n\}$

$\hookrightarrow$ denboraren independentea den Schrödingeren ekuazioa

$$\hookrightarrow (2) \quad i\hbar\cdot\frac{1}{\varphi}\frac{d\varphi}{dt} = E \rightarrow i\hbar\frac{d\varphi}{dt} = E\varphi \leftrightarrow \frac{d\varphi}{\varphi} = \frac{E}{i\hbar}dt = -\frac{i}{\hbar}E\,dt \rightarrow$$

$$\ln\frac{\varphi}{\varphi_0} = -\frac{i}{\hbar}Et \rightarrow \frac{\varphi}{\varphi_0} = e^{-iEt/\hbar} \rightarrow \varphi = \varphi_0\, e^{-\frac{iEt}{\hbar}}$$

E_n-ak

$\hookrightarrow$ denboraren menpekoa den Schrödingeren ekuazioa:

$$\Rightarrow \Psi_n = \psi_n\, e^{-\frac{i}{\hbar}E_n t}\cdot A \; ; \quad \Psi = \sum_{n=0}^{\infty} A_n \psi_n\, e^{-\frac{iE_n t}{\hbar}} \quad \text{(guztien konbinazio lineala)}$$

$\hookrightarrow$ modu iraunkorrak, geldikorrak

• UHIN FUNTZIOEN DENBORAREN GARAPENA:

Demagun ezagutzen dugula $t=0$-n uhin funtzioa $\Rightarrow \Psi(x,0)$, baina nolakoa da t-ren funtzioan? $\Psi(x,t)$?

* Funtzio geldikorrak erabili $\Rightarrow \Psi_n(x,t) = A\psi_n e^{-i\frac{E_n}{\hbar}t}$ (Demagun normalizatuta daudela ψ_n-ak $\Rightarrow A=1$)
 ↳ egoera geldikorren denboraren garapena

$\Psi(x,0)$ edozein izan daiteke, ez du zertan hamiltondarraren autofuntzio bat izan. Horrela, lehendabizi hamiltondarraren autofuntzioak eta autobalioak kalkulatuko ditugu: $\hat{H}\psi_n = E_n\psi_n$, izan ere, Schrödingerren ekuazioa betetzen duen edozein egoera, egoera geldikorren bitartez garatu daiteke,
↳ $\Psi(x,t)$
oinarri bat osatzen baitute, $\{\psi_n\}$ (Garrera bati aukera dezakegu oinarri ortonormala) $\leftrightarrow$ $(\psi_n, \psi_m) = \delta_{nm}$

* Hortaz $\Rightarrow$ $\Psi(x,t) = \sum_{n=0}^{\infty} c_n \Psi_n = \sum_{n=0}^{\infty} c_n \psi_n e^{-i\frac{E_n}{\hbar}t}$, eta modu berean $t=0$ aldiuneen garatu $\Rightarrow$ $\Psi(x,0) = \sum_{n=0}^{\infty} c_n\psi_n$ Baina c_n?

↳ $(\psi_m, \Psi) = (\psi_m, \sum_{n=0}^{\infty} c_n\psi_n) = \sum_{n=0}^{\infty} c_n \underbrace{(\psi_m, \psi_n)}_{\delta_{nm}} = c_m$

Orain, $\Psi(x,0)$-ren garapena ezagututa, ψ_n bakoitza denboraren funtzioan nola aldatzen den badakigunez, bakoitzari egokituko diogu denboraren garapen hori $\Rightarrow$ $\boxed{\Psi(x,t) = \sum_{n=0}^{\infty} c_n\psi_n e^{-i\frac{E_n}{\hbar}t}}$

• EGOERA IRAUNKORRAK eta EZ-IRAUNKORRAK:

Schrödingerren ekuazioa betetzen duen edozein uhin-funtzio hamiltondarraren autofuntzioen konbinazio lineal modura adierazi daiteke: $\Psi(x,t) = \sum_{n=0}^{\infty} c_n\psi_n e^{-i\frac{E_n}{\hbar}t}$
↳ $\psi_n(x)$

edo zuzenean hamiltondarraren autofuntzioa

a) Egoera iraunkorrak: $\Psi_i(x,t) = \psi_n e^{-i\frac{E_n}{\hbar}t}$ → Hamiltondarraren autofuntzioen ekarpen bakarra dugunean.

→ $P_i = |\Psi_i(x,t)|^2 = |\psi_n|^2$ ↔ denboraren independentea ↔ iraunkorra

b) Egoera ez-iraunkorrak: Beste edozein egoerak, non hamiltondarraren autofuntzioen ekarpen bat baino gehiago dagoen → $\Psi_{ei}(x,t) = \sum_{n=0}^{\infty} c_n \psi_n e^{-i\frac{E_n}{\hbar}t}$ →

$$P_{ei} = |\Psi_{ei}(x,t)|^2 = \underbrace{\left(\sum_{n=0}^{\infty} c_n^* \psi_n^* e^{\frac{iE_n t}{\hbar}}\right)\left(\sum_{m=0}^{\infty} c_m \psi_m e^{\frac{-iE_m t}{\hbar}}\right)}_{=\sum_{n,m} c_n^* c_m \psi_n^* \psi_m e^{-i\frac{E_m - E_n}{\hbar}t}}$$

↔ ez da denboraren independentea

• **HAMILTONDARRAREN AUTOFUNTZIOEN KALKULUAREN BI ADIBIDE: PARTIKULA ASKEAREN AUTOFUNTZIOAK eta POTENTZIAL OSIN-INFINITUA:**

Partikula askea: $V=0 \rightarrow \hat{H} = \hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \Rightarrow \hat{H}\psi = \hat{T}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = \varepsilon\psi$

$\psi = e^{rx}$ ukin funtzioak saiatu $\Rightarrow -\frac{\hbar^2}{2m} r^2 e^{rx} = \varepsilon e^{rx} \rightarrow -\frac{\hbar^2}{2m} r^2 = \varepsilon \rightarrow r = \pm \underbrace{\sqrt{\frac{2m\varepsilon}{\hbar^2}}}_{K}\, i$

$\varepsilon > 0$ ($V=0$ delako) $T \geq 0$ *

* Bestela $\varepsilon < 0$ balitz esponentziala erreala izango litzateke eta ondorioz ez litzateke integragarria izango $(-\infty,\infty)$ mugetan → dentsitate probabilitatea ez litzateke ondo definituta egongo

$\Rightarrow \varepsilon = \frac{\hbar^2 K^2}{2m} \Rightarrow \psi_K = Ae^{iKx} + Be^{-iKx}$ ⇒ energia endekatua da, bi egoerei energia bera dagozkielako (momentu lineal bera ez, kontrakoa) ($\hbar K$ eta $-\hbar K$)

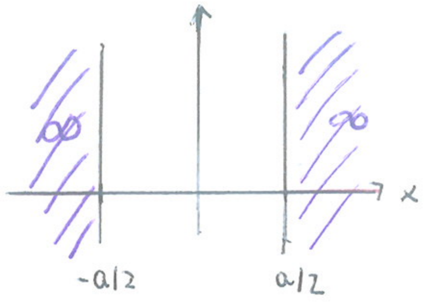
ψ_K orokorrean irudikaria da baina hamiltondarraren ezagutza erreala denez aukera dezakegu erreala den autofuntzioa. Izan ere ψ autofuntzioa bada

ψ^* ere → $\hat{H}\psi^* = \varepsilon\psi^*$, orduan $\psi' = \frac{\psi + \psi^*}{2} = Re(\psi) \in \mathbb{R}$,

orduan, $\psi_K' = A'\sin Kx + B'\cos Kx$ ($A', B' \in \mathbb{R}$) defini dezakegu

(Nahi duguna har dezakegu, ψ_K edo ψ_K')

Potentzial - osin infinitua:



$$V(x) = \begin{cases} 0 & x \in (-a/2, a/2) \\ \infty & x \in (-\infty, -a/2) \cup (a/2, \infty) \end{cases}$$

↳ Jatorrian zentratuta

* Uhin funtzioak bete behar diren baldintzak esanguratsuak izateko:

Partikularen energia finkatuta badago partikula $[-a/2, a/2]$ tartean mugituko da eta hormen kontra jotzean errebotatuko du abiadura konstante lineala; eta honela denbora osoan.

1. Energia potentziala infinitua den tartean uhin funtzioa nulua izan behar da bestela energia infinitua izango delako; $\Psi = 0$ $V = \infty$ tartean

↳ $\hat{H}\Psi = E\Psi$

$x \in (-a/2, a/2)$ tartean $\Rightarrow$ $-\dfrac{\hbar^2}{2m}\dfrac{\partial^2\Psi}{\partial x^2} = \hat{H}\Psi = E\Psi \rightarrow \dfrac{\hbar^2}{2m}\dfrac{\partial^2\Psi}{\partial x^2} + E\Psi = 0 \rightarrow$

$$\frac{\partial^2\Psi}{\partial x^2} + \underbrace{\frac{2mE}{\hbar^2}}_{K^2 \,\rightarrow\, E>0 \text{ delako}}\Psi = 0 \leftrightarrow \frac{\partial^2\Psi}{\partial x^2} + K^2\Psi = 0 \rightarrow \Psi = Ae^{iKx} + Be^{-iKx} \qquad K = \sqrt{\frac{2mE}{\hbar^2}}$$

$x \in (-a/2, a/2)$

2. $V \neq \infty$ den tartean uhin funtzioa eta uhin funtzioaren lehen deribatua jarraituak izan behar dira; $x = -a/2$ eta $x = a/2$ -n jarraitua izan behar da uhin funtzioa. Hala ere, gure kasuan muga horietatik kanpo energia potentziala infinitua denez, ezin da aplikatu lehenengo deribatuaren jarraitutasuna.

$x = a/2 \rightarrow \Psi(a/2^+) = \Psi(a/2^-) = 0 = Ae^{iKa/2} + Be^{-iKa/2}$ →

$x = -a/2 \rightarrow \Psi(-a/2^-) = \Psi(-a/2^+) = 0 = Ae^{-iKa/2} + Be^{iKa/2}$

Soluzio tribiala ez izateko

$$\begin{vmatrix} e^{iKa/2} & e^{-iKa/2} \\ e^{-iKa/2} & e^{iKa/2} \end{vmatrix} = e^{iKa} - e^{-iKa} = 0 = 2i\sin Ka \leftrightarrow Ka = n\pi \quad n \in \mathbb{N}$$

$K_n = \dfrac{n\pi}{a}$ → ezin da edozein izan, balio diskretuak hartzen ditu

Beraz, energiak ezin dira edozein izan $\Rightarrow E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2} = \frac{1}{2m}\left(\frac{\hbar n\pi}{a}\right)^2$

Izan ere, egoera lotuak baditugu non partikula tarte finitu batean baino ezin den mugitu energia diskretua da.

Halaber, gure baldintzetatik lortzen dugu $B=-Ae^{ika}$ dela, hortaz,

$$\boxed{\Psi_n = Ae^{ik_nx} + Be^{-ik_nx} = A\left(e^{ik_nx} - e^{ika - ik_n x}\right) = Ae^{ik_n a/2}\left(e^{-ik_n a/2}e^{ik_nx} - e^{ik_n a/2}e^{-ik_nx}\right) = 2iAe^{ik_na/2}\sin[k_n(x-a/2)] = B_n \sin[k_n(x-a/2)]}$$

(B_n normalizazio baldintzak definitzen du) $\rightarrow \Psi_n = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}(x-a/2)$

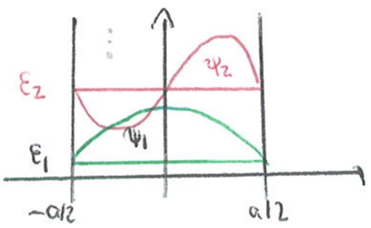
Sistema endekatuta ez dagoenez badakigu Ψ_n-ak ortogonalak izango direla,

$(\Psi_n, \Psi_m) = \delta_{nm}$

Hala ere, uhin funtzioak beste moduetan adieraz daitezke:

- $$\underset{x\in(-a/2,a/2)}{\Psi_n(x)} = \begin{cases} \sqrt{\frac{2}{a}}\cos\frac{n\pi x}{a} & n=2m+1 \\ \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} & n=2m \end{cases} \qquad (m\in\mathbb{N})$$

- Jatorria ertz batean jarriz $\rightarrow \underset{x\in(0,a)}{\Psi_n'(x)} = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$



• PARTIKULA ASKEARI DAGOKION FARDEL-GAUSSIARRAREN DENBORA-GARAPENA:

Demagun $\Psi(x,0) = \left(\frac{2}{\pi a^2}\right)^{1/4} e^{-\frac{x^2}{a^2}} e^{ik_0x}$ $(a\in\mathbb{R})$, gainera $P(x,0) = \left(\frac{2}{\pi a^2}\right)^{1/2} e^{-\frac{2x^2}{a^2}}$.

↗ gaussiarraren zabalerarekin lotuta

↳ normalizazio koefizientea

$\Delta x = \frac{a}{2} \Rightarrow$ Garatu nahi dugu dekonposatuko $\rightarrow$ garatu hamiltondarraren autofuntzioetan.

goian egin dugun bezala

$\{\Psi_n\} = \left\{\frac{e^{ikx}}{\sqrt{2\pi}}\right\}$

↳ uhin-lauak → errealak adieraz daitezke

Lehenengo, uhin paketearen Fourieren transformatua $A(k)$ kalkulatuko dugu:

$$A(k,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \left(\frac{2}{\pi a^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2}} e^{i(k_0-k)x} dx =$$

$* \int_{-\infty}^{\infty} e^{-\alpha^2(x-\beta)^2} dx = \frac{\sqrt{\pi}}{\alpha}$

$$\frac{1}{\sqrt{2\pi}} \left(\frac{2}{\pi a^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-\left(\frac{x^2}{a^2} - i(k_0-k)x\right)} dx =$$

$$\frac{1}{\sqrt{2\pi}} \left(\frac{2}{\pi a^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-\left(\left[\frac{x}{a} - i\frac{(k_0-k)a}{2}\right]^2 + \frac{(k_0-k)a^2}{4}\right)} dx = e^{-\frac{(k_0-k)a^2}{4}} \cdot \frac{1}{\sqrt{2\pi}} \left(\frac{2}{\pi a^2}\right)^{1/4} \cdot$$

$$\int_{-\infty}^{\infty} e^{-\frac{1}{a^2}\left[x - i\frac{(k_0-k)a^2}{2}\right]^2} dx = e^{-(k_0-k)\frac{a^2}{4}} \cdot \frac{1}{\sqrt{2\pi}} \left(\frac{2}{\pi a^2}\right)^{1/4} \cdot \frac{\sqrt{\pi}}{1/a} = \frac{a}{\sqrt{2}} \left(\frac{2}{\pi a^2}\right)^{1/4} e^{-(k_0-k)\frac{a^2}{4}}$$

$$\hookrightarrow P(k) = |A(k,0)|^2 = \frac{a}{\sqrt{2\pi}} e^{-\frac{a^2}{2}(k_0-k)^2} \rightarrow \langle p \rangle = \hbar \langle k \rangle = \hbar k_0$$

* Uhin funtzioa, Ψ, e^{ik_0x}-rekin biderkatzean $\langle p \rangle = p_0$ bada momentu hasierakoa linealaren batez bestekoa, $\langle p \rangle$ berria ($\langle p \rangle'$) $\langle p \rangle' = p_0 + \hbar k_0$ izango da

(Kasu honetan hasieran, e^{ik_0x} kendu $\langle p \rangle = 0$ zen, $\Psi \in \mathbb{R}$ delako espazioan kontuta)

uhin paketea garatuta → bardin du serie / integral → integral bat denez $(-\infty,\infty)$ mugetan ez da e^{ikx} jarri behar

Orduan, orain, $\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\sqrt{a}}{(2\pi)^{1/4}} e^{-\frac{a^2}{4}(k_0-k)^2} e^{ikx} dk \Rightarrow$ $\Psi(x,t)$ lortzeko $\cdot\, e^{-i\frac{E_k}{\hbar}t}$

$$* \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\sqrt{a}}{(2\pi)^{1/4}} e^{-\frac{a^2}{4}(k_0-k)^2} e^{ikx} \cdot e^{-i\frac{\hbar k^2}{2m}t} dk =$$

$$\left(\frac{2a^2}{\pi}\right) \frac{e^{i\varphi}}{\left(a^4 + \frac{4\hbar^2t^2}{m^2}\right)^{1/4}} e^{ik_0x} e^{-\left[\frac{x - \frac{\hbar k_0}{m}t}{a^2 + \frac{4\hbar t}{m}}\right]}$$

φ: a-ren menpekoa

$$\hookrightarrow P(x,t) = \sqrt{\frac{2}{\pi a^2}} \cdot \frac{1}{\sqrt{1 + \frac{4\hbar^2t^2}{ma^4}}} e^{\frac{-2a^2\left(x - \frac{\hbar k_0}{m}t\right)^2}{a^4 + \frac{4\hbar^2t^2}{m}}} \rightarrow \text{Gaussiarra}$$

$$x_{max} = \frac{\hbar k_0}{m} t \qquad v_{max} = \frac{\hbar k_0}{m} = kte$$

• NEURKETEN EMAITZAK ETA HAUEN PROBABILITATEAK:

* $\hat{H}\psi_n = \mathcal{E}_n \psi_n \Rightarrow \{\psi_n\}$ autofuntzioak eta $\{\mathcal{E}_n\}$ autobalioak

$\Rightarrow$ autofuntzioek oinarri ortogonala osatzea aukera dezakegu (egoki aukeratuz, Gram-Smith) eta errealak izatea ($\hat{H} \in \mathbb{R}$ delako)

* Autobalioek badute esangura fisikoa, lor ditzakegun neurketen emaitzak hamiltondarren autobalioetan lokatuta daude.

Bestalde, uhin funtzioa hamiltondarraren autofuntzioen oinarrian garatu dezakegu $\rightarrow$

$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n e^{-i\frac{E_n t}{\hbar}}$ $\rightarrow$ autofuntzio askoren menpe garatuta, orduan

zein izango litzateke neurtu ondoren lortuko genukeen Ψ-ri dagokion egoera horren energia? zein $\mathcal{E}_n$?

Interpretazio probabilistikoa: ((openhagueko interpretazioa) kenduta

• $(\Psi,\Psi) = \left(\sum_{n=0}^{\infty} c_n \psi_n e^{-i\frac{E_n t}{\hbar}}, \sum_{m=0}^{\infty} c_m \psi_m e^{-i\frac{E_m t}{\hbar}}\right) =$

$n\neq m \rightarrow 0$ orduan $n=m$ hartuz $\rightarrow$ batukari bat

$$\sum_{n,m} c_n^* c_m e^{i\frac{E_n t}{\hbar}} e^{-i\frac{E_m t}{\hbar}} \underbrace{(\psi_n,\psi_m)}_{=\delta_{nm}} = \sum_{n=0}^{\infty} c_n^* c_n = \sum_{n=0}^{\infty} |c_n|^2 = 1$$

Ψ normalizatuta badago

$|c_n|^2$-ren elkarren arteko batura bat bada, interpretazio probabilistikoa

emanez $|c_n|^2$ elkarren balioitzak probabilitate bat adierazten du, sistema

egoera balioitzen energia bat $\Leftrightarrow$ zein energia izateko probabilitatea

n egoeran egoteko probabilitatea. Aldez aurretik gure sistema zein egoeratan

dagoen ezin dugunez jakin, egoera balioitzen egoteko probabilitatea

baino ezin dugu ezagutu. $\Rightarrow$ $P_{\mathcal{E}_1} = |c_1|^2$, $P_{\mathcal{E}_2} = |c_2|^2, \ldots, P_{\mathcal{E}_n} = |c_n|^2$

Orduan, $\langle H \rangle = \sum_{n=0}^{\infty} |c_n|^2 \mathcal{E}_n$, eta hau orokortzean edozein magnitudetarako

$A \rightarrow \hat{A} \rightarrow \hat{A}\psi_n^a = a_n \psi_n^a$ $\{\psi_n\}$ oinarria eta $\{a_n\}$ autobalioak

$\hookrightarrow$ magnitude fisiko bat

$\hookrightarrow (\psi_n^a, \psi_m^a) = \delta_{nm}$

Orduan, edozein uhin funtzio oinarri honetan garatuz $\rightarrow$ $\Psi = \sum_{n=0}^{\infty} c_n^a \psi_n^a$

$\langle A \rangle = \sum_{n=0}^{\infty} |c_n^a|^2 a_n$ izango da. $\quad (P(a_n) = |c_n^a|^2)$

$$* \quad c_n^a = (\psi_n^a , \Psi)$$

$\hookrightarrow$ egoera jakin batean edozein magnitude fisikoren balio bereziak lortzeko, edo balio baten probabilitatea.

- MOMENTU LINEALAREN AUTOFUNTZIOAK:
  - Momentu linealaren eragilea $\rightarrow$ $\hat{p} = -i\hbar \frac{\partial}{\partial x}$

    $\hookrightarrow$ $\hat{p}\psi_p = p\psi_p = -i\hbar \frac{\partial \psi_p}{\partial x}$ (lehen ordenako deribatu partzialeko ekuazio diferentzial lineala, koefiziente konstanteekoa)

  - $e^{rx} = \psi_p$ soluzio $\rightarrow$ $-i\hbar r e^{rx} = p e^{rx}$ $\rightarrow$ $r = \frac{p}{-i\hbar} = \frac{ip}{\hbar} = ik$ $\quad \hookrightarrow p = \hbar k$

    $\psi_k = e^{ikx}$ (Printzipioz mugalde baldintzik ez dugunez k edozein izan daiteke)

    $\hookrightarrow$ k-ren menpe dagoelako

    $\hookrightarrow$ oinarri bat osatu $\{ e^{ikx} \}$

  - Autofuntzioak konplexuak dira eta ezin dira erreal bihurtu, konplexuak izango dira beti. Izan ere, ψ_k^* autofuntzioa ere da baina ez dute autobalio bera, $-\hbar k$ baizik. Honen arrazoia eragilea irudikari purua izatea da. (Hamiltondarraren kasuan, erreala denez hori ez da gertatzen eta posiblea da autofuntzioak errealak bihurtzea $\psi' = \frac{\psi + \psi^*}{2}$ definituz)

- Autofuntzioak ortogonalak dira $(\psi_k , \psi_{k'}) = \int_{-\infty}^{\infty} e^{-ikx} \cdot e^{ik'x} dx = \int_{-\infty}^{\infty} e^{i(k'-k)x} dx =$

  $2\pi \delta(k'-k)$

  (Diskretuak direnean k.k $(\psi_n, \psi_m) = \delta_{nm}$ jartzen da n, m zenbaki naturalak izanik, baina honetan jarraituak direnez balioak dirac-en delta erabiltzen da $\rightarrow$

  $\Psi = \int_{-\infty}^{\infty} c(k) \psi_k \, dk$ eta ez $\Psi = \sum_n c_n \psi_n$)

  $\quad \quad \quad \quad \; = A(x)$ (Fourieren transformatua)

Autofuntzioak $\left\{ \frac{e^{ikx}}{\sqrt{2\pi}} \right\}$ bezala definitu dugu $(\psi_k, \psi_{k'}) = \delta(k'-k)$ izan dadin

- Edozein funtzio oinarri horretan garatu daiteke → Fourier → balioak jarraituak direnez eta ez diskretuak integral bidez adierazi dugu eta ez serie bidez:

$$* \quad \psi(x) = \int A(k)\psi_k \, dk = \frac{1}{\sqrt{2\pi}} \int A(k) e^{ikx} dx$$

Uhin funtzioen arazo batlora normalizagarriak ez direla da → $\psi(x) \cdot \psi^*(x) = \frac{1}{2\pi}$ → honen integrala $(-\infty, \infty)$ infinitua da. → beraz ez dira funtzio fisikoki esanguratsuak → ez dugu horietan hala uhin funtzioa egoera batean duen partikularik aurkitu

- **OSOTASUNAREN edo ITXIDURA-ERLAZIOA:**

A behagarri bat badugu (magnitude fisiko bat...) komenigarria da haren eragileari dagokion autofuntzioak kalkulatzea → autofuntzio horiek oinarri bat osatzen dute, ortonormala izatea aukera dezakeguna, eta ψ edozein funtzio oinarri horretan garatu daiteke → $\psi = \sum_n c_n \psi_n$; $c_n = (\psi_n, \psi)$

$$\psi(x) = \sum_n c_n \psi_n = \int \psi(x')\underbrace{\delta(x'-x)}\,dx' = \sum_n \int \psi_n^*(x')\psi(x')\psi_n(x)\,dx' =$$

$$\int \psi(x') \underbrace{\sum_n \psi_n^*(x')\psi_n(x)}\, dx'$$ Berdintza hau edozein uhin funtziorako bete behar denez ezinbestekoa da $\boxed{\delta(x'-x) = \sum_n \psi_n^*(x')\psi_n(x)}$ izatea. Honi uhin funtzioen osotasunaren edo itxiduraren-erlazioa deritzo. Hauxe da oinarriak bete behar duen erlazioa edozein uhin funtzio oinarri horretan garatzea posible izan dadin

Askotan ez da oso erreza, eta indizea jarraia denean ere bete behar da. (Σ ordez $\int$). Kasu horretan hauxe gertatzen da (uhin-lauak):

$\left\{ \frac{e^{ikx}}{\sqrt{2\pi}} \right\} \rightarrow$ momentu linealaren autofuntzioak:

$\rightarrow$ ortonormalak

- ortogonalak: $(\psi_k, \psi_{k'}) = \delta(k-k')$ (jarraitua delako, bestela Kroneckeren delta)

$$\hookrightarrow \int_{-\infty}^{\infty} \psi_k^* \psi_{k'} \, dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} \cdot e^{ik'x} \, dx = \frac{1}{2\pi} \int e^{i(k'-k)x} \, dx = \delta(k-k')$$

- Itxidura erlazioa: Beharrezkoa betetzea, edozein uhin-funtzio oinarri horietan garatu daitekeelako (Fourier):

$\hookrightarrow$ modu jarraituan $\rightarrow$ $\delta(x'-x) = \int \psi_k^*(x') \psi_k(x) \, dk$

k da aldatzen dena

Froga: $\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx'} e^{ikx} \, dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} \, dk = \delta(x'-x)$

FISIKA KUANTIKOA:

16-09-13

- Partikula erlatibista askeari dagokion fase eta talde abiadura, eta haien arteko erlazioa:

V=0 (askea)

$$E = \sqrt{c^2p^2+m^2c^4} = \hbar\omega \rightarrow \hbar^2\omega^2 = c^2\hbar^2K^2 + m^2c^4 = c^2(\hbar^2K^2+m^2c^2) \rightarrow \omega = \frac{c}{\hbar}\sqrt{\hbar^2K^2+m^2c^2}$$

$\left(\begin{array}{l} E = \hbar\omega = h\nu \\ p = \hbar K = \frac{h}{\lambda} \end{array} \right.$ Einsteinen erlazioak $\Big)$

$$v_T = \frac{d\omega}{dK} = \frac{K\hbar^{\cancel{2}} c}{\hbar\sqrt{\hbar^2K^2+m^2c^2}} = \frac{K\hbar c}{\sqrt{\hbar^2K^2+m^2c^2}} = \frac{p\cdot c}{\sqrt{p^2+m^2c^2}} = \frac{c}{\sqrt{1+\frac{m^2c^2}{p^2}}}$$

$$v_f = \frac{\omega}{K} = \frac{c}{\hbar K}\sqrt{\hbar^2K^2+m^2c^2} = \frac{c}{p}\sqrt{p^2+m^2c^2} = c\sqrt{1+\frac{m^2c^2}{p^2}}$$

$$v_T \cdot v_f = \frac{c}{\cancel{\sqrt{1+\frac{m^2c^2}{p^2}}}} \cdot c\cancel{\sqrt{\frac{1+m^2c^2}{p^2}}} = c^2$$

- Partikula askeari dagokion Hamiltondarra: $(V=0)$

$$\hookrightarrow \hat{H}\cdot\varphi = E\cdot\varphi = -\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} \rightarrow \frac{2mE}{\hbar^2} = -\frac{1}{\varphi}\frac{d^2\varphi}{dx^2} = K^2 \rightarrow \varphi K^2 + \frac{d^2\varphi}{dx^2} = 0 \Rightarrow \varphi = Ae^{iKx} + Be^{-iKx}$$

V=0

$$K = \frac{\sqrt{2mE}}{\hbar}$$

$\{e^{iKx}\}_{K=-\infty}^{\infty}$ Oinarria

partikula existitzen da espazio osoan

Arazoa $\Rightarrow$ ez da normalizagarria $\Rightarrow$ $\varphi = Ae^{iKx}$ $\quad 1 = \int_{-\infty}^{\infty} |A|^2 dx = \infty$ (Beraz partikula askearen idea idealizazio bat da)

* Partikula askeari dagokion autofuntzioa al da $\varphi = \cos ax$? $\Rightarrow$ Bete beharko du

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \text{ ekuazioa} \rightarrow \frac{d\psi}{dx} = -a\sin ax \quad \frac{d^2\psi}{dx^2} = -a^2\cos ax \Rightarrow$$

$$\frac{\hbar^2}{2m}a^2\cos ax = E\cos ax \leftrightarrow E = \frac{\hbar^2a^2}{2m} = \frac{p^2}{2m} \leftrightarrow p^2 = \hbar^2a^2 \rightarrow p = \hbar a = \hbar K \rightarrow K = a$$ Betetzen da!

Gainera $\psi = \cos ax = \frac{e^{iax}+e^{-iax}}{2}$ da $\rightarrow$ e^{iKx} eta e^{-iKx}-ren arteko konbinazio lineala

* Ba al da $\varphi = \cos^2 ax$?

16-09-15

$$\Psi(x,0) = e^{-\left(\frac{x^2}{a^2}+iK_0x\right)} \qquad K?,\ \Delta x?$$

$$\hookrightarrow \Psi(x,0) = e^{-x^2/a^2}\cdot e^{-iK_0x}$$

$P(x,0) = |\Psi(x,0)|^2 = e^{-\frac{2x^2}{a^2}}$ $\Rightarrow$ normalizatu $\Rightarrow$ $1 = \int_{-\infty}^{\infty} P(x,0)\cdot A\,dx = \int_{-\infty}^{\infty} A e^{-\frac{2x^2}{a^2}} dx =$

$$A\int_{-\infty}^{\infty} e^{-\frac{2x^2}{a^2}} dx = \frac{A}{2}\sqrt{\frac{\pi}{2}}\, a \,\mathrm{erf}\left(\frac{\sqrt{2}x}{a}\right)\Big]_{-\infty}^{\infty} = \frac{A}{\cancel{2}\sqrt{2}}\sqrt{\pi}\, a\,(1-\cancel{(-1)}) = \frac{A\sqrt{\pi}\,a}{\sqrt{2}} \Rightarrow$$

$A = \sqrt{\frac{2}{\pi}}\cdot\frac{1}{a}$ $\Rightarrow$ Beraz $P'(x,0) = \sqrt{\frac{2}{\pi}}\cdot\frac{1}{a}\, e^{-\frac{2x^2}{a^2}}$

funtzio bakoitia $P'(x,0)$

$$\bar{x} = \int_{-\infty}^{\infty} P'(x,0)\, x\, dx = \sqrt{\frac{2}{\pi}}\cdot\frac{1}{a}\int_{-\infty}^{\infty} e^{-\frac{2x^2}{a^2}} x\, dx = \sqrt{\frac{2}{\pi}}\cdot\frac{1}{\cancel{a}}\left(-\frac{1}{4}a^2 e^{-\frac{2x^2}{a^2}}\right)\Big]_{-\infty}^{\infty} = 0$$

$$\Delta x = \sqrt{|\overline{x^2} - \bar{x}^2|} = \sqrt{\overline{x^2}} \Rightarrow \left|\int_{-\infty}^{\infty} P'(x,0)\, x^2\, dx\right| = \sqrt{\frac{2}{\pi}}\cdot\frac{1}{a}\left|\int_{-\infty}^{\infty} e^{-\frac{2x^2}{a^2}} x^2\, dx\right| =$$

$$\sqrt{\frac{2}{\pi}}\cdot\frac{1}{\cancel{a}}\left|\frac{1}{16}a^2\left(\sqrt{2\pi}\, a\,\mathrm{erf}\left(\frac{\sqrt{2}x}{a}\right) - 4x e^{-\frac{2x^2}{a^2}}\right)\Big]_{-\infty}^{\infty}\right| = \sqrt{\frac{2}{\cancel{\pi}}}\cdot\frac{2}{16}a^2\sqrt{2\cancel{\pi}} = \frac{a^2}{4} = \overline{x^2} \rightarrow$$

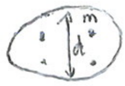
$\Delta x = \sqrt{\overline{x^2}} = \frac{a}{2}$; $\bar{x} = 0$, $\Delta x = \frac{a}{2}$ ($P(x,0)$ Gaussiarra)

$A e^{-\frac{x^2}{2\sigma^2}} \rightarrow \sigma^2 = \frac{a^2}{4} = \Delta x^2$

$\Psi(x,0) = A e^{-\left(\frac{x^2}{a^2} + ik_0x\right)} \neq A e^{-\frac{2x^2}{a^2}}$, x-ren menpekoa den fase bat daukalako $\Rightarrow$ Hamiltondarrean aplikatzean eragin ezberdinak lortu, E ezberdina (momentua ezberdina da)

* x-ren menpekoa ez balitz baliokideak izango lirateke, uhinetan sartuko genukeelako (ad. $e^{ik_0}A = \tilde{B} \in \mathbb{C}$)

Problema: Beste unibertso batean $\hbar = 10^4$ erg·s ; meloi bat (haziekin)



$d = 20$ cm
$m = 2$g

Meloia apurtuko balitz amiskuitsua izango litzateke gurentzat? (Kortasa oso gogorra da) Zenbatekoa da hazien gutxi gorabeherako abiadura?

Heissenbergen ziurgabetasun printzipioa: $\Delta x\Delta p \geq \frac{\hbar}{2}$ $\quad \Delta x = d = 20$ cm $= 0'2$ m

$\Delta p = m\Delta v \rightarrow \quad \Delta p \geq \frac{\hbar}{2\Delta x} \rightarrow \Delta v \geq \frac{\hbar}{2m\Delta x} = 1'25$ m/s

Potentzial osin infinitu esferikoa. Oinarrizko egoeran daudela suposatu : $E_1 = \frac{h^2}{8m}\cdot\frac{1}{r^2} = 0'246$ J $\rightarrow$

$r = d/2$ $\quad E_1 = \frac{1}{2}mv^2 \rightarrow v = 15'71$ m/s $\rightarrow v = (15'71 \pm 1'25)$ m/s

16-09-20

- $\psi = \frac{\sin x}{x^2}$ → $x=0$ puntuan ez da jarraitua eta ez da limitea existitzen → ez da normalizagarria eta ez da bere Fourieren seriea existitzen. ↗ esanahia fisikorik ez dauka uhin funtzioak

Kalkulatu daiteke V energia potentzial bat non ψ hamiltondarraren autofuntzioa den? $\hat{H}\cdot\psi = E\cdot\psi \rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\cdot\psi = E\cdot\psi \rightarrow V = E + \frac{\hbar^2}{2m}\cdot\frac{1}{\psi}\frac{d^2\psi}{dx^2}$

(Esanahia fisikorik ez badu ere izan daiteke hamiltondarraren autofuntzioa *)

Kasu honetan, $x=0$-n ez denez deribagarria ez da existitzen hamiltondarrik, ezin da definitu

- $2a$ zabalerako tarte batean (k-ren neurrian) $\hbar k$ momentua lortzeko probabilitatea konstantea da. Momentuaren batezbestekoa k_0 da. Zein da baldintza hori betetzen duen normalizatutako uhin funtzioa? Momentuaren probabilitatea kte ⟺ k-ren probabilitatea kte

$$P(k,t) = kte = B = \hbar|A(k)|^2 \rightarrow A(k) = \sqrt{B}e^{i\gamma_k} = Ce^{i\alpha}$$

↗ kte bat denez batezbestekoa zentruan

$$\bar{k} = \cancel{k_0} = \int_{-\infty}^{\infty} k\, P(k,t)\,dk = \int_{k_0-a}^{k_0+a} k\cdot B\,dk = B\int_{k_0-a}^{k_0+a} k\,dk = B\cdot\frac{k^2}{2}\Big] = B\left(\frac{4ak_0}{2}\right) = 2Bak_0$$

$$B = \frac{1}{2a} \rightarrow A(k) = \frac{1}{\sqrt{2a}}\cdot e^{i\gamma}, \quad \int_{-\infty}^{\infty} P(k,t)\,dk = \int_{k_0-a}^{k_0+a} B\,dk = B\cdot 2a = 1 \rightarrow B = \frac{1}{2a}$$

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(k)e^{ikx}\,dk = \frac{1}{\sqrt{2\pi}}\cdot\frac{1}{\sqrt{2a}}\int_{k_0-a}^{k_0+a} e^{ikx}\,dk = \frac{1}{2}\cdot\frac{1}{\sqrt{a\pi}}\left(-\frac{i}{x}e^{ikx}\right)\Big]_{k_0-a}^{k_0+a} =$$

$\gamma = 0$ jar daiteke

$$\frac{1}{2\sqrt{a\pi}}\left(-\frac{i}{x}\left(e^{i(k_0+a)x} - e^{i(k_0-a)x}\right)\right) = \frac{1}{2i\sqrt{a\pi}}\cdot\frac{1}{x}\left(e^{ix(k_0+a)} - e^{ix(k_0-a)}\right) = \frac{1}{2i\sqrt{a\pi}}\cdot\frac{1}{x}e^{ixk_0}\left(e^{ixa} - e^{-aix}\right) = \frac{1}{\sqrt{\pi a}}e^{ik_0x}\frac{\sin ax}{x}$$

16-09-21

- $\Psi(x,0) = e^{-\alpha|x|}$ uhin funtzio honen momentuaren batezbestekoa.

Normalizatu $\Rightarrow$ $\displaystyle\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = \int_{-\infty}^{\infty} e^{-2\alpha|x|} dx = \int_{-\infty}^{0} e^{2\alpha x} dx + \int_{0}^{\infty} e^{-2\alpha x} dx =$

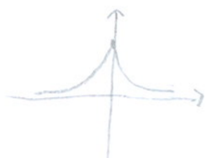
$$\frac{1}{2\alpha} e^{2\alpha x}\Big]_{-\infty}^{0} - \frac{1}{2\alpha} e^{-2\alpha x}\Big]_{0}^{\infty} = \frac{1}{2\alpha} + \frac{1}{2\alpha} = \frac{1}{\alpha} \Rightarrow \Psi'(x,0) = \sqrt{\alpha}\, e^{-\alpha|x|}$$

(Normalizatuta)

* $\bar{p} = \left(\Psi', -i\hbar \frac{\partial \Psi'}{\partial x}\right) = \displaystyle\int_{-\infty}^{\infty} -\Psi'^{*}\, i\hbar \frac{\partial \Psi'}{\partial x} dx$

$$\Psi'(x,0) = \begin{cases} \sqrt{\alpha}\, e^{-\alpha x} & x \geq 0 \\ \sqrt{\alpha}\, e^{\alpha x} & x < 0 \end{cases} \rightarrow \frac{\partial \Psi'}{\partial x}(x,0) = \begin{cases} -\alpha^{3/2} e^{-\alpha x} & x \geq 0 \\ \alpha^{3/2} e^{\alpha x} & x < 0 \end{cases}$$

Funtzioa ez da deribagarria $x=0$ puntuan.



Hala ere, puntu bakarrean baino ez denez deribagarria ez du garrantzi handirik

* $\bar{p} = \displaystyle\int_{-\infty}^{\infty} -\Psi'^{*}\, i\hbar \frac{\partial \Psi'}{\partial x} dx = \int_{0}^{\infty} \sqrt{\alpha}\, e^{-\alpha x}\, i\hbar\, \alpha^{3/2} e^{-\alpha x} dx + \int_{-\infty}^{0} -\sqrt{\alpha}\, e^{\alpha x}\, i\hbar\, \alpha^{3/2} e^{\alpha x} dx =$

$$\alpha^{5/2} i\hbar \int_{0}^{\infty} e^{-2\alpha x} dx - \alpha^{5/2} i\hbar \int_{-\infty}^{0} e^{2\alpha x} dx = \alpha^{5/2} i\hbar \left(\int_{0}^{\infty} e^{-2\alpha x} dx - \int_{-\infty}^{0} e^{2\alpha x} dx \right) =$$

$$\alpha^{5/2} i\hbar \left(\frac{-1}{2\alpha} e^{-2\alpha x}\Big]_{0}^{\infty} - \frac{1}{2\alpha} e^{2\alpha x}\Big]_{-\infty}^{0} \right) = \alpha^{5/2} i\hbar \left(+\frac{1}{2\alpha} - \frac{1}{2\alpha} \right) = 0$$

- Frogatu bi uhin funtzioen arteko biderkadura eskalarra banakorra, trukakorra eta elkarkorra den.

$\Psi, \varphi \Rightarrow$ bi uhin funtzio

* Banakorra: $\xi(x,t)$, $\displaystyle(\Psi + \xi, \varphi) = \int_{-\infty}^{\infty} (\Psi + \xi)^{*} \varphi\, dx = \int_{-\infty}^{\infty} (\Psi^{*} + \xi^{*}) \varphi\, dx =$

$$\int_{-\infty}^{\infty} (\Psi^{*}\varphi + \xi^{*}\varphi) dx = \int_{-\infty}^{\infty} \Psi^{*}\varphi\, dx + \int_{-\infty}^{\infty} \xi^{*}\varphi\, dx = (\Psi, \varphi) + (\xi, \varphi)$$

Banakorra da

* Trukakorra: $\leftrightarrow$ $(\psi, \varphi) = (\varphi, \psi)$

$$(\psi, \varphi) = \int_{-\infty}^{\infty} \psi^* \varphi \, dx = \int_{-\infty}^{\infty} (\psi \varphi^*)^* \, dx = \left(\int_{-\infty}^{\infty} \psi \varphi^* \, dx \right)^* = (\varphi, \psi)^* \neq$$

(φ, ψ) Ez da trukakorra (Uhin funtzio errealetan bai)

* Elkarkorra: $\leftrightarrow$ $\lambda \in \mathbb{C}$ $\quad (\lambda \psi, \varphi) = \lambda (\psi, \varphi) = (\psi, \lambda \varphi)$

$$\circ \ \lambda (\psi, \varphi) = \lambda \int_{-\infty}^{\infty} \psi^* \varphi \, dx \neq \int_{-\infty}^{\infty} (\lambda \psi)^* \varphi \, dx = \int_{-\infty}^{\infty} \lambda^* \psi^* \varphi \, dx =$$

$$\lambda^* \int_{-\infty}^{\infty} \psi^* \varphi \, dx = \lambda^* (\psi, \varphi)$$

ez da betetzen

betetzen da

$$\circ \ \lambda (\psi, \varphi) = \lambda \int_{-\infty}^{\infty} \psi^* \varphi \, dx = \int_{-\infty}^{\infty} \psi^* \lambda \varphi \, dx = \lambda \int_{-\infty}^{\infty} \psi^* \varphi \, dx = (\psi, \lambda \varphi)$$

Ez da elkarkorra

16-09-22

∘ $\Psi(x,0) = e^{-\alpha |x|}$ uhin funtzio honen egoeraren energia zinetikoaren batez-bestekoa:

$$* \ \bar{T} = (\Psi, \hat{T} \Psi) \quad ; \quad \hat{T} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

Normalizatuz →
$$\Psi(x,0) = \sqrt{\alpha} e^{-\alpha |x|} = \begin{cases} \sqrt{\alpha} e^{-\alpha x} & x \geq 0 \\ \sqrt{\alpha} e^{\alpha x} & x < 0 \end{cases}$$

$$\circ \ \frac{\partial \Psi}{\partial x}(x,0) = \begin{cases} -\alpha^{3/2} e^{-\alpha x} & x \geq 0 \\ \alpha^{3/2} e^{\alpha x} & x < 0 \end{cases} \rightarrow \frac{\partial^2 \Psi}{\partial x^2}(x,0) = \begin{cases} \alpha^{5/2} e^{-\alpha x} & x \geq 0 \\ \alpha^{5/2} e^{\alpha x} & x < 0 \end{cases}$$

$$* \ \bar{T} = \int_{-\infty}^{\infty} \Psi^* \cdot \hat{T} \Psi \, dx = \int_{-\infty}^{\infty} \Psi^* \cdot \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \right) dx = \int_{-\infty}^{0} -\frac{\hbar^2}{2m} \sqrt{\alpha} e^{\alpha x} \cdot \alpha^{5/2} e^{\alpha x} \, dx +$$

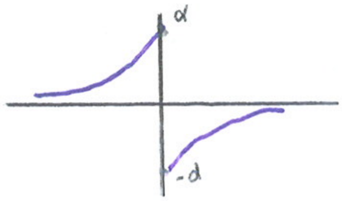
$$\int_{0}^{\infty} -\frac{\hbar^2}{2m} \sqrt{\alpha} e^{-\alpha x} \cdot \alpha^{5/2} e^{-\alpha x} \, dx = -\frac{\hbar^2}{2m} \alpha^3 \left(\int_{-\infty}^{0} e^{2\alpha x} \, dx + \int_{0}^{\infty} e^{-2\alpha x} \, dx \right) = -\frac{\hbar^2}{2m} \alpha^3 \left(\left[\frac{e^{2\alpha x}}{2\alpha} \right]_{-\infty}^{0} + \right.$$

$$\left. -\frac{1}{2\alpha} e^{-2\alpha x} \Big]_{0}^{\infty} \right) = -\frac{\hbar^2}{2m} \alpha^3 \left(\frac{1}{2\alpha} + \frac{1}{2\alpha} \right) = -\frac{\hbar^2 \alpha^2}{2m} < 0$$

ezinezkoa (T>0 BETI)

* Abisua → $x=0$-n ez da deribagarria, salto bat dago.

$$\frac{\partial \Psi}{\partial x} = \begin{cases} \alpha^{3/2} e^{\alpha x} & x<0 \\ -\alpha^{3/2} e^{-\alpha x} & x>0 \end{cases}$$



→ Heaviside-ren funtzioaren antzekoa → deribatzerakoan 0-n brezia → dirac-en delta

$$\frac{\partial^2 \Psi}{\partial x^2} = \begin{cases} \alpha^{5/2} e^{\alpha x} & x<0 \\ -2\alpha^{3/2}\delta(x) & x=0 \\ \alpha^{5/2} e^{-\alpha x} & x>0 \end{cases}$$

↓

$\frac{\partial \Psi}{\partial x}$ $x=0$-n ez-jarraitua delako

(-2α → tartea $[2\alpha]$ delako eta $\ominus$ goitik behera doalako saltoa)

dunelakoa ↗ gutxi gorabehera

$$\rightarrow \bar{T} = -\frac{\hbar^2}{2m}\left(\Psi, \frac{\partial^2 \Psi}{\partial x^2}\right) = \ldots\ldots -\frac{\hbar^2}{2m}\int_{0^-}^{0^+} \Psi(-2\alpha^{3/2}\delta(x))\,dx =$$

$$-\frac{\hbar^2}{2m}\alpha^2 + \frac{\hbar^2}{2m}\cdot 2\alpha^{3/2}\Psi(0) = \frac{\hbar^2}{2m}\left(2\alpha^{3/2}\cdot\sqrt{\alpha} - \alpha^2\right) =$$

$$\frac{\hbar^2}{2m}\alpha^2 > 0 \quad !$$

• Ψ funtzioaren momentu linealaren batezbestekoa → $\bar{P}_\Psi = P_0$ → zein da Ψ^*-ri dagokion $\bar{P}_{\Psi^*}$?

$$* \ \bar{P}_\Psi = \left(\Psi, -i\hbar\frac{\partial \Psi}{\partial x}\right) = -i\hbar\left(\Psi, \frac{\partial \Psi}{\partial x}\right) = -i\hbar\int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x}\,dx = P_0 \rightarrow \left(\Psi, \frac{\partial \Psi}{\partial x}\right) = \frac{P_0 i}{\hbar}$$

$$* \ \bar{P}_{\Psi^*} = \left(\Psi^*, -i\hbar\frac{\partial \Psi^*}{\partial x}\right) = -i\hbar\left(\Psi^*, \frac{\partial \Psi^*}{\partial x}\right) = -i\hbar\int_{-\infty}^{\infty} \Psi \frac{\partial \Psi^*}{\partial x}\,dx = -i\hbar\int_{-\infty}^{\infty} \Psi\left(\frac{\partial \Psi}{\partial x}\right)^* dx =$$

$$-i\hbar\left(\frac{\partial \Psi}{\partial x}, \Psi\right) = -i\hbar\underbrace{\left(\Psi, \frac{\partial \Psi}{\partial x}\right)^*}_{\parallel} = -i\hbar\left(\frac{P_0 i}{\hbar}\right)^* = -i\cancel{\hbar}\left(\frac{-P_0 i}{\cancel{\hbar}}\right) = -P_0$$

$$\left(i\hbar\left(\Psi, \frac{\partial \Psi}{\partial x}\right)\right)^* = -\left(-i\hbar\left(\Psi, \frac{\partial \Psi}{\partial x}\right)\right)^* = -P_0^* = -P_0$$

Hermitikoa denez → $\bar{P}_{\Psi^*} = \left(\Psi^*, -i\hbar\frac{\partial \Psi^*}{\partial x}\right) = \left(-i\hbar\frac{\partial \Psi^*}{\partial x}, \Psi^*\right) = (-i\hbar)^*\left(\frac{\partial \Psi^*}{\partial x}, \Psi^*\right) =$

$$i\hbar\int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x}\,dx = -P_0$$

16-09-26

- Fourier-en transformatuta ($A(k,t)$) lor daiteke $\bar{x}$ kalkulatzeko eragile bat uhin funtzioa ($\psi(x,t)$) erabili gabe?

$\bar{x} = (\psi(x,t), x\psi(x,t))$ *

$\rightarrow \langle p \rangle = (A, \hbar k A) = \int_{-\infty}^{\infty} A^* A \hbar k \, dk = (A, pA) =$

$$\begin{cases} \psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k,t) e^{ikx} dk \\ \psi^*(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A^*(k,t) e^{-ikx} dk \end{cases}$$

$(\psi, -i\hbar \frac{\partial}{\partial x}\psi) \Rightarrow$ konparaketa bat egin

$\langle x \rangle = (\psi, x\psi) = (A, C \cdot \frac{\partial}{\partial k} A)$

$$* \quad \bar{x} = \int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx = \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A^*(k',t) e^{-ik'x} dk' \right) x \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k,t) e^{ikx} dk \right) dx =$$

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} A^*(k',t) e^{-ik'x} dk' \right) \left(\int_{-\infty}^{\infty} A(k,t) e^{ikx} dk \right) x \, dx =$$

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x \cdot A^*(k',t) A(k,t) e^{i(k-k')x} dx\, dk'\, dk$$

$$\bar{x} = (A(k), \hat{B} A(k)) = (A(k), C \frac{\partial A}{\partial k}) = \int_{-\infty}^{\infty} A^*(k)\, C \frac{\partial A}{\partial k} dk = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} C \cdot \frac{1}{\sqrt{2\pi}} \psi^*(x) e^{ikx} \cdot$$

$$\frac{\partial}{\partial k} \left[\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \psi(x') e^{-ikx'} dx' \right] dx\, dk = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} C \cdot \frac{1}{2\pi} \psi^*(x) e^{ikx} (-ix') \psi(x') e^{-ikx'} dx'\, dk\, dx =$$

$$\frac{-iC}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi^*(x) \psi(x') x' e^{ik(x-x')} dx\, dx'\, dk = -iC \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi^*(x) \psi(x') x' \delta(x-x')\, dx\, dx' =$$

$$-iC \int_{-\infty}^{\infty} x' \psi^*(x') \psi(x') dx' = -iC \bar{x'} \leftrightarrow -iC = 1 \rightarrow C = i \Rightarrow \text{eragilea } \boxed{\hat{B} = i \frac{\partial}{\partial k}}$$

($A \in \mathbb{R}$ bada $\bar{x} = 0$)

- $\hat{A} = x^2 \frac{\partial^2}{\partial x^2}$ eragilearen adjuntua lortu eta esan Hermitikoa den.

$$\hat{A} = x^2 \frac{\partial}{\partial x} \left(\frac{\partial}{\partial x} \right), \quad \hat{A}^+ = \left(x^2 \frac{\partial}{\partial x} \left(\frac{\partial}{\partial x} \right) \right)^+ = \left(\frac{\partial}{\partial x} \right)^+ \left(x^2 \frac{\partial}{\partial x} \right)^+ = \left(\frac{\partial}{\partial x} \right)^+ \left(\frac{\partial}{\partial x} \right)^+ (x^2)^+ =$$

$$\left(\left(\frac{\partial}{\partial x} \right)^+ \right)^2 (x^2)^+ = \frac{\partial^2}{\partial x^2} x^2 \Rightarrow \text{ez da hermitikoa}$$

deribatu x^2 ere $\rightarrow \hat{A}^+ \psi = \frac{\partial^2}{\partial x^2} (x^2 \psi) = \frac{\partial}{\partial x} (2x\psi + x^2 \frac{\partial \psi}{\partial x})$

• Eragile baten infinito autofuntzio endakatuak izan daitezke? Nola ortogonalizatu?

Adib.: eragilea kte bat bada $\Rightarrow \hat{A} = K \iff \hat{A}\psi_n = K\psi_n = a_n\psi_n \iff$

$K = a_n \quad \forall n \in \mathbb{N}$, guztiak endakatuak izango dira

Ortogonalizatzeko prozedura arrunta $\Rightarrow$ Gram-Smith-en metodoa

• $\hat{C}\psi = \psi^*$ bada $\hat{C}$-ren autobalioak konplexuak izango dira?

Frogatuko dugu ea hermitikoa den $\Rightarrow$ hermitikoa bada autobalioak errealak izango dira.

$$(\psi, \hat{C}\psi) = (\hat{C}\psi, \psi) \rightarrow \int_{-\infty}^{\infty} \psi^* \psi^* dx \neq \int_{-\infty}^{\infty} (\psi^*)^* \psi \, dx = \int_{-\infty}^{\infty} \psi \cdot \psi \, dx$$

Ez da hermitikoa $\rightarrow$ baina ezin dugu guztiz ziurtatu autobalioak errealak izango ez direnik $\rightarrow$ kalkulatu beharko ditugu autobalioak.

↳ arkatza ebatzia

$\rightarrow f, g$ funtzio errealak

$\hat{C}\psi = \psi^* = \lambda\psi$. defini dezagun $\psi = f(x) + ig(x)$ modura $\Rightarrow (f+ig)^* = \lambda(f+ig) \rightarrow$

$$f - ig = \lambda f + \lambda i g \xrightarrow{\lambda \in \mathbb{R}} \begin{cases} f = \lambda f \rightarrow \lambda = 1 \rightarrow g = 0 \rightarrow \psi \in \mathbb{R} \\ -ig = \lambda i g \rightarrow -g = \lambda g, \ \lambda = -1 \rightarrow f = 0 \rightarrow \psi \in \mathbb{C} \end{cases}$$

derrigorrezkoa λ x-ren independentea delako, kte bat.

bestela $f = \lambda i g \rightarrow \lambda = \frac{f}{ig} \Rightarrow$ x-ren menpekoa

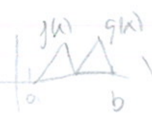
• Zein da hasierako aldiuneko dimentsio bateko uhin funtzioak bete behar duen erlazioa bere Fourieren transformatua erreala izateko?

$\psi(x,0)$, $A(k) \in \mathbb{R}$? $\quad A(k) \in \mathbb{R} \iff A(k) = A^*(k)$

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,0) e^{-ikx} dx = A^*(k) = \frac{1}{\sqrt{2\pi}} \left(\int_{-\infty}^{\infty} \psi(x,0) e^{-ikx} dx \right)^* =$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi^*(x,0) e^{ikx} dx \rightarrow$$

barnekoak ez du zertan berdina izan



$f(x) \neq g(x) \iff \int_a^b f(x)dx = \int_a^b g(x)dx$

$$\rightarrow \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \psi(x,0)e^{-ikx}dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \psi^*(x,0)e^{ikx}dx \underset{x=-x}{=} \frac{-1}{\sqrt{2\pi}}\int_{\infty}^{-\infty} \psi^*(-x,0)e^{-ikx}dx =$$

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \psi^*(-x,0)e^{-ikx}dx \Rightarrow \psi(x,0) = \psi^*(-x,0) \Leftrightarrow \psi(-x,0) = \psi^*(x,0)$$

↳ ez dagoen baldintza erabiltzen den edo ez

Adb: $\psi(x) = e^{-x^2}(1-ix)$ (zati erreala bikoitia eta zati irudikaria bakoitia)

16-09-28

- Edozein uhin funtzio emanda izan daiteke Hamiltondar baten autofuntzioa?

$$\left(\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right) \leftrightarrow \text{autofuntzioa bada } \hat{H}\psi = \varepsilon\psi =$$

$\psi = \psi(x)$; $\frac{\partial}{\partial x} = \frac{d}{dx}$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = \varepsilon\psi \leftrightarrow V = \varepsilon + \frac{1}{\psi}\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$$

(V ψ-ren menpekoa izango da eta $\varepsilon \in \mathbb{R}$ edozein konstante izan daiteke → infinito aukera → infinitu hamiltondar)

- Partikula askean dagoen $\hat{H}$-ren autofuntzioa izan ahal da edozein uhin funtzio? $\hat{H}\psi = \varepsilon\psi$

partikula askea

$$V = \varepsilon + \frac{1}{\psi}\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = 0 \rightarrow \frac{1}{\psi}\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -\varepsilon = \text{kte}$$

baldintza hau betetzen duten uhin funtzioak bakarrik. (Beraz edozein ez)

$$\Rightarrow \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \varepsilon\psi = 0 \rightarrow \frac{d^2\psi}{dx^2} + \frac{2m\varepsilon}{\hbar^2}\psi = 0 = \frac{d^2\psi}{dx^2} + k^2\psi = 0 \rightarrow$$

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad k = \sqrt{\frac{2m\varepsilon}{\hbar^2}}$$

$(\forall\varepsilon \in \mathbb{R})$ funtzioak bakarrik

↳ uhin lauak (autofuntzioa)

Fourier

edozein funtzio esponentzial moduan konbinazio lineal moduan jarri ahal bada ere hauek k bera izan behar dute

* Hamiltondarraren autofuntzioen konbinazio lineala, $\psi = a\psi_1 + b\psi_2$ adibidez,

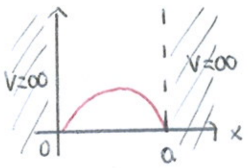
$$\begin{matrix} \psi_1 & \psi_2 \\ \downarrow & \downarrow \\ \varepsilon_1 & \varepsilon_2 \end{matrix}$$

ez da hamiltondarraren autofuntzioa, $\varepsilon_1 \neq \varepsilon_2$ badira.

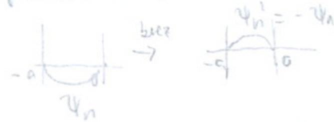
16-09-29

- Frogatu potentzial osin infinituaren autofuntzioak ortogonalak direla:

Potentzial osin infinituaren autofuntzioak: $\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$



jatorria erpin batean → $[-a,0]$ tartea hartuz uhin funtzioa autofuntzioa ere da, autofuntzioa bider -1 bat baino ez delako



* $$(\psi_n, \psi_m) = \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \sqrt{\frac{2}{a}} \sin\left(\frac{m\pi x}{a}\right) dx = \frac{\cancel{2}}{a\cancel{2}} \int_0^a \left(\cos\left(\frac{\pi x}{a}(n-m)\right) - \cos\left(\frac{\pi x}{a}(n+m)\right)\right) dx =$$

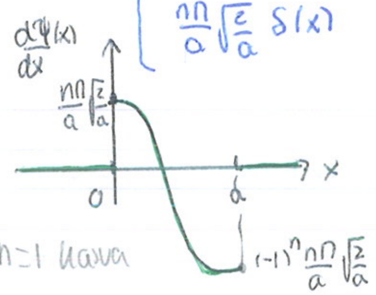
$$\frac{1}{a}\int_0^a \cos\left(\frac{\pi x}{a}(n-m)\right) - \cos\left(\frac{\pi x}{a}(n+m)\right) dx \overset{n \neq m}{=} \frac{1}{\cancel{a}} \left[\frac{\cancel{a}}{\pi(n-m)} \sin\left(\frac{\pi x}{a}(n-m)\right) - \frac{\cancel{a}}{\pi(n+m)} \sin\left(\frac{\pi x}{a}(n+m)\right)\right]_0^a =$$

$$\frac{1}{\pi}\left(\frac{\sin\left(\frac{\pi x}{a}(n-m)\right)}{n-m} - \frac{\sin\left(\frac{\pi x}{a}(n+m)\right)}{n+m}\right)\Bigg]_0^a = 0$$

- Potentzial osin infinituko autofuntzioak $\hat{T}$-ren autofuntzioak dira?

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \quad ; \quad \psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) & 0 \leq x \leq a \\ 0 & \text{kanpoan.} \end{cases}$$

$$\frac{d\psi}{dx} = \begin{cases} \frac{n\pi}{a}\sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right) & 0 < x < a \\ (-1)^n \frac{n\pi}{a}\sqrt{\frac{2}{a}}\, \delta(x-a) & x = a \\ 0 & \text{kanpoan} \\ \frac{n\pi}{a}\sqrt{\frac{2}{a}}\, \delta(x) & x = 0 \end{cases} \quad ; \quad \frac{d^2\psi}{dx^2} = \begin{cases} -\left(\frac{n\pi}{a}\right)^2 \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) & 0 < x < a \\ 0 & \text{kanpoan} \end{cases}$$



Puntu guztietan ez dira, $(-\infty, \infty)$-ra ez.

16-10-03

- $\Psi(x) = e^{2ix} - 5e^{-3ix}$ uhin-funtzioa normalizagarria da?

Ψ uhin-lauen konbinazio lineala da, eta uhin lauak normalizagarriak ez badira ere, normalizagarria izan daiteke.

- $\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = \int_{-\infty}^{\infty} \Psi \cdot \Psi^* dx = \int_{-\infty}^{\infty} (e^{2ix} - 5e^{-3ix})(e^{-2ix} - 5e^{3ix}) dx = \int_{-\infty}^{\infty} (1 - 5e^{3ix+2ix} - 5e^{-3ix-2ix} + 25) dx =$

$-\int_{-\infty}^{\infty} (-26 + 5e^{5ix} + 5e^{-5ix}) dx = -\int_{-\infty}^{\infty} (10\cos(5x) - 26) dx = \int_{-\infty}^{\infty} (26 - 10\cos(5x)) dx = 26x - \frac{10}{5}\sin(5x) \Big]_{-\infty}^{\infty}$

Integral hau ez da integragarria sinua ez dagoelako definituta infinituan. $\Rightarrow$

uhin funtzioa ez da normalizagarria

berez ez dira normalizagarriak

Modu berean, ez da partikula askearen autofuntzioa, autobalio ezberdineko bi autofuntzioen konbinazio lineala delako. (e^{2ix} eta e^{-3ix})

- Izan daiteke $\Psi(x) = e^{2ix} - 5e^{-3ix}$ partikula askeari dagokion uhin-funtzio onargarria?

$\Psi(x)$ autofuntzioen oinarrian dago garatuta: $\Psi(x) = e^{2ix} - 5e^{-3ix}$ $(\{e^{ikx}\})$

orduan denboraren menpe garatuz honela izango da:

$$* \ \Psi(x,t) = e^{2ix} \cdot e^{-\frac{i\hbar 2^2}{2m}t} - 5e^{-3ix} e^{-\frac{i\hbar 3^2}{2m}t} = e^{2ix - \frac{i\hbar 2}{m}t} - 5e^{-3ix - \frac{i\hbar 9}{2m}t}$$

Orduan, uhin-funtzio onargarria den jakiteko Schrödingerren ekuazioan sartuko dugu, eta betetzen bada onargarria izango da.

$V = 0$ (partikula askea)

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi = i\hbar \frac{\partial \Psi}{\partial t} \stackrel{?}{=} -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}$$

$$* \ \frac{\partial \Psi}{\partial x} = 2i\left(e^{2ix - \frac{i\hbar 2}{m}t}\right) + 15i\left(e^{-3ix - \frac{i\hbar 9}{2m}t}\right) \qquad * \ \frac{\partial^2 \Psi}{\partial x^2} = -4\left(e^{2ix - \frac{i\hbar 2}{m}t}\right) + 45\left(e^{-3ix - \frac{i\hbar 9}{2m}t}\right)$$

$$* \ \frac{\partial \Psi}{\partial t} = -\frac{i\hbar 2}{m}\left(e^{2ix - \frac{i\hbar 9}{2m}t}\right) + \frac{45 i\hbar}{2m}\left(e^{-3ix - \frac{i\hbar 9}{2m}t}\right) \longrightarrow +\frac{\hbar^2}{2m}\left(+4e^{2ix - \frac{i\hbar 2}{m}t}\right) - \frac{45\hbar^2}{2m} e^{-3ix - \frac{i\hbar 9}{2m}t} =$$

$$\frac{2\hbar^2}{m} e^{2ix - \frac{i\hbar 9}{2m}t} - \frac{45\hbar^2}{2m} e^{-3ix - \frac{i\hbar 9}{2m}t}$$ ✓ → onargarria da

Ez da autofuntzioa baina bada egoera

16-10-04

- Partikula askea dugu eta bere momentua neurtzen dugu edozein t aldiunetan. Zein da momentu honek izan ditzakeen balioa eta bere probabilitatea?

$$* \ \Psi(x,0) = e^{2ix} - 5e^{-3ix} \rightarrow \text{partikula askea } \{e^{ikx}\} \text{ oinarria eta } E_k = \frac{\hbar^2 k^2}{2m} \rightarrow$$

(Gure kasuan Ψ_2 eta Ψ_{-3} → E_2 eta E_3, orduan p, p_2 eta p_3 izan daitezke)

denborarekiko garatu → $$\Psi(x,t) = e^{i(2x - \frac{E_2}{\hbar}t)} - 5e^{-i(3x + \frac{E_3}{\hbar}t)} = C_2\Psi_2 + C_{-3}\Psi_{-3}$$

↳ $\Psi(x,0)$ partikula askearen autofuntzioen oinarrian garatu dugulako

$$C_2 = e^{-i\frac{E_2 t}{\hbar}}, \quad C_{-3} = -5e^{-i\frac{E_3 t}{\hbar}} \longleftrightarrow P(E_2) = \frac{|C_2|^2}{\underbrace{|C_2|^2 + |C_3|^2}_{P \text{ osoa}}} = \frac{1}{1+25} = \frac{1}{26}$$

ez dagoelako normalizatua

C_2, E_3 aukera posible bakarrak direlako

ez dagoelako normalizatuta

$$P(E_3) = \frac{|C_3|^2}{|C_2|^2 + |C_3|^2} = \frac{25}{1+25} = \frac{25}{26}$$

$$(P(E_3) + P(E_2) = 1)$$

$$* \ E_2 = \frac{p_2^2}{2m} \longleftrightarrow P(\underset{2\hbar}{\overset{\|}{p_2}}) = P(E_2) = \frac{1}{26}, \quad E_3 = \frac{p_3^2}{2m} \longleftrightarrow P(\underset{-3\hbar}{\overset{\|}{p_3}}) = P(E_3) = \frac{25}{26}$$

Edo zuzenean Ψ $\hat{p}$-ren autofuntzioetan garatu → $\Psi = \sum_n C_n^p \Psi_n^p$ → $P(p_n) = |C_n^p|^2$

- Energia zehaztuta badago partikula askearen kasuan p momentu unean zehaztuta dago?

Partikula askea → $E_k = \frac{\hbar^2 k^2}{2m} = \frac{p_k^2}{2m}$, $\quad \hat{H} \Rightarrow \Psi_k = Ae^{ikx} + Be^{-ikx}$

$\hat{p} \Rightarrow \Psi_k^p = Ce^{ikx}$ ez dira berdinak

$p_k = \pm\sqrt{2E_k m} = \pm\hbar k$

Ez dago guztiz zehaztuta. Energia zehaztuk badago $\Psi_k = Ae^{ikx} + Be^{-ikx}$ beraloko egoera batean gaude, eta ez da $\Psi_k^p = Ce^{ikx}$ egoeraren berdina izan behar.

(Berdina izango balitz p zehaztuta egongo litzateke) → p-ren bi balio posible: $\pm\hbar k$

↳ $A, B \neq 0$ egoera hori ez da $\hat{p}$-ren autofuntzioa ($\hat{p}$-ren bi autobalio ezberdinen konb lineala delako)

Potentzial osin infinituan jaude, jatorrian zentratuta: $\Psi(x,0) = \psi_1 + 2i\psi_3$

$$\psi_n = \begin{cases} \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} & n \text{ bikoitia} \\ \sqrt{\frac{2}{a}} \cos \frac{n\pi x}{a} & n \text{ bak.} \end{cases}$$

Energia neurtzen dugu. Zein da $\langle E(t) \rangle$?

Kasu honetan $E = H \rightarrow \langle E(t) \rangle = \langle H(t) \rangle = \langle H \rangle$

* $\psi(x,0) = \psi_1 + 2i\psi_3 \rightarrow$ Normalizatu $\rightarrow \int_{-a/2}^{a/2} \psi^*(x,0)\, \psi(x,0)\, dx = (\psi_1 + 2i\psi_3, \psi_1 + 2i\psi_3) =$

$(\psi_1 + 2i\psi_3, \psi_1) + (\psi_1 + 2i\psi_3, 2i\psi_3) = (\psi_1, \psi_1) + \cancel{(2i\psi_3, \psi_1)}^{0} + \cancel{(\psi_1, 2i\psi_3)}^{0} +$

$(2i\psi_3, 2i\psi_3) = (\psi_1, \psi_1) + 2i(-2i)(\psi_3, \psi_3) = (\psi_1, \psi_1) + 4(\psi_3, \psi_3) =$

normalizatuta daudelako ψ_n-ak

$1 + 4 = 5 \leftrightarrow \psi(x,0) = \frac{1}{\sqrt{5}} \cdot \psi_1 + \frac{2i}{\sqrt{5}} \cdot \psi_3$

* Potentzial osin infinituaren autofuntzioetan garatuta dagoenez $\Psi(x,0) \rightarrow$

$$\Psi(x,t) = \frac{1}{\sqrt{5}} \psi_1 e^{-i\frac{E_1}{\hbar}t} + \frac{2i}{\sqrt{5}} \psi_3 e^{-i\frac{E_3}{\hbar}t}$$

Energia posibleak $\rightarrow E_1$ eta $E_3 \rightarrow P(E_1) = \left| \frac{e^{-i\frac{E_1}{\hbar}t}}{\sqrt{5}} \right|^2 = \frac{1}{5}$

$P(E_3) = \left| \frac{e^{-i\frac{E_3}{\hbar}t}}{\sqrt{5}} \cdot 2i \right|^2 = \frac{4}{5}$

$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$

$\langle E \rangle = P(E_1) \cdot E_1 + P(E_3) \cdot E_3 = \frac{E_1}{5} + \frac{4E_3}{5} = \frac{1}{5}(E_1 + 4E_3) =$

ψ_1, ψ_3 autofuntzioak

$\frac{1}{5} \frac{\hbar^2 \pi^2}{2ma^2}(1 + 4 \cdot 9) = \frac{37}{10} \frac{\hbar^2 \pi^2}{ma^2}$

Edo $\langle \hat{H} \rangle_\Psi = (\Psi, \hat{H}\Psi) = \left(\frac{1}{\sqrt{5}} e^{-i\frac{E_1}{\hbar}t} \psi_1 + \frac{2i}{\sqrt{5}} \psi_3 e^{-i\frac{E_3}{\hbar}t}, \hat{H}\left(\frac{1}{\sqrt{5}} \psi_1 e^{-i\frac{E_1}{\hbar}t} + \frac{2i}{\sqrt{5}} \psi_3 e^{-i\frac{E_3}{\hbar}t} \right) \right) =$

$\left(\frac{1}{\sqrt{5}} e^{-i\frac{E_1}{\hbar}t} \psi_1 + \frac{2i}{\sqrt{5}} e^{-i\frac{E_3}{\hbar}t} \psi_3, \frac{1}{\sqrt{5}} \cdot E_1 e^{-i\frac{E_1}{\hbar}t} \psi_1 + \frac{2i}{\sqrt{5}} E_3 e^{-i\frac{E_3}{\hbar}t} \psi_3 \right) = \frac{1}{5} E_1 (\psi_1, \psi_1) + \frac{(-2i)(2i)}{5} E_3 (\psi_3, \psi_3) = \frac{E_1}{5} + \frac{4E_3}{5}$

$$P(x,0) = |\psi(x,0)|^2 = \frac{1}{5}\left((\psi_1 + 2i\psi_3)(\psi_1^* - 2i\psi_3^*)\right) = \frac{1}{5}\left[|\psi_1\psi_1^* - 2i\psi_1\psi_3^* + 2i\psi_3\psi_1^* + 4\psi_3^*\psi_3|\right] =$$

$\downarrow$ $\psi_K \in \mathbb{R}$

$\frac{1}{5}(\psi_1^2 + 4\psi_3^2) \rightarrow$ simetrikoa da

simetrikoa $x=0$-rekiko

- Non dago probabilitate handiagoa partikula (ezkerrean, eskuinean edo erdialdean)?

$P(x,0) = \frac{1}{5}\left(\frac{2}{a}\cos^2\frac{\pi x}{a} + \frac{8}{a}\cos^2\frac{3\pi x}{a}\right)$ bikoitia denez, bere integrala

$(-a/2,0)$ tartean eta $(0,a/2)$ tartean berdina izango da,

hau da $P(x<0) = P(x>0) = \frac{1}{2} \rightarrow \langle x\rangle = 0$

- $\psi(x,0) = \frac{1}{\sqrt5}(\psi_1 + 2i\psi_2) \rightarrow \Psi(x,t) = \frac{1}{\sqrt5}\left(\psi_1 e^{-\frac{i\varepsilon_1 t}{\hbar}} + 2i\psi_2 e^{-\frac{i\varepsilon_2 t}{\hbar}}\right) \rightarrow$ zein da probabilitatea partikula eskuinean eta ezkerrean egoteko?

ψ_K errealak

$$P(x,t) = |\Psi(x,t)|^2 = \frac{1}{5}\left(\left(\psi_1 e^{-\frac{i\varepsilon_1 t}{\hbar}} + 2i\psi_2 e^{-\frac{i\varepsilon_2 t}{\hbar}}\right)\left(\psi_1^* e^{\frac{i\varepsilon_1 t}{\hbar}} - 2i\psi_2^* e^{\frac{i\varepsilon_2 t}{\hbar}}\right)\right) =$$

$$\frac{1}{5}\left[\psi_1^2 - 2i\psi_1\psi_2 e^{-\frac{i(\varepsilon_1-\varepsilon_2)t}{\hbar}} + 2i\psi_2\psi_1 e^{\frac{i(\varepsilon_1-\varepsilon_2)t}{\hbar}} + 4\psi_2^2\right] =$$

$$\frac{1}{5}\left[\psi_1^2 + 4\psi_2^2 + 2i\psi_1\psi_2\left(e^{\frac{i(\varepsilon_1-\varepsilon_2)t}{\hbar}} - e^{-\frac{i(\varepsilon_1-\varepsilon_2)t}{\hbar}}\right)\right] = \frac{1}{5}\left[\psi_1^2 + 4\psi_2^2 - 4\psi_1\psi_2\sin\left(\frac{(\varepsilon_1-\varepsilon_2)t}{\hbar}\right)\right]$$

Orain ez da simetrikoa. (ψ_3 edukiko bagenu ψ_2 ordez, simetrikoa, bikoitia izango litzateke eta probabilitatea berdina)

$$P(x<0) = \int_{-a/2}^{0} P(x,t)\,dx \neq P(x>0) = \int_0^{a/2} P(x,t)\,dx$$

(bakoitiak)

$$\langle x\rangle = \int_{-a/2}^{a/2} x\cdot\frac{1}{5}\left(\psi_1^2 + 4\psi_2^2 - 4\psi_1\psi_2\sin\left(\frac{(\varepsilon_1-\varepsilon_2)t}{\hbar}\right)\right)dx = \underbrace{\int_{-a/2}^{a/2} x\cdot\cancel{\frac{2}{5a}\cos^2\frac{\pi x}{a}}\,dx}_{0} + \underbrace{\int_{-a/2}^{a/2} x\cdot\cancel{\frac{8}{5a}\cos^2\frac{2\pi x}{a}}\,dx}_{0} +$$

$$-4\sin\left(\frac{(\varepsilon_1-\varepsilon_2)t}{\hbar}\right)\int_{-a/2}^{a/2} x\cos\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx = -4\sin\left(\frac{(\varepsilon_1-\varepsilon_2)t}{\hbar}\right)\frac{16a}{18\pi^2} = \frac{-32}{9\pi^2}a\sin\left(\frac{(\varepsilon_1-\varepsilon_2)t}{\hbar}\right)$$

FISIKA KUANTIKOA

16-10-05

2. FORMALISMOA:

• MEKANIKA KUANTIKOAREN POSTULATUAK:

Mekanika kuantikoaren postulatuak → arrazt hartzen ditugun ezinbesteko puntuak mekanika kuantikoan.

1. postulatua: uhin funtzioa, $\Psi(x,t)$ → sistemaren egoera deskribatzen duena → interpretazio probabilistikoa; $P(x,t) = |\Psi(x,t)|^2$... Normalean ezin da zuzenean neurtu baina sistemaren informazio guztia darama.

2. postulatua: eragileak. A magnitude fisiko bat bada, horrekin lotuta $\hat{A}$ eragilea definitu dezakegu → hermitikoa ($\hat{A} = \hat{A}^+$) eta lineala.

3. postulatua: neurketak eta autobalioak. $\Psi(x,t)$ uhin funtzioa bada eta sistema egoera horretan badago, A magnitudea neurtzen badugu neurketa horretatik lor ditzakegun balioak $\hat{A}$-ren autobalioak baino ezin dira izan. ($\hat{A}\psi_n = a_n\psi_n$)

4. postulatua: emaitza ezberdinen probabilitateak. Neurketetan, magnitude horren eragilearen autobalioak baino ezin dira neurtu, baina balioek probabilitate bat izango du. $\Psi(x,t)$ gure egoera izanda $\hat{A}$-ren autofuntzioetan garatu dezakegu → $\Psi(x,t) = \sum_n c_n\psi_n$

Orduan, a_n neurtzeko probabilitatea $|c_n|^2 = P(a_n)$ izango da ($c_n = (\psi_n, \Psi)$)

5. postulatua: neurketa baten ondoko egoera kuantikoa. Demagun gure sistema $\Psi(x,t)$ egoeran dagoela eta t_0 aldiunean neurketa bat egiten dugula → lortu dugu $A = a_n$ dela (autobalio bat) → nahiz eta neurketa baino lehen edozein a_n neurtzea posible den orain ez, egoera aldatu da t_0-n → $\Psi(x,t_0) = \psi_n$ (a_n-ri dagokion

↳ Orain t_0-n a_n neurtzeko probabilitatea 1 da, balio hori neurtu dugulako autofuntzioa) $\longleftrightarrow$ uhin funtzioa kolapsatu egin da neurketen ondorioz eta hemendik

aurrera $\Psi(x,t_0) = \Psi_n$ denborarekin aldatuko da. denboraren garapena nolakoa izango da

6. postulatua: uhin-funtzioaren denboraren garapena Schrödingeren ekuazioak ematen du:

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial t^2} + V(x,t)\Psi$$

Postulatu hauekin eta hauetan oinarrituta mekanika kuantikoaren garapena egiten dira.

• TRUKATZAILEAK:

Bi eragile trukakorrak diren edo ez jakiteko eragile bat definitu dugu: trukatzaileen eragiketa.

Mekanika klasikoan adibidez, bi magnitude beti dira trukakorrak ($x \cdot p = p \cdot x$ ad.) funtzioen biderkadura beti delako trukakorra. Baina mekanika kuantikoan magnitude horiei lotuta eragileak ditugunez ez dute zertan trukakorrak izan.

Demagun $\hat{A}$ eta $\hat{B}$ eragileak ditugunez $\rightarrow$ bi eragileen arteko trukatzailea hauxe da:

$* \; [\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \longleftrightarrow [\hat{A},\hat{B}] = 0$ trukakorrak dira

$[\hat{A},\hat{B}] \neq 0$ ez dira trukakorrak

Trukatzailearen propietateak:

$\lambda \in \mathbb{C}$ delako, bestela ez

1. $\lambda \in \mathbb{C}$; $[\lambda\hat{A},\hat{B}] = \lambda[\hat{A},\hat{B}]$

   $\hookrightarrow$ eragile linealak: $[\lambda\hat{A},\hat{B}] = \lambda\hat{A}\hat{B} - \hat{B}\lambda\hat{A} = \lambda(\hat{A}\hat{B} - \hat{B}\hat{A})$

2. $\hat{A}, \hat{B}$ eta $\hat{C}$ eragileak ; $[\hat{A}+\hat{B},\hat{C}] = [\hat{A},\hat{C}] + [\hat{B},\hat{C}]$

3. $\hat{A}, \hat{B}$ eta $\hat{C}$ eragileak ; $[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B}$

• TRUKATZAILEEN ADIBIDEAK:

deribatu $x\Psi$

1.- $[\hat{x},\hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = x\left(-i\hbar\frac{\partial}{\partial x}\right) - \left(-i\hbar\frac{\partial}{\partial x}\right)x = -i\hbar x\frac{\partial}{\partial x} + i\hbar\frac{\partial}{\partial x}x = -i\hbar x\frac{\partial}{\partial x} + i\hbar\left(1 + x\frac{\partial}{\partial x}\right) =$

$\cancel{-i\hbar x\frac{\partial}{\partial x}} + i\hbar + \cancel{i\hbar x\frac{\partial}{\partial x}} = i\hbar \neq 0$ ez dira trukakorrak

2- $[\hat{x}, \hat{T}] = \hat{x}\hat{T} - \hat{T}\hat{x} = \hat{x}\frac{\hat{p}^2}{2m} - \frac{\hat{p}^2}{2m}\hat{x} = \frac{1}{2m}[\hat{x}, \hat{p}^2] \Longrightarrow$ Bi modu hau aztertzeko:

- $\hat{p}^2 = \hat{p}\hat{p} = -i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial}{\partial x}\right) = -\hbar^2\frac{\partial^2}{\partial x^2}$

$$[\hat{x}, \hat{p}^2] = -\hbar^2\left[x, \frac{\partial^2}{\partial x^2}\right] = -\hbar^2\left(x\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x^2}x\right) = -\hbar^2\left(x\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x}\left(1 + x\frac{\partial}{\partial x}\right)\right) =$$

$$-\hbar^2\left(x\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} - \frac{\partial}{\partial x}\left(x\frac{\partial}{\partial x}\right)\right) = -\hbar^2\left(\cancel{x\frac{\partial^2}{\partial x^2}} - \frac{\partial}{\partial x} - \frac{\partial}{\partial x} \cancel{-x\frac{\partial^2}{\partial x^2}}\right) = 2\hbar^2\frac{\partial}{\partial x} \neq 0$$

ez dira trukakorrak

$$[\hat{x}, \hat{T}] = \frac{\hbar^2}{m}\frac{\partial}{\partial x}$$

- $[\hat{x}, \hat{p}^2] = [\hat{x}, \hat{p}\hat{p}] = (\hat{p}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{p}) \overset{\text{aurretik}}{=} \hat{p}(i\hbar) + i\hbar\hat{p} = 2i\hbar\hat{p} \longleftrightarrow$

$$[\hat{x}, \hat{T}] = \frac{2i\hbar}{2m}\hat{p} = \frac{i\hbar}{m}\left(-i\hbar\frac{\partial}{\partial x}\right) = \frac{\hbar^2}{m}\frac{\partial}{\partial x}$$

ez dira trukakorrak

- **BEHAGARRI BATERAGARRIAK:**

Behagarri bateragarriak aldi berean zehaztasun osoz neurtu ditzakegun behagarriak, magnitude fisikoak, dira. Zehaztasun osoz neurtzeko, behagarri horren eragilearen autofuntzio batean egon behar da sistema:

- $\hat{A} \to \hat{A}\Psi_n^a = a_n\Psi_n^a \to$ Sistema $\hat{A}$-ren autofuntzio batean badago eta egoera horretan A neurtzen badugu a_n autobalioa lortuko dugu. Bestalde, sistema autofuntzioen konbinazio lineal batean badago ezinez aurretik ezin dezakegu esan zein izango den A neurketaren emaitza (badakigu autobalioetako bat izango dela baina ez zein → ez dago zehaztuta)

- $\hat{B}$ eragilea badugu (B magnitudeari dagokiona) → $\hat{B}\Psi_n^b = b_n\Psi_n^b$ autofuntzio eta autobalio batzuk izango ditu.
  B zehaztasun osoz ere neurtu ahal izateko sistema bere autofuntzioetako batean egon beharko da.

A eta B bateragarriak izateko ezinbestekoa da biak zehaztasun osoz neurtu ahal izatea aldi berean. $\longleftrightarrow$ Egoera bien autofuntzioa izan behar da $\longleftrightarrow$ $\{\psi_n^a\} \equiv \{\psi_n^b\}$ autofuntzioak berdinak izan behar dira

Autofuntzioak berdinak izateko eragileek bete behar duten baldintza hauxe da:

$$[\hat{A}, \hat{B}] = 0 \qquad \text{TRUKAKORRAK IZATEA}$$

Froga: $\hat{A}$ eta $\hat{B}$ endakatuak ez direla suposatuz (adibide honetan)

$$\hat{A}\hat{B}\psi_n^b = \hat{A}(\hat{B}\psi_n^b) = \hat{A}(b_n\psi_n^b) = b_n(\hat{A}\psi_n^b) \underset{\substack{\downarrow \\ \text{trukakorrak } \hat{A}\hat{B}=\hat{B}\hat{A}}}{=} \hat{B}\hat{A}\psi_n^b = \hat{B}(\hat{A}\psi_n^b) =$$

$$\hat{B}(\hat{A}\psi_n^b) \longleftrightarrow \hat{B}(\underbrace{\hat{A}\psi_n^b}_{\psi}) = b_n(\underbrace{\hat{A}\psi_n^b}_{\psi}) \longleftrightarrow \hat{B}\psi = b_n\psi \longleftrightarrow$$

n → bere autobalioa b_n delako

ψ $\hat{B}$-ren autofuntzioa da $\rightarrow \psi = \alpha\psi_n^b \longleftrightarrow \hat{A}\psi_n^b = \alpha\psi_n^b \longleftrightarrow$

ψ_n^b $\hat{A}$-ren autofuntzioa da. eta α autofuntzio horren autobalioa

$$\longleftrightarrow \{\psi_n^a\} = \{\psi_n^b\}$$

- **BEHAGARRI TRUKAKORREKO MULTZO OSOA:**

* Bi behagarri aldi berean zehaztasun osoz neurtu ahal izateko trukakorrak izan behar dira → egoerak behagarri horien autofuntzioak dira.

* Multzo osoa behar den behagarrien kopuru minimoa da autofuntzio horiek erabat zehaztu ahal izateko:

autobalio guztiak ez-berdinak izatea

- $\hat{A}$: $\hat{A}\psi_n = a_n\psi_n$ a_n ez bada endekatua A-ren balioa neurtzen badugu jakingo dugu zer egoeratan gauden, erabat zehaztuta dago. → Kasu honetan multzo osoa A behagarriaz baino ez da osatuta egongo, nahikoa delako egoera guztiz zehazteko. $\{\hat{A}\}$

• $\hat{A}$; $\hat{A}\psi_n = a_n\psi_n$ badugu eta endakatua bada kasu ezberdina:

beste guztiak ez daude endakatuta

Demagun bi egoera endakatu ditugula: $\hat{A}\psi_1 = a\psi_1$, $\hat{A}\psi_2 = a\psi_2$

Orduan, a autobalioa emanda, A-ren balioa neurtuan, ez dago guztiz zehaztuta ze egoeratan gauden → beste behagarri bat behar da, endekapen hori ez daukan behagarri bat $[\hat{A},\hat{B}]=0$ izanda:

$\hat{B}$; $\hat{B}\psi_1 = b_1\psi_1$, $\hat{B}\psi_2 = b_2\psi_2$ → ez dago endakatuta ψ_1 eta ψ_2 autofuntzioetan (beste batzuetan egon daiteke)

Honela, B-ren balioa behar genuke eta hori ezagututa jakin ahal izango genuke zer egoeratan gauden zehaztasunez.

Modu berean, A beste egoeretan endakatuta ez dagoenez eta egoera horietan B endekatuta egon daitekeenez, A-rekin nahiko izango litzateke egoera guztiz zehaztea. Hanregatik, multzo osoa kasu honetan, 2 behagarri dira.

$\{\hat{A},\hat{B}\}$

• Endekapenak handiagoak badira gerta daiteke behagarri gehiago behar izatea.

• ZIURGABETASUNAREN PRINTZIPIOA FORMALISMOAREN BARRUAN:

Ziurgabetasunaren printzipioa → $\Delta x \Delta p \geq \hbar/2$

Ziurgabetasun beste magnitude batzuekin lotuta ere → ziurgabetasun printzipio orokorra:

$$(\Delta\hat{A})^2(\Delta\hat{B})^2 \geq -\frac{1}{4}\left(\overline{[\hat{A},\hat{B}]}\right)^2$$

Froga:

magnitude fisiko bat delako

1. A magnitudea → $\hat{A}=\hat{A}^+$, B magnitudea → $\hat{B}=\hat{B}^+$

Definitu $\delta\hat{A} = \hat{A}-\bar{\hat{A}}$ $\delta\hat{B}=\hat{B}-\bar{\hat{B}}$ → $\delta\hat{A}$ eta $\delta\hat{B}$ hermitikoak dira

egoera batean balioaldia (zenbaki bat) → $\bar{\hat{B}} = \langle B\rangle$, $\bar{\hat{A}}=\langle A\rangle$

* $[\hat{A},\hat{B}] = [\delta\hat{A},\delta\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = \delta\hat{A}\delta\hat{B} - \delta\hat{B}\delta\hat{A} = (\hat{A}-\bar{\hat{A}})(\hat{B}-\bar{\hat{B}}) - (\hat{B}-\bar{\hat{B}})(\hat{A}-\bar{\hat{A}}) =$

$\hat{A}\hat{B} - \cancel{\hat{A}\bar{\hat{B}}} - \cancel{\bar{\hat{A}}\hat{B}} + \cancel{\bar{\hat{A}}\bar{\hat{B}}} - \hat{B}\hat{A} + \cancel{\hat{B}\bar{\hat{A}}} + \cancel{\bar{\hat{B}}\hat{A}} - \cancel{\bar{\hat{B}}\bar{\hat{A}}} = \hat{A}\hat{B} - \hat{B}\hat{A}$

$\bar{\hat{A}}$ eta $\bar{\hat{B}}$ zenbakiak direlako

2. $\overline{\hat{C}\hat{C}^+} \geq 0$; $\overline{\hat{C}^+\hat{C}} \geq 0$

kasu honetan $\hat{C}$-k ez du hermitikoa izan behar

* $(\hat{C}^+)^+ = \hat{C}$; $\overline{\hat{C}\hat{C}^+} = (\Psi, \hat{C}\hat{C}^+\Psi) = (\hat{C}^+\Psi, \hat{C}^+\Psi) = \int |\hat{C}^+\Psi|^2 dx \geq 0$

$$\overline{\hat{C}^+\hat{C}} = (\Psi, \hat{C}^+\hat{C}\Psi) = (\hat{C}\Psi, \hat{C}\Psi) = \int |\hat{C}\Psi|^2 dx \geq 0$$

$\delta\hat{A}$ eta $\delta\hat{B}$ hermitikoak

3. $\hat{C}$ eragilea $\rightarrow$ $\hat{C} = \delta\hat{A} + i\lambda\delta\hat{B}$ $(\lambda \in \mathbb{R})$ $\quad \hat{C}^+ = (\delta\hat{A})^+ + (i\lambda\delta\hat{B})^+ = \delta\hat{A} - i\lambda\delta\hat{B}$

$\overline{\hat{C}\hat{C}^+} = \overline{(\delta\hat{A} + i\lambda\delta\hat{B})(\delta\hat{A} - i\lambda\delta\hat{B})} = \overline{(\delta\hat{A}^2 - i\lambda\delta\hat{A}\delta\hat{B} + i\lambda\delta\hat{B}\delta\hat{A} + \lambda^2\delta\hat{B}^2)} = \overline{\delta\hat{A}^2} - i\lambda\overline{\delta\hat{A}\delta\hat{B}} +$

definizioa $\Delta A = \sqrt{\overline{(A-\overline{A})^2}}$

$i\lambda\overline{\delta\hat{B}\delta\hat{A}} + \lambda^2\overline{\delta\hat{B}^2} = \overline{\delta\hat{A}^2} - i\lambda(\overline{\delta\hat{A}\delta\hat{B} - \delta\hat{B}\delta\hat{A}}) + \lambda^2\overline{(\delta\hat{B})^2} = (\Delta\hat{A})^2 + \lambda^2(\Delta\hat{B})^2 - i\lambda\overline{[\delta\hat{A}, \delta\hat{B}]} =$

$$(\Delta\hat{A})^2 + \lambda^2(\Delta\hat{B})^2 - i\lambda\overline{[\hat{A}, \hat{B}]} \geq 0 \xrightarrow{\cdot (\Delta\hat{B})^2} (\Delta\hat{A})^2(\Delta\hat{B})^2 + \lambda^2(\Delta\hat{B})^4 - i\lambda\overline{[\hat{A}, \hat{B}]}(\Delta\hat{B})^2 \geq 0 \rightarrow$$

uhin funtzio baten gainean $\rightarrow$ nudulen proba

$$(\Delta\hat{A})^2(\Delta\hat{B})^2 \geq \underbrace{i\lambda\overline{[\hat{A}, \hat{B}]}(\Delta\hat{B})^2 - \lambda^2(\Delta\hat{B})^4}_{f(\lambda)}$$

$f(\lambda) \rightarrow \lambda$-ren funtzio bat $\rightarrow$ ereala

Kalkulatuko dugu λ-ren zer baliotarako daukagun f-ren minimoa $\rightarrow$

$$\frac{df}{d\lambda} = i\overline{[\hat{A}, \hat{B}]}(\Delta\hat{B})^2 - 2\lambda(\Delta\hat{B})^4 = 0 \rightarrow i\overline{[\hat{A}, \hat{B}]} = +2\lambda(\Delta\hat{B})^2 \rightarrow$$

$$\lambda = +\frac{i}{2}\frac{\overline{[\hat{A}, \hat{B}]}}{(\Delta\hat{B})^2}$$

Orduan $\rightarrow$ $(\Delta\hat{A})^2(\Delta\hat{B})^2 \geq -\frac{1}{2}\overline{[\hat{A}, \hat{B}]}^2 - \frac{1}{2}\overline{[\hat{A}, \hat{B}]}^2 = -\frac{1}{4}\overline{[\hat{A}, \hat{B}]}^2$

Beraz, lehen bezala, zehaztasun osoz neurtzeko bi magnitudeak

$[\hat{A}, \hat{B}] = 0$ izan behar da

↳ hau betetzen denean posible da $\Delta\hat{A}$ eta $\Delta\hat{B}$ biak 0 izatea

- **BEHAGARRIEN DENBORA-GARAPENAREN EKUAZIOA:**

* Behagarrien batez bestekoaren denboraren-garapenaren ekuazioa:

Demagun $\Psi(x,t)$ uhin-funtzioa dugula eta A magnitude-fisiko bateri lotutako (behagarria) eragile hermitikoa, $\hat{A}$.

Magnitude honen neurketak egiten badira normala izan daiteke neurketa balio ezberdinak lortzea, denborarekin aldatu daitekelako $\Rightarrow$ bataz bestekoak

batez bestekoa Ψ-rekiko

ekuazio bat betetzen du: $\dfrac{d\langle \hat{A} \rangle_\Psi}{dt} = \dfrac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle_\Psi + \left\langle \dfrac{\partial \hat{A}}{\partial t} \right\rangle_\Psi$

Froga:

- $\langle \hat{A} \rangle_\Psi = (\Psi, \hat{A}\Psi) = \int \Psi^* \hat{A} \Psi \, dx$

gerta daiteke $\hat{A}$ t-ren menpekoa izatea

- $\dfrac{d}{dt} \langle \hat{A} \rangle_\Psi = \dfrac{d}{dt} \left(\int \Psi^* \hat{A} \Psi \, dx \right) = \int \dfrac{\partial \Psi^*}{\partial t} \hat{A} \Psi \, dx + \int \Psi^* \dfrac{\partial \hat{A}}{\partial t} \Psi \, dx + \int \Psi^* \hat{A} \dfrac{\partial \Psi}{\partial t} \, dx =$

$\Psi(x,t)$ denez $dt \rightarrow \partial t$

$\int \dfrac{\partial \Psi^*}{\partial t} \hat{A} \Psi \, dx + \int \Psi^* \hat{A} \dfrac{\partial \Psi}{\partial t} \, dx + \left\langle \dfrac{\partial \hat{A}}{\partial t} \right\rangle_\Psi$

$\hat{x}, \hat{p}$ kasuetan nulua baina ad
V t-ren menpekoa bada $\hat{H}$ ere

- Bestalde, $\hat{H}\Psi = i\hbar \dfrac{\partial \Psi}{\partial t}$ da, $\Psi(x,t)$-k Schrödingeren ekuazioa betetzen duelako, orduan,

$\dfrac{\partial \Psi}{\partial t} = -\dfrac{i}{\hbar} \hat{H} \Psi$. eta modu berean $\left(\dfrac{\partial \Psi}{\partial t} \right)^* = \left(-\dfrac{i}{\hbar} \hat{H} \Psi \right)^* = \dfrac{i}{\hbar} \hat{H} \Psi^* = \dfrac{\partial \Psi^*}{\partial t}$

- $\dfrac{d}{dt} \langle \hat{A} \rangle_\Psi = \int \dfrac{i\hat{H}}{\hbar} \Psi^* \hat{A} \Psi \, dx - \int \dfrac{i}{\hbar} \Psi^* \hat{A} \hat{H} \Psi \, dx + \left\langle \dfrac{\partial \hat{A}}{\partial t} \right\rangle_\Psi = \left\langle \dfrac{\partial \hat{A}}{\partial t} \right\rangle_\Psi +$

$\dfrac{i}{\hbar} (\hat{H}\Psi, \hat{A}\Psi) - \dfrac{i}{\hbar} (\Psi, \hat{A}\hat{H}\Psi) \underset{\hat{H} = \hat{H}^+}{=} \left\langle \dfrac{\partial \hat{A}}{\partial t} \right\rangle_\Psi + \dfrac{i}{\hbar} (\Psi, \hat{H}\hat{A}\Psi) - \dfrac{i}{\hbar} (\Psi, \hat{A}\hat{H}\Psi) =$

$\left\langle \dfrac{\partial \hat{A}}{\partial t} \right\rangle_\Psi + \dfrac{i}{\hbar} \left(\Psi, (\hat{H}\hat{A} - \hat{A}\hat{H})\Psi \right) = \boxed{\dfrac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle_\Psi + \left\langle \dfrac{\partial \hat{A}}{\partial t} \right\rangle_\Psi}$

· EHRENFEST

$\hat{A}$-k denborarekiko menpekotasunik ez badu, edozein egoeran batean $\langle \hat{A} \rangle$ konstante izateko

$\hat{H}$ eta $\hat{A}$ trukakorrak izan behar dira ; $[\hat{H}, \hat{A}] = 0 \rightarrow \langle \hat{A} \rangle_\Psi = \text{kte}$ edozein egoera

batean (neurketa guztietan ez da balio bera lortuko, alda daiteke, baina batazbestekoa

edozein egoeratan, edozein Ψ-rako konstantea izango da) Horretarako Ψ magnitude honen autofuntzio bat izan behar da

↳ Horregatik $\hat{H}$ denborarekiko independentea denean (V t-ren menpekoa ez denean) bere

batez bestekoa konstantea da.

• HIGIDURA-KONSTANTEAK:

Higidura-konstanteak ⟺ denboran zehar konstante mantentzen diren magnitude fisikoak dira:

1. Demagun sistema Ψ egoeran dagoela eta A behagarria neurtzen dugula ($\hat{A}$ bere eragilea izanik) eta egoera horretan egonik beti balio bera lortzen dugula (A beti da berdina) ⟷ Ψ $\hat{A}$-ren autofuntzioetariko bat izan behar da.

$(\Psi = \psi^a)$ eta egoera, Ψ, denborarekin ez aldatzea, beti izan dadin $\hat{A}$-ren autofuntzioa → horretarako egoera hori $\hat{A}$-ren autofuntzio bat izan behar da, ere.

$(\hat{A}\psi^a = \varepsilon\psi^a)$ $\Psi = \psi^a e^{-i\frac{E}{\hbar}t}$ modukoa izan dadin (badakigu horrelakoa dela $\hat{A}$-ren autofuntzioan denboraren garapena → $P(a) = 1$) Oso kasu berezia

2. Demagun sistema $\Psi(x,t)$ egoeran dagoela eta A-rekin lotutako eragilea $\hat{A}$ dela.

$\langle \hat{A} \rangle_\Psi = \text{kte}$ izateko: $\left(\frac{d}{dt}\langle \hat{A} \rangle_\Psi = \frac{i}{\hbar}\langle [\hat{H},\hat{A}] \rangle_\Psi + \langle \frac{\partial \hat{A}}{\partial t} \rangle_\Psi \right)$

a) $\frac{\partial \hat{A}}{\partial t} = 0$ ⟹ edozein egoeraren independentea ⟹ hau betetzen bada (a) eta b)) → higidura konstantea

b) $[\hat{H},\hat{A}] = 0$

• EHRENFEST-EN TEOREMAK:

Teoremen helburua: $\langle \hat{x} \rangle$ eta $\langle \hat{p} \rangle$-k betetzen duten eboluzioa denboran.

1. $\hat{x}$ ⟹ $\frac{d}{dt}\langle \hat{x} \rangle = \frac{i}{\hbar}\langle [\hat{H},\hat{x}] \rangle + \cancel{\langle \frac{\partial \hat{x}}{\partial t} \rangle} = \frac{i}{\hbar}\langle [\hat{H},\hat{x}] \rangle$ $\quad -[\hat{x},\hat{p}] = [\hat{p},\hat{x}] = -i\hbar$

$\hat{H} = \frac{\hat{p}^2}{2m} + V(x,t)$; $[\hat{H},\hat{x}] = \frac{1}{2m}[\hat{p}^2, x] + \overset{0}{\cancel{[V(x,t),x]}} = \frac{1}{2m}(\hat{p}[\hat{p},x] + [\hat{p},x]\hat{p}) =$

$\frac{1}{2m}(\hat{p}(-i\hbar) + (-i\hbar)\hat{p}) = \frac{-2i\hbar\hat{p}}{2m} = -\frac{i\hbar}{m}\hat{p}$

$$\frac{d}{dt}\langle \hat{x} \rangle = \frac{i}{\hbar}\langle -\frac{i\hbar}{m}\hat{p} \rangle = -\frac{i\cancel{\hbar}}{m}\cdot\frac{i}{\cancel{\hbar}}\langle \hat{p} \rangle = \frac{\langle \hat{p} \rangle}{m}$$

2. $\hat{p}$ ⟹ $\frac{d}{dt}\langle \hat{p} \rangle = \frac{i}{\hbar}\langle [\hat{H},\hat{x}] \rangle + \cancel{\langle \frac{\partial \hat{p}}{\partial t} \rangle} = \frac{i}{\hbar}\langle [\hat{H},\hat{p}] \rangle$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x,t) \quad ; \quad [\hat{H},\hat{p}] = \frac{1}{2m}[\hat{p}^2,\hat{p}]^{*} + [V(x,t),\hat{p}] = V\hat{p} - \hat{p}V = -i\hbar V\frac{\partial}{\partial x} + i\hbar\frac{\partial (V)}{\partial x} =$$

$$-i\hbar \cancel{V\frac{\partial}{\partial x}} + i\hbar\frac{\partial V}{\partial x} + i\hbar \cancel{V\frac{\partial}{\partial x}} = i\hbar\frac{\partial V}{\partial x}$$

$$\frac{d\vec{p}}{dt} = \vec{F} = -\nabla\vec{V} = -\frac{\partial V}{\partial x}$$

1 dimentsio

$$* \; [\hat{p}^2,\hat{p}] = \hat{p}[\hat{p},\hat{p}] + [\hat{p},\hat{p}]\hat{p} = 0 + 0 = 0$$

$$\langle F \rangle = \frac{d}{dt}\langle \hat{p} \rangle = \frac{i}{\hbar}\langle i\hbar\frac{\partial V}{\partial x}\rangle = -\langle \frac{\partial V}{\partial x} \rangle \rightarrow \text{mekanika klasikoaren ekuazioaren antza}$$

Gradientea

◦ EHRENFEST-EN ERLAZIOEN LIMITE KLASIKOA:

Ehrenfesten ekuazioek aukera ematen dute kuantika eta mekanika klasikoaren arteko erlazioa ulertzeko → erlazioek mekanika klasikoaren antzeko erlazioak jarraitzen dituzte

Baina mekanika kuantikoan posizioa bezalako magnitudeak ezin direnez definitu batez bestekoak erabiltzen ditugu, eta batez bestekoek betetzen dituzte mekanika klasikoaren erlazioak:

$$\frac{d\langle \hat{x} \rangle}{dt} = \frac{\langle \hat{p} \rangle}{m} \quad ; \quad \langle F \rangle^{*} = -\langle \frac{\partial V}{\partial x} \rangle = \frac{d\langle \hat{p} \rangle}{dt}$$

* Mekanika klasikoan dugun Newtonen 2. legearen antzekoa izateko $\langle F \rangle$-ren ordez $F(\langle x \rangle)$ izan beharko genuke (printzipioz ez dira berdinak) →

x-ren batez bestekoan ebaluatuta

$$\langle F \rangle \neq F(\langle x \rangle) \quad \text{(Normalean)}$$

Froga:

$$F(x) = F(\langle x \rangle) + (x - \langle x \rangle)\frac{\partial F}{\partial x}\Big|_{x=\langle x \rangle} + \frac{1}{2}(x-\langle x \rangle)^2 \frac{\partial^2 F}{\partial x^2}\Big|_{x=\langle x \rangle} + \ldots \longrightarrow$$

Taylor
$\langle x \rangle$-ren inguruan

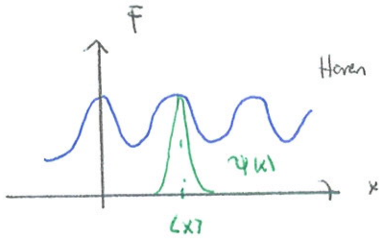
zenbaki bat da, ez dugu zertan batez bestekoa egin

$$\langle F(x) \rangle = F(\langle x \rangle) + \underbrace{\langle (\cancel{x - \langle x \rangle}) \rangle}_{0} \frac{\partial F}{\partial x}\Big|_{x=\langle x \rangle} + \frac{1}{2}\underbrace{\langle (x-\langle x \rangle)^2 \rangle}_{\Delta x^2} \frac{\partial^2 F}{\partial x^2}\Big|_{x=\langle x \rangle} + \ldots \Rightarrow$$

Orokorrean ez berdinak ($\frac{\partial^n F}{\partial x^n} = 0$ bada salbu ez) $n \geq 2$

Hurbilketa egiten $\Delta x \ll 1$ denean $\langle F(x) \rangle \simeq F(\langle x \rangle)$ bai

↳ uhin funtzioa oso estua denean F-k duen aldaketarekiko



Horen Modulua kasua dugunean adibidez. , $\Delta x << 1$ (Hurbilketan)

Hala ere, nahiz eta $\langle F\rangle = F(\langle x\rangle)$ izan eta adierazpen klasikoa bete ezin dugu esan ekarpen kuantikorik ez dagoela (adibidez osziladore harmonikoaren kasuan $\langle F(x)\rangle = F(\langle x\rangle)$ da baina ekarpen kuantikoak daude) $\Rightarrow$ ezin da esan sistema klasikoa dela

↳ energiaren kuantizazioa

• VIRIALAREN TEOREMA:

↳ Latinetik artua denez, vis = indarra, energia

*Teorema: Ψ_E egoera iraunkor bat badugu bertan lortutako energiaren balioa E izanik

↓ $|\Psi_E|^2 = P(x)$ t-ren independentea denean ↔ $\hat H$-ren autofuntzio balioa denean

$\Psi_E(x,t) = \psi_E(x)\, e^{-i\frac{E}{\hbar}t}$ dugu (x eta t banangarriak) eta egoera horretan kalkulatutako energia zinetikoaren batazbestekoa energia potentzialaren adierazpenarekin dago lotuta:

$$\langle \hat T\rangle_{\Psi_E} = \frac{1}{2}\left\langle x\frac{\partial V}{\partial x}\right\rangle_{\Psi_E} = -\frac{1}{2}\langle xF\rangle_{\Psi_E}$$

Froga: $\frac{d\langle\hat A\rangle}{dt} = \frac{i}{\hbar}\langle[\hat H,\hat A]\rangle + \left\langle\frac{\partial\hat A}{\partial t}\right\rangle$ aplikatu $\hat A = \frac{\hat x\hat p+\hat p\hat x}{2}$ -n.

hau gehitu hermitikoa izateko

* Teorema hau betetzeko ezinbestekoa da Ψ_E egoera iraunkorra izatea

1. $\langle\hat A\rangle_{\Psi_E} = (\Psi_E, \hat A\Psi_E) = (\psi_E e^{-i\frac{E}{\hbar}t}, \hat A(\psi_E e^{-i\frac{E}{\hbar}t})) = (\psi_E, \hat A\psi_E) \neq f(t)$

↓ $\hat A$ lineala (definizioagatik)

↘ denboraren menpekotasuna desagertu

$$\frac{d\langle\hat A\rangle_{\Psi_E}}{dt} = 0$$

2. $\frac{\partial\hat A}{\partial t}=0$ denez, $\left\langle\frac{\partial\hat A}{\partial t}\right\rangle=0$ ere eta 1.-ren ondorioz $\langle[\hat H,\hat A]\rangle=0$ izango da.

$$[\hat H,\hat A] = \frac{1}{2}\{[\hat H,\hat x\hat p]+[\hat H,\hat p\hat x]\} = \frac{1}{2}\{\hat x[\hat H,\hat p]+[\hat H,\hat x]\hat p+\hat p[\hat H,\hat x]+[\hat H,\hat p]\hat x\}=$$

$$\hat{T}=\hat{p}^2/2m$$

$$\frac{1}{2}\{\hat{x}[\hat{V},\hat{p}]+\hat{x}\cancel{[\hat{T},\hat{p}]}^{0}+\cancel{[\hat{V},\hat{x}]}^{0}\hat{p}+[\hat{T},\hat{x}]\hat{p}+\hat{p}\cancel{[\hat{V},\hat{x}]}+\hat{p}[\hat{T},\hat{x}]+\cancel{[\hat{T},\hat{p}]}\hat{x}+[\hat{V},\hat{p}]\hat{x}\}\overset{*}{=}$$

$$\frac{1}{2}\{xi\hbar\frac{\partial V}{\partial x}+\left(-\frac{i\hbar}{m}\hat{p}\right)\hat{p}+\hat{p}\left(-\frac{i\hbar}{m}\hat{p}\right)+i\hbar\frac{\partial V}{\partial x}\cdot x\}=xi\hbar\frac{\partial V}{\partial x}-\frac{i\hbar}{m}\hat{p}^2\neq 0 \quad \text{baina}$$

$$= i\hbar\{x\frac{\partial V}{\partial x}-\frac{\hat{p}^2}{m}\}$$

batazbestekoa bai.

$$* \; [\hat{V},\hat{p}]=\hat{V}\hat{p}-\hat{p}\hat{V}=-i\hbar V\frac{\partial}{\partial x}+i\hbar\frac{\partial}{\partial x}V=-i\hbar\cancel{V\frac{\partial}{\partial x}}+i\hbar\frac{\partial V}{\partial x}+\cancel{Vi\hbar\frac{\partial}{\partial x}}=i\hbar\frac{\partial V}{\partial x}$$

$$[\hat{T},\hat{x}]=\frac{1}{2m}[\hat{p}^2,\hat{x}]=\frac{1}{2m}\left(\hat{p}[\hat{p},\hat{x}]+[\hat{p},\hat{x}]\hat{p}\right)=\frac{1}{2m}\left(\hat{p}(-i\hbar)+(-i\hbar)\hat{p}\right)=-\frac{2i\hbar\hat{p}}{2m}=$$

$$-\frac{i\hbar}{m}\hat{p}$$

$$\langle[\hat{H},\hat{A}]\rangle_{\psi_E}=0=i\hbar\left\langle x\frac{\partial V}{\partial x}-\frac{\hat{p}^2}{m}\right\rangle_{\psi_E}=0 \iff \left\langle x\frac{\partial V}{\partial x}-\frac{\hat{p}^2}{m}\right\rangle_{\psi_E}=0\rightarrow$$

$$\left\langle x\frac{\partial V}{\partial x}\right\rangle_{\psi_E}-2\langle\hat{T}\rangle_{\psi_E}=0\rightarrow \quad \langle\hat{T}\rangle_{\psi_E}=\frac{1}{2}\left\langle x\frac{\partial V}{\partial x}\right\rangle_{\psi_E}=-\frac{1}{2}\langle xF\rangle_{\psi_E}$$

(* Ad. $V=\alpha x^n$ badugu, $\frac{\partial V}{\partial x}=\alpha n x^{n-1}$, $x\frac{\partial V}{\partial x}=\alpha n x^n=nV\propto V\Rightarrow$

$\langle\hat{T}\rangle_{\psi_E}=\frac{1}{2}n\langle V\rangle_{\psi_E}$ → $\hat{T}$ eta V-ren arteko erlazioa eman)

↳ egoera geldikorrean badaugu $\langle\hat{T}\rangle_{\psi_E}+\langle\hat{V}\rangle_{\psi_E}=\langle\hat{H}\rangle_{\psi_E}=E$, bi ekuazio hauetatik $\langle\hat{T}\rangle_{\psi_E}$ eta $\langle\hat{V}\rangle_{\psi_E}$ lortu ditzakegu

DENBORAREN INDEPENDENTEA DEN SCHRÖDINGER-EN EKUAZIOAREN EBAZPENAREN IKUSTARAZPENA:

Denboraren independentea den schrödingerren ekuazioa grafikoki aztertuko dugu eta kualitatiboki bada ere, uhin-funtzioaren formaren inguruko ondorioak aterako ditugu.

Denboraren independentea den Schrödingeren ekuazioa: $\hat{H}\Psi=E\Psi$;

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}+V\Psi=E\Psi \; ; \quad \frac{d^2\Psi}{dx^2}=\frac{2m}{\hbar^2}(V-E)\Psi$$

↳ honek uhin-funtzioaren "kurbatitatearen" informazioa ematen du (ahurra, ganbila...)

Uhin funtzioak bete behar dituen baldintza orokorrak:

1.) $\int |\psi|^2 dx = 1$ (interpretazio probabilistikoa dela eta) ; $|\psi|^2$ integragarria izan behar da

eta $\lim_{x\to\pm\infty} \psi = 0$ izan behar da.

gerta daiteke, ad. potentzial oso infinituan, esate baterako

2.) Bigarren deribatua existitu behar da (ad. energia potentzialean infinituak ezin da egon...);

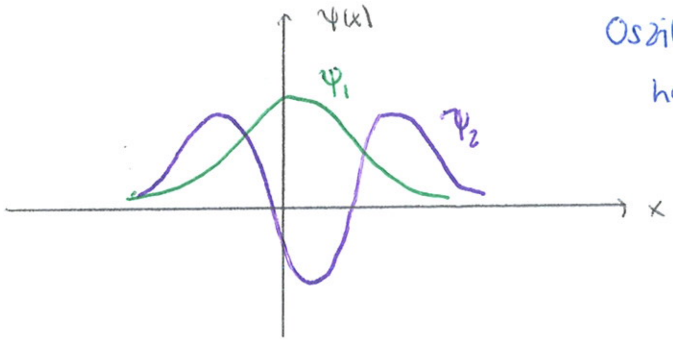
ψ eta $\frac{d\psi}{dx}$ finituak izan behar dira, balio bakarrekoak eta jarraituak. (Ager daiteke

lehenengo deribatuan ez-jarraitasun bat, potentzial oso infinituan...)

* Funtzioa ahurra edo ganbila izango den jakiteko, 2. deribatua aztertu behar da:

- $(V-\varepsilon)\psi > 0 \Rightarrow$ ahurra $\cup$
- $(V-\varepsilon)\psi < 0 \Rightarrow$ ganbila $\cap$

*



Oszilazio gehiago daudenean bigarren deribatua handiagoa da $|\psi_2|$ eta leunagoa denean $|\psi_1|$ txikiagoa.

- $\left|\frac{d^2\psi_1}{dx^2}\right| < \left|\frac{d^2\psi_2}{dx^2}\right|$

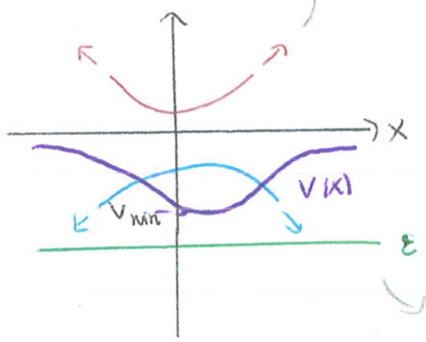
Hau V eta ε-ren arteko aldearen araberakoa da, aldea zenbat eta

handiagoa izan $\left|\frac{d^2\psi}{dx^2}\right|$ gero eta handiagoa izango da eta oszilazio gehiago egongo dira.

EZINEZKO ENERGIAK:

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V-\varepsilon)\psi$$

Kasu konkretua:



infinituetan infinitura jo, ezinezkoa → $\cancel{\int|\psi|^2 dx} \neq 1$

Kasu honetan $(V-\varepsilon) \geq 0$ izango da, eta ψ-ren ikurraren arabera $\frac{d^2\psi}{dx^2} > 0$ edo < 0 izango da.

- Demagun $\psi > 0$ dela $\Rightarrow$ ahurra

$\Rightarrow \varepsilon < V_{min}$

Klasikoki ezinezkoa $V \leq \varepsilon$ BETI

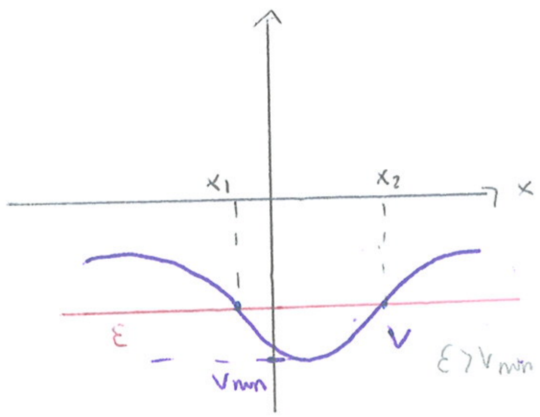
Infinituetan infinitura jo dezakeenez, uhin-funtzio honek ez du zentzu fisikoki izango. Posiblea da Schrödingeren denboraren independentea den ekuazioa bete baina zentzu fisikorik ez duen uhin-funtzio bat aurkitzea.

- Demagun $\psi < 0$ dela ⇒ ganbila
  Arazo bera daukagu → infinituetan infinitura doa → ezin da integragarria izan eta ondorioz ezin dezake zentzu fisikorik izan.
- $\psi = 0$ bada baldintzak betetzen dira, integragarria da, baina kasu honetan ez dugu uhin-funtziorik.

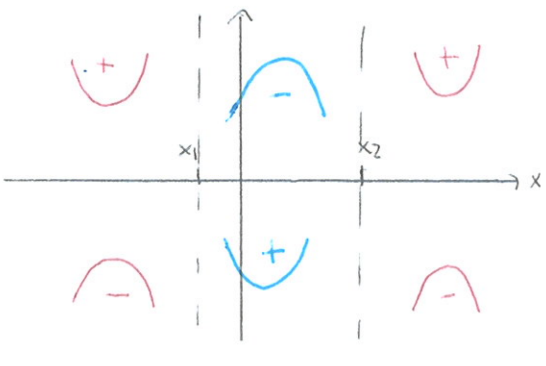
Beraz, ez dago esangura fisikoa duen holako Schrödingeren ekuazioa betetzen duen uhin-funtziorik ⇒ klasikoki daukagun arazo bera, $V \leq E$!

EGOERA-LOTUAK eta ENERGIAREN KUANTIZAZIOA:

Denboraren independentea den Schrödingeren ekuazioa: $\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V-E)\psi$



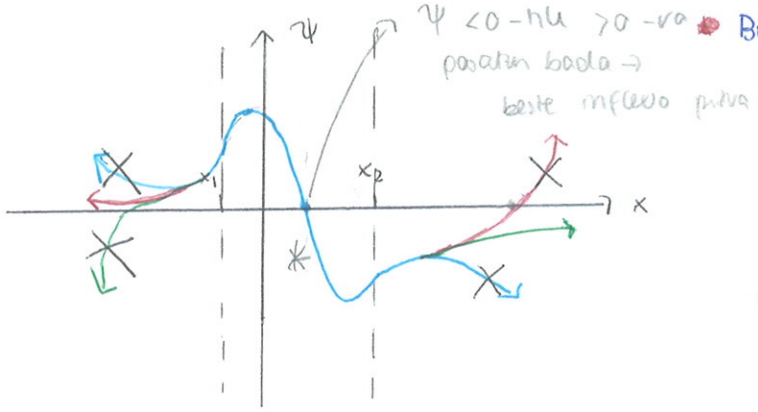
* x_1 eta x_2 puntuetan $E=V$ dugu, beraz puntu haietan abiadura 0 izango da. eta klasikoki partikula x_1 eta x_2 artean baino ezin da mugitu $E \geq V$ den tartean. ⇒ tarte finitu eta mugatua



* x_1 eta x_2 puntuetan $\frac{d^2\psi}{dx^2} = 0$ betetzen da, beraz puntu horietan uhin-funtzioak inflexio puntu bat izango du

* $x < x_1$ edo $x > x_2$ → $(V-E) > 0$; $\begin{cases} \psi > 0 \Rightarrow \frac{d^2\psi}{dx^2} > 0 \text{; ahurra} \\ \psi < 0 \Rightarrow \frac{d^2\psi}{dx^2} < 0 \text{; ganbila} \end{cases}$

* $x_1 < x < x_2$ → $(V-E) < 0$ $\begin{cases} \psi > 0 \to \text{ganbila} \\ \psi < 0 \to \text{ahurra} \end{cases}$



• Bigarren ordenako ekuazio diferentziala denez, Ψ guztiz zehazteko bi hasierako baldintza izan beharko ditugu (ad. Ψ-ren balioa puntu batean eta $\frac{d\Psi}{dx}$-rena)

Demagun ezagutzen dugula Ψ eta $\frac{d\Psi}{dx}$ puntu batean

•, •, • → hiru aukera

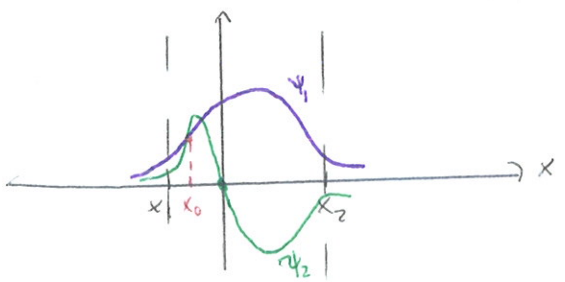
Bat edo bestea izango dugu ε-ren arabera ⇒ baliagarri bakarra berdea da, ε baliogarria duen bakarra (ε-ren balio batzuetarako izango dugu bakarrik fisikoki onargarria den Ψ bat) ⇒ Energiaren kuantizazioa

↳ hori esker Ψ-ren forma grafikoa suposatu

* Hemen ez du zertan 0-tik pasatu behar

• Klasikoki murgaitua daudegun zonaldean oszilazioak egon daitezke eta kanpoan derrigorrez uhin-funtzioa 0-ra joan behar da ⇒ klasikoki debekatuta dagoen zonaldean uhin-funtzioa derrigorrez ez da 0 izan behar, uhin funtzioak badu balio bat, partikula zonalde honetan egon daiteke, baina probabilitatea murrizten da

• Klasikoki baimendutako zonaldeko oszilazioak:



(Azterketa kualitatiboa, Ψ-ren balioak ezin dugu zehaztu horrela)

(Posibilitate bakoitza kolore batez egingo dut)

• oszilaziorik ez. (Ψ_1)
• oszilazio bakarra → beste inflexio puntu bat; (Ψ_2)

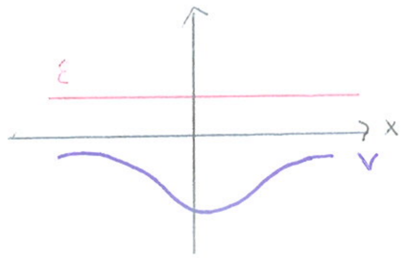
Har dezagun bi uhin-funtzioek balio bera hartzen duten puntu bat, $x_0 \to \Psi_1(x_0)=\Psi_2(x_0)$

$$\left|\frac{d^2\Psi_2}{dx^2}\right|_{x_0} > \left|\frac{d^2\Psi_1}{dx^2}\right|_{x_0} \Rightarrow |(V-\varepsilon_2)\Psi_2|_{x_0} > |(V-\varepsilon_1)\Psi_1|_{x_0} \Rightarrow$$

$|(V-\varepsilon_2)| > |(V-\varepsilon_1)| \to \Psi_2$-ren kasuan energia aldea V eta ε-ren artean handiagoa da → V ε_2-tik urrunago egon behar da ⇒ $E_2 > E_1$

• EGOERA EZ-LOTUAK:

Denboraren independentea den Schrödingeren ekuazioa: $\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V-E)\psi$



• $E > V \quad \forall x \in \mathbb{R}$

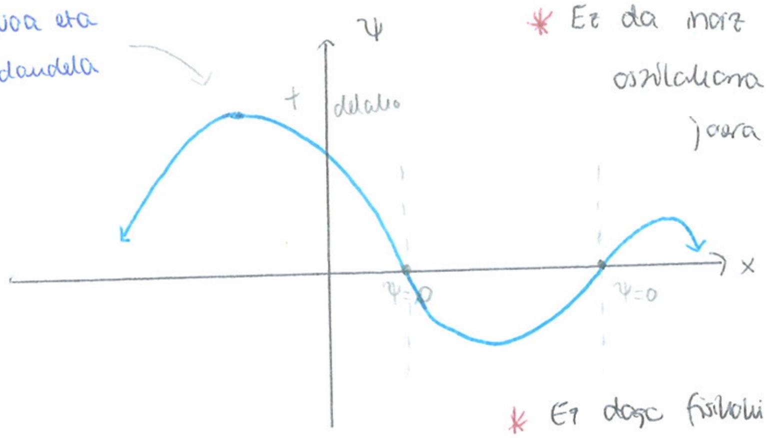
Mekanika klasikoan $T > 0$ da beti eta beraz partikula $-\infty < x < \infty$ tartean mugi daiteke $\Rightarrow$ ez dago tarte baten mugatuta, ez dago ezer boterantz lotuta $\Leftrightarrow$ egoera ez-lotua

• Inflexio puntu balioetan $\psi = 0$ denean, $V \neq E$ delako eta beti dauka $\frac{d^2\psi}{dx^2}$-k ψ-ren aurkako zeinua

$\psi < 0 \rightarrow \frac{d^2\psi}{dx^2} > 0$; ahurra

$\psi > 0 \rightarrow \frac{d^2\psi}{dx^2} < 0$; ganbila

• Demagun hasierako balioa eta deribatuak emanda daudela



* Ez da inoiz infinitura joango → oszilakorra; <0 denean gora joateko joera duelako eta >0 denean behera joateko joera

* Ez dago fisikoki esangura duen ezer den emaitzik $E > V$ denean → E-ren balio jarraituak, edozein balio du $E > V$ den bitartean

• SIMETRIA eta FISIKA:

Sistema baten simetria jakin bat badu ondorio fisikoak izango ditu (klasikoan ere).

Ad: sistemak rotazio simetria duenean, zentrala, momentu angeluarra kontserbatzen da.

Beraz simetria dagoenean zenbait kantitate kontserbatzen dira. Nolakoa da lotura hau (simetria $\Leftrightarrow$ ondorio fisikoak) mekanika kuantikoan?

Simetria izateak esan nahi du gure sistema ez dela aldatzen transformazio baten aurrean. Mekanika kuantikoan transformazio hori eragile baten bidez adierazten dugu

Kasu konkretua: inbertsio transformazioa $\rightarrow$ $x \leftrightarrow -x$ bihurtzea. $\hat{I}\,\psi(x) = \psi(-x)$

$\hat{I}\hat{H}(x) = \hat{H}(-x)$. Demagun gure Hamiltondarra simetrikoa dela:

$$\hat{I}\hat{H}(x) = \hat{H}(-x) = \hat{H}(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

* $\hat{T}$ simetrikoa da beti, beraz $\hat{V}$ simetrikoa bada $\hat{H}$ simetrikoa izango da

* Zer ondorio lortzen ditugu egoeren gainean Hamiltondarra (energia potentziala) simetrikoa denean?

gero $\hat{I}$ uhin-funtzioaren gainean aplikatuko — simetrikoa

- $[\hat{I}, \hat{H}] = \hat{I}\hat{H} - \hat{H}\hat{I} = \hat{I}\hat{H}(x) - \hat{H}(x)\hat{I} = \hat{H}(-x)\hat{I} - \hat{H}(x)\hat{I} = \hat{H}(x)\hat{I} - \hat{H}(x)\hat{I} = 0 \rightarrow$

  Trukakorrak dira $\rightarrow$ $\hat{I}$ eta $\hat{H}$-ren aldi-bereko autofuntzioak aurkitu daitezke

- $\hat{I}\underset{\text{autof}}{\psi(x)} = \underset{\text{autob.}}{\lambda}\psi(x) = \psi(-x)$; $\hat{I}(\hat{I}\psi(x)) = \hat{I}(\lambda\psi(x)) = \hat{I}(\psi(-x)) = \psi(x) = \lambda\psi(-x) =$

  $\lambda \cdot \lambda\psi(x) = \lambda^2\psi(x) \leftrightarrow \lambda^2 = 1$!

  konplexua izan daiteke

  λ baina Hermitikoa bada

  erreala izango da

- $\hat{I}$ hermitikoa? $\underbrace{(\psi, \hat{I}\varphi)}_{1} = \underbrace{(\hat{I}\psi, \varphi)}_{2}$ (suposizioa) $\leftrightarrow \underbrace{\int_{-\infty}^{\infty}\psi^*(x)\,\hat{I}\,\varphi(x)\,dx}_{1} = \underbrace{\int_{-\infty}^{\infty}\psi^*(x)\,\varphi(-x)\,dx}_{1} =$

$$\underbrace{\int_{-\infty}^{\infty}(\hat{I}\psi(x))^*\varphi(x)\,dx}_{2} = \underbrace{\int_{-\infty}^{\infty}\psi^*(-x)\,\varphi(x)\,dx}_{2} \underset{x=-x}{=} \int_{+\infty}^{-\infty}\psi^*(x)\,\varphi(-x)\,(-dx) = \underbrace{\int_{-\infty}^{\infty}\psi^*(x)\,\varphi(-x)\,dx}_{1}$$

Ondorioz $\Longrightarrow (\psi, \hat{I}\varphi) = (\hat{I}\psi, \varphi)$ Hermitikoa da $\leftrightarrow \lambda \in \mathbb{R}$, $\lambda^2 = 1$, $\lambda = \pm 1$

$\hat{I}\psi(x) = \lambda\psi = \pm\psi = \psi(-x)$ $\Rightarrow$ autofuntzioak bakoitiak edo bikoitiak $\Rightarrow$ hamiltondarraren autofuntzioak ere ($\hat{H}$ simetrikoa denean autofuntzioak funtzio bakoitiak edo bikoitiak dira)

* Simetrian, transformazio bakoitzarekin eragile bat lotu eta horren autofuntzioak bilatuko ditugu aztertuko

• DENTSITATE PROBABILITATEAREN KORRONTE-DENTSITATEA:

∗ Jarraikitasunean partikulen kopurua kontserbatu behar da ⇒ jarraipen ekuazioa ⇒ $\underbrace{\frac{\partial n}{\partial t}}^{\text{partikulen dentsitatea}} + \operatorname{div} \underbrace{\vec{j}}_{\text{partikulen korronte dentsitatea}} = 0$

Bolumen diferentzial batean aldatzen diren partikulen kopurua ihes egiten dutenenen berdina izan behar da.

$\vec{j} = n\vec{v}$; $\int n\,dV = \int n\,dx = N$ ↔ $\int \frac{n}{N}\,dx = 1$

↓ abiadura · partikulen dentsitatea; dV ↓ 1D; N: partikula kopuru osoa; $\frac{n}{N} = P(x)$

Probabilitate bat bezela izan daiteke, x puntu batean partikula bat aurkitzeko probabilitatea

∗ Mekanika kuantikoan: $\int P(x,t)\,dx = 1$, $P(x,t) = \Psi^* \Psi$; antzekotasun bat bilatu.

Jarraikitasunean probabilitate dentsitate bat badugu eta hari lotuta korronte dentsitate bat, mekanika kuantikoan defini dezakegu $P(x,t)$-rekin lotuta dagoen korronte dentsitaterik? Horrela bada, jarraitasun ekuazio bat bete beharko litzateke, baina zer ondorioa?

Dimentsio bakar batean egingo dugunez azterketa $\frac{\partial n}{\partial t} + \operatorname{div}\vec{j} \leftrightarrow \frac{\partial n}{\partial t} + \frac{\partial j}{\partial x}$

• $\frac{\partial P}{\partial t} = \frac{\partial(\Psi^*\Psi)}{\partial t} = \frac{\partial \Psi^*}{\partial t}\Psi + \Psi^* \frac{\partial \Psi}{\partial t}$ (1)

↓ $P(x,t) = \Psi^*\Psi$

• Ψ-k Schrödingeren ekuazioa bete beharko du: $-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi(x) = i\hbar \frac{\partial \Psi}{\partial t}$;

$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{Vi}{\hbar}\Psi$ (2) ; $\left(\frac{\partial \Psi}{\partial t}\right)^* = \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*$ (3)

(2) eta (3) (1)-en ordezkatu ⇒ $\frac{\partial P}{\partial t} = -\frac{i\hbar}{2m}\Psi\frac{\partial^2 \Psi^*}{\partial x^2} + \cancel{\frac{i}{\hbar}V\Psi\Psi^*} + \frac{i\hbar}{2m}\Psi^*\frac{\partial^2 \Psi}{\partial x^2} - \cancel{\frac{Vi}{\hbar}\Psi\Psi^*} =$

$\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2 \Psi}{\partial x^2} - \Psi\frac{\partial^2 \Psi^*}{\partial x^2}\right) = \frac{i\hbar}{2m}\left(\frac{\partial}{\partial x}\left[\Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x}\right]\right)$ ⇒ ordenatu ⇒

partikula bakarra $N=1$

$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}\left\{\underbrace{\frac{i\hbar}{2m}\left(\Psi\frac{\partial \Psi^*}{\partial x} - \Psi^*\frac{\partial \Psi}{\partial x}\right)}_{j}\right\} = -\frac{\partial j}{\partial x}$ $\left(\frac{\partial n}{\partial t} + \frac{\partial j}{\partial x} = 0 \text{ forma bera}\right)$

(dimentsio bakar batean ez bada $\vec{\nabla}$ jarri, grad)

KORRONTE-DENTSITATEAREN ADIBIDE BATZUK:

$$* \; j = \frac{i\hbar}{2m}\left\{ \psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right\}$$ Adibide batzuk:

1- $\psi = Ae^{iKx}$; $p = \hbar K$, $v = \frac{p}{m} = \frac{\hbar K}{m}$

↳ uhin laua

$$j = \frac{i\hbar}{2m}\left(Ae^{iKx} \frac{\partial (A^* e^{-iKx})}{\partial x} - A^* e^{-iKx} \frac{\partial (Ae^{iKx})}{\partial x} \right) = \frac{i\hbar}{2m}|A|^2\left(e^{iKx}(-iKe^{-iKx}) - e^{-iKx}(iKe^{iKx}) \right) =$$

$$\frac{i\hbar}{2m}|A|^2(-iK)\left(\underbrace{\cancel{e^{iKx}} \cdot e^{-iKx}}_{=1} + \underbrace{e^{iKx} \cdot e^{-iKx}}_{=1} \right) = \frac{2\hbar K|A|^2}{2m} = |A|^2 \frac{\hbar K}{m} = |A|^2 v = P(x)\, v \Rightarrow$$

↳ dentsitate probabilitatea, $P(x)$

partikulen antzekotasuna: $j = n v$

2- $\psi = Ae^{-\alpha x^2}$ (Gaussiarra) , $A \in \mathbb{R}$ bada $\to \psi \in \mathbb{R}$ $\langle p \rangle = 0 \to j = 0$

↓

normalizazio ktea

($\in \mathbb{R}$ aukera daiteke)

$$j = \frac{i\hbar}{2m}\left(Ae^{-\alpha x^2} \frac{\partial}{\partial x}(Ae^{-\alpha x^2}) - Ae^{-\alpha x^2} \frac{\partial}{\partial x}(Ae^{-\alpha x^2}) \right) = 0$$

Baina, zenbaki irudikari batekin biderkatuz (modulua 1 izanik):

$\psi = Ae^{iK_0 x} e^{-\alpha x^2}$ $\langle p \rangle = K_0$ $\left(= \langle p \rangle_{Ae^{-\alpha x^2}} + K_0 = 0 + K_0 \right)$

1 ikusita 1. gaian

$$j = \frac{i\hbar}{2m}\left(Ae^{iK_0 x - \alpha x^2} \frac{\partial}{\partial x}(A^* e^{-iK_0 x - \alpha x^2}) - A^* e^{-iK_0 x - \alpha x^2} \frac{\partial}{\partial x}(Ae^{iK_0 x - \alpha x^2}) \right) =$$

$$|A|^2 \frac{i\hbar}{2m}\left(e^{iK_0 x - \alpha x^2}\left[-2\alpha x\, e^{-\alpha x^2 - iK_0 x} - iK_0 e^{-\alpha x^2 - iK_0 x}\right] - e^{-iK_0 x - \alpha x^2}\left[-2\alpha x\, e^{-\alpha x^2 + iK_0 x} + iK_0 e^{-\alpha x^2 + iK_0 x}\right] \right) =$$

$$|A|^2 \frac{i\hbar}{2m}\left(\cancel{-2\alpha x\, e^{-2\alpha x^2}} - iK_0 e^{-2\alpha x^2} \cancel{+2\alpha x\, e^{-2\alpha x^2}} - iK_0 e^{-2\alpha x^2} \right) = +|A|^2 \frac{\hbar K_0}{m} e^{-2\alpha x^2} =$$

$$\underbrace{\frac{\hbar K_0}{m}}_{=\langle v \rangle_x} \underbrace{|A|^2 e^{-2\alpha x^2}}_{P(x)}$$ ⇒ berriz lortu partikuletan dugun korrontearen irudia.

edozein neurri dezakegu

↑

↳ honetan ez dugu v, ez dagoelako guztiz zehaztuta, bata-bestelakoa dugu

BEHAGARRIEN ADIERAZPEN MATRIZIALA:

- Behagarriak matrizeen bidez adierazi daitezke.

Demagun A behagarriarekin lotutako $\hat{A}$ eragilearen autofuntzioak eta autobalioak kalkulatu nahi ditugula: $\hat{A}\Psi = \lambda\Psi$.

Izan bedi $\left((\varphi_n, \varphi_m) = \delta_{nm} \text{ izanik} \right)$ $\{\varphi_n\}$ oinarri ortonormala ⇒ edozein uhin-funtzio uhin horretan garatu daiteke, Ψ ere.

$$* \quad \Psi = \sum_j c_j \varphi_j \quad ; \quad \hat{A}\Psi = \hat{A}\left(\sum_j c_j \varphi_j\right) = \lambda\left(\sum_j c_j \varphi_j\right) \rightarrow \hat{A} \text{ lineala denez} \rightarrow$$

$$\sum_j c_j \hat{A}\varphi_j = \sum_j \lambda c_j \varphi_j \longrightarrow \left(\varphi_i, \sum_j c_j \hat{A}\varphi_j\right) = \left(\varphi_i, \lambda \sum_j c_j \varphi_j\right) =$$

$$\sum_j c_j \underbrace{(\varphi_i, \hat{A}\varphi_j)}_{\substack{= \\ A_{ij} \\ \text{(zenbaki bat)}}} = \lambda \sum_j c_j \underbrace{(\varphi_i, \varphi_j)}_{\substack{= \\ \delta_{ij}}} = \lambda c_i \rightarrow$$

↗ dimentsioa printzipioz inf.

$$* \quad \sum_j A_{ij} c_j = \lambda c_i \rightarrow \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ \vdots & & & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_i \\ \vdots \end{pmatrix} = \lambda \begin{pmatrix} c_1 \\ c_2 \\ c_i \\ \vdots \end{pmatrix}$$

- $\hat{A}$-ri dagokion adierazpen matriziala → $\boxed{A \cdot \vec{C} = \lambda \vec{C}}$; $A_{ij} = (\varphi_i, \hat{A}\varphi_j)$

($\hat{A}$-ren autofuntzioak kalkulatzeko
adierazpen matriziala → c_i ezagutzea oinarria garatu: $\Psi = \sum_i c_i \varphi_i$)

$$\text{Ordenatuz} \rightarrow \underbrace{\begin{pmatrix} A_{11}-\lambda & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22}-\lambda & A_{23} & \cdots \\ \vdots & \vdots & A_{33}-\lambda & \ddots \end{pmatrix}}_{A-\lambda I} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \text{sistema homogeneoa} \Rightarrow$$

↘ ezezagunak

↳ identitate matrizea

Emaitza tribiala ez izateko $(c_i = 0 \quad \forall i) \Rightarrow |A - \lambda I| = 0 \rightarrow$ hemendik A-ren autobalioak lortu, eta λ (autobalio) balioetarako c_i batzuk lortuko ditugu → autofuntzioak (autobaliori dagokiona)

- Adierazpen matrizialarekin zenbait kalkulu egin daitezke:

Demagun A matrizea kalkulatu dugula. $\hat{A} = A_{ij}$, $\{\varphi_n\}$ ↗ zein oinarritan garatuta

1. $\Psi \rightarrow \langle \hat{A} \rangle_\Psi = (\Psi, \hat{A}\Psi) = \left(\sum_i c_i \varphi_i , \hat{A} \sum_j c_j \varphi_j \right) = \sum_{i,j} c_j\, c_i^* (\varphi_i, \hat{A}\varphi_j) =$

$\Psi = \sum_j c_j \varphi_j$

$(\varphi_i, \hat{A}\varphi_j) = A_{ij}$

$$\sum_{j,i} c_j c_i^* A_{ij} = (c_1^* \; c_2^* \; c_3^* \ldots) \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ & & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$$

2. $A_{ij} = (\varphi_i, \hat{A}\varphi_j) = (\hat{A}\varphi_i, \varphi_j) = (\varphi_j, \hat{A}\varphi_i)^* = A_{ji}^* \Rightarrow A_{ij} = A_{ji}^*$

A behagarria, hermitikoa; $\hat{A}^+ = \hat{A}^1$

$\Downarrow$ iraganolikoak eIR

$A = (A^t)^*$

Hermitikoa delako

MATRIZEEN eta BEKTOREEN OINARRI-ALDAKETA:

$\hat{A}$-ren autofuntzioak garatzeko oinarri ezberdinak erabiltzen baditugu matrize ezberdinak lortuko ditugu, A_{ij} ezberdinak $\rightarrow$ nola aldatzen dira matrizeak eta bektoreen $(c_1, c_2, \ldots)$ elementuak?

$\hookrightarrow$ Baita bektore (c_j) ezberdinak

oinarri horren konbinazio lineala

* $\{\varphi_i\}$ oinarria, ortonormala $\rightarrow \Psi = \sum_i c_i \varphi_i$

Modu berean, oinarri horretan matrize baten elementuak adieraz daitezke: U

beste oinarri baten gaudela adierazteko

* $\{\varphi_i'\}$ oinarri ortonormala $\rightarrow \Psi' = \sum_i c_i' \varphi_i'$, matrizean elementuak U'

Nola erlazionatzen dira hauek? $U \leftrightarrow U'$?, $\Psi \leftrightarrow \Psi'$?, $\{\varphi_i\} \leftrightarrow \{\varphi_i'\}$

- φ_i' aurreko oinarrian garatu $\Rightarrow \varphi_i' = \sum_j^N a_{ij}\varphi_j \rightarrow T = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{i1} & \cdots & a_{N1} \\ \vdots & \vdots & & a_{i2} & & \vdots \\ \vdots & \vdots & & \vdots & & \vdots \\ a_{1N} & & & a_{iN} & & a_{NN} \end{pmatrix} \Rightarrow$

i=1-ri dagokion a_{ij} osagaiak

Bektoreak:

* $\Psi = T\Psi'$; (bektorea, bektorea) $\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} = T \begin{pmatrix} c_1' \\ c_2' \\ \vdots \\ c_N' \end{pmatrix}$

$\updownarrow$

$\Psi' = T^{-1}\Psi$ $\begin{pmatrix} c_1' \\ c_2' \\ \vdots \\ c_N' \end{pmatrix} = T^{-1} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$

Matrizeak:

* $U' = T^{-1} U T$; $U = T U' T^{-1}$

Adibidea:

2x2-ko espazioa $\rightarrow$ $\{\varphi_1, \varphi_2\}$ oinarria $(\varphi_1, \varphi_2)=0$, $(\varphi_1, \varphi_1)=1$, $(\varphi_2, \varphi_2)=1$ (orton.)

$U = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ aurreko oinarrian $\rightarrow$ oinarri berria $\{\varphi_1', \varphi_2'\}$;

Erlazioa; $\varphi_1' = \frac{1}{\sqrt{2}}(\varphi_1 + i\varphi_2)$, $\varphi_2' = \frac{1}{\sqrt{2}}(\varphi_1 - i\varphi_2)$ $\Rightarrow T = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ i/\sqrt{2} & -i/\sqrt{2} \end{pmatrix} =$

$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$, U' ? (U $\{\varphi_1', \varphi_2'\}$ oinarrian)

$U' = T^{-1} U T$, $T^{-1} = \mathrm{adj}(T)^t \cdot \frac{1}{|T|} \overset{*}{=} \frac{i}{\sqrt{2}}\begin{pmatrix} -i & -i \\ -1 & 1 \end{pmatrix}^t = \frac{i}{\sqrt{2}}\begin{pmatrix} -i & -1 \\ -i & 1 \end{pmatrix} =$

$* \ |T| = \left(\frac{1}{\sqrt{2}}\right)^2(-i-i) = -i$

$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} = T^{t}$ (Matrize unitarioa)

*

* Bi oinarri ortonormalen arteko matrizeak unitarioak dira

$U' = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} U \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} =$

$\frac{1}{2}\begin{pmatrix} 1 & -i \\ -1 & -i \end{pmatrix}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Rightarrow U$ diagonalizatu

$\downarrow$

autobalioak ± 1,

autobektoreak φ_1', φ_2'

MOMENTUEN ADIERAZPIDEA:

- Normalean x espazioan lan egiten dugu; $\Psi(x,t)$, eragileak x espazioan definitu,

  Schrödingeren ekuazioa x espazioan definituta... $\left(i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi\right)$

- Fourier-en transformatuaren bitartez: $\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(k,t)e^{ikx}dk$ $\longrightarrow$ Ψ-k

  Schrödingerren ekuazioa betetzen badu $A(k,t)$-k beste ekuazio bat

  beteko du. Gainera, eragileak k espazioan defini ahal izango ditugu.

  $\hookrightarrow$ k-ren espazioan definituta

k-ren (momentuaren espazioan, $p=\hbar k$) espazioan lan egiten badugu uhin-funtzioa

$A(k,t)$ izango genuke. Honi momentuen adierazpidea deritzo, k-ren espazioan lan egitea.

1. Zein da Schrödingeren ekuazioari dagokion momentuaren adierazpidea?

$$i\hbar\frac{\partial A}{\partial t} \underset{*}{=} i\hbar\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{d\psi}{dt}e^{-ikx}dx \underset{\substack{\downarrow \\ \text{Schrö.} \\ \text{ek.}}}{=} \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}e^{-ikx}+V\psi e^{-ikx}\right)dx =$$

$$\left(* \quad A(k,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi e^{-ikx}dx\right)$$

$$\frac{1}{\sqrt{2\pi}}\left[\underbrace{-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{\partial^2\psi}{\partial x^2}e^{-ikx}dx}_{1}+\underbrace{\int_{-\infty}^{\infty}V\psi e^{-ikx}dx}_{2}\right]$$

1) $$\int_{-\infty}^{\infty}\frac{\partial^2\psi}{\partial x^2}e^{-ikx}dx = \cancel{\left.e^{-ikx}\frac{\partial\psi}{\partial x}\right]_{-\infty}^{\infty}}+ik\int_{-\infty}^{\infty}\frac{\partial\psi}{\partial x}e^{-ikx}dx = ik\int_{-\infty}^{\infty}\frac{\partial\psi}{\partial x}e^{-ikx}dx =$$

$$\begin{cases} u=e^{-ikx}, & du=-ik\,e^{-ikx}dx \\ dv=\frac{\partial^2\psi}{\partial x^2}dx, & v=\frac{\partial\psi}{\partial x}\end{cases} \qquad \begin{cases} u=e^{-ikx}, & du=-ik\,e^{-ikx}dx \\ dv=\frac{\partial\psi}{\partial x}dx & v=\psi\end{cases}$$

0 izan behar da fisikoki esanguratsua izateko (bestela ez da normalizagarria)

$$ik\left(\cancel{\left.\psi e^{-ikx}\right]_{-\infty}^{\infty}}+ik\int_{-\infty}^{\infty}e^{-ikx}\psi\,dx\right)=-k^2\int_{-\infty}^{\infty}e^{-ikx}\psi\,dx \Rightarrow$$

$$*\ -\frac{\hbar^2}{2m}\cdot\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{\partial^2\psi}{\partial x^2}e^{-ikx}dx = +\frac{\hbar^2}{2m}\cdot\frac{k^2}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-ikx}\psi\,dx = \overset{T}{\frac{\hbar^2k^2}{2m}}A(k,t)$$

Suposatu $V=V(x)$ dela

2) $$\int_{-\infty}^{\infty}V\psi e^{-ikx}dx \underset{\substack{\downarrow\\ \text{Fourier}}}{=} \int_{-\infty}^{\infty}V\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k',t)e^{ik'x}dk'\right]e^{-ikx}dx = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}V A(k',t)e^{ix(k'-k)}dk'dx =$$

V-ren Fourieren transf. $V(k-k')$

$$\int_{-\infty}^{\infty}V(k-k')A(k',t)dk'$$

$$\Rightarrow \boxed{i\hbar\frac{\partial A}{\partial t}=\frac{\hbar^2k^2}{2m}A+\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}V(k-k')A(k',t)dk'}$$

dena (k,t)-ren menpe

2. Nola aldatzen dira eragileak momentuaren espazioan?

$\hat{p}=\hbar k$ (x-n $\hat{p}=-i\hbar\frac{\partial}{\partial x}$)

$$\langle\hat{p}\rangle=(A(k,t),\hbar k\,A(k,t))=\int_{-\infty}^{\infty}|A(k,t)|^2\hbar k\,dk$$

$\hat{x}$? $\rightarrow$ $\hat{x} = i\frac{\partial}{\partial k}$, $\langle \hat{x} \rangle = (\psi, x\psi) = \left(A(k,t), i\frac{\partial}{\partial k}A(k,t)\right) = \int_{-\infty}^{\infty} A^* i\frac{\partial A}{\partial k}\, dk =$

$$i\int_{-\infty}^{\infty} A^* \frac{\partial A}{\partial k}\, dk \underset{\downarrow}{=} i\int_{-\infty}^{\infty}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi^* e^{ikx'}dx'\right]\frac{1}{\sqrt{2\pi}}(-ix)\left[\int_{-\infty}^{\infty}\psi e^{-ikx}dx\right]dk =$$

$$A = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi e^{-ikx}dx$$

$$\underbrace{\frac{1}{2\pi}\int_{-\infty}^{\infty}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi^*(x',t)\psi(x,t)\,x\,\underbrace{e^{ik(x'-x)}}\,dx'\,dx\,\underbrace{dk}_{\delta(x'-x)} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi^*(x',t)\psi(x,t)\,x\,\delta(x'-x)dx'dx =$$

$$\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)\,x\,dx = \int_{-\infty}^{\infty} x\,|\psi(x,t)|^2 dx$$

- **POSIZIOAREN AUTOFUNTZIOAK:**

zentrua hartu ballambe x_0 puntuan

* $\hat{x}\psi_{x_0} = x_0\psi_{x_0}$; $x\psi_{x_0} = x_0\psi_{x_0} \rightarrow \psi_{x_0} = \delta(x-x_0)$

* Frogatu k-ren espazioan: $\hat{x} = i\frac{\partial}{\partial k}$ (momentuaren adierazpidean)

$\psi_{x_0} \leftrightarrow A_{x_0}$; $\hat{x}A_{x_0} = x_0 A_{x_0} \rightarrow i\frac{\partial}{\partial k}A_{x_0}(k) = x_0 A_{x_0}(k)$

$e^{rk} = A_{x_0}$ suposatu $\rightarrow$ $ri\cancel{e^{rk}} = x_0\cancel{e^{rk}} \rightarrow r = \frac{x_0}{i} = -ix_0 \Rightarrow A_{x_0} = Be^{-ix_0k}$

$$A_{x_0} \leftrightarrow \psi_{x_0} \rightarrow \psi_{x_0} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A_{x_0}e^{+ikx}dk = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}B\,e^{-ikx_0}e^{ikx}dk =$$

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{C}{\sqrt{2\pi}}e^{ik(x-x_0)}dk = \frac{C}{2\pi}\int_{-\infty}^{\infty}e^{ik(x-x_0)}dk = C\cdot\delta(x-x_0)$$

FISIKA KUANTIKOA:

2. FORMALISMOA:

16-10-10

- $[\hat{A}\hat{B}, \hat{C}\hat{D}]$ garatu trukatzaileen propietateak erabiliz eragile bakoitzeren funtzioan.

$$[\hat{A}\hat{B}, \hat{C}\hat{D}] = \hat{A}[\hat{B}, \hat{C}\hat{D}] + [\hat{A}, \hat{C}\hat{D}]\hat{B} = \hat{A}\left(\hat{C}[\hat{B},\hat{D}] + [\hat{B},\hat{C}]\hat{D}\right) + \left(\hat{C}[\hat{A},\hat{D}] + [\hat{A},\hat{C}]\hat{D}\right)\hat{B} =$$

$$\hat{A}\hat{C}[\hat{B},\hat{D}] + \hat{A}[\hat{B},\hat{C}]\hat{D} + \hat{C}[\hat{A},\hat{D}]\hat{B} + [\hat{A},\hat{C}]\hat{D}\hat{B}$$

batez bestekoa [illegible] $(\psi, [A,B]\psi)$

- $(\Delta A)^2_\psi (\Delta B)^2_\psi \geq -\frac{1}{4}\underbrace{\overline{[A,B]}^2_\psi}_{\text{hau } <0 \text{ izan behar da } *}$ bada frogatu Heisenbergen ziurgabetasuna: $\Delta x \Delta p \geq \hbar/2$

↳ Herendik $(\Delta x)^2(\Delta p)^2 \geq -\frac{1}{4}\overline{[x,p]}^2 = -\frac{1}{4}\overline{(i\hbar)}^2 = -\frac{1}{4}(-\hbar^2) = \frac{\hbar^2}{2^2} \longleftrightarrow$

badakigu $[x,p] = i\hbar$

$$\Delta x \Delta_p \geq \frac{\hbar}{2}$$

[Trukakorrak ez badira, ezinezkoa da biak aldi berean zehaztuta egon ahal izatea.]

* $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \Rightarrow ([\hat{A},\hat{B}])^+ = (\hat{A}\hat{B})^+ - (\hat{B}\hat{A})^+ = \hat{B}^+\hat{A}^+ - \hat{A}^+\hat{B}^+ = \hat{B}\hat{A} - \hat{A}\hat{B} = -[\hat{A},\hat{B}]$

$\hat{B}$ eta $\hat{A}$ hermitikoak dira, $\hat{B} = \hat{B}^+$, $\hat{A} = \hat{A}^+$ Ez da hermitikoa

Orduan bere batez bestekoak ez du zertan erreala izan.

$i[\hat{A},\hat{B}]$ ordea hermitikoa da $\rightarrow (i[\hat{A},\hat{B}])^+ = -i([\hat{A},\hat{B}])^+ = i[\hat{A},\hat{B}]$

Beraz $\overline{i[\hat{A},\hat{B}]} \in \mathbb{R}$ izango da $\rightarrow \overline{i[\hat{A},\hat{B}]} = i\overline{[\hat{A},\hat{B}]} \in \mathbb{R}$ horretarako

$\overline{[\hat{A},\hat{B}]}$ irudikari purua izan behar du $\longleftrightarrow \overline{[\hat{A},\hat{B}]}^2 < 0$

16-10-11

- $[\hat{A},\hat{B}] = 0$ bada, $\hat{A}$ eta $\hat{B}$ bateragarriak dira; aukera daitezke $\hat{A}$ eta $\hat{B}$-ren

autofuntzio berdinak. Baina beti dira berdinak? Gerta daiteke $\hat{A}$ eta $\hat{B}$-ren autofuntzioak berdinak ez izatea?

Ad: $\hat{p}$ eta $\hat{T}$.

- $\hat{p} = -i\hbar \frac{\partial}{\partial x}$ • $\hat{T} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ $\Rightarrow$ $[\hat{p}, \hat{T}] = \hat{p}\hat{T} - \hat{T}\hat{p} = -i\hbar \frac{\partial}{\partial x}\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right) + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(-i\hbar\frac{\partial}{\partial x}\right) =$

$+\frac{i\hbar^3}{2m}\frac{\partial^3}{\partial x^3} - \frac{i\hbar^3}{2m}\frac{\partial^3}{\partial x^3} = 0$ trukakorrak dira $\leftrightarrow$ $\hat{p}$ eta $\hat{T}$ bateragarriak dira.

- $\hat{p}\psi = p\psi = -i\hbar\frac{\partial \psi}{\partial x} = p\psi$ saiatu $\psi = e^{ikx}$; $\frac{\partial \psi}{\partial x} = ike^{ikx}$ $\Rightarrow$ $+\hbar k e^{ikx} = pe^{ikx}$ $\rightarrow$

$p = \hbar k$ $k \in \mathbb{R}$ $\rightarrow$ $\{\psi_k = e^{ikx}\}$ $\hat{p}$-ren autofuntzioak eta $p = \hbar k$ autobalioak.

- $\hat{T}\psi = T\psi = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = T\psi$. , partikula askearen hamiltondarraren autofuntzioak:

$\psi_k' = Ae^{ikx} + Be^{-ikx}$ $k \in \mathbb{R}$ eta $T = \frac{\hbar^2 k^2}{2m}$ $\hat{T}$-ren autobalioak.

↳ endakapena, bi autofuntzio T bera dagozkie.

- Beraz ψ_k' eta ψ_k ez dira berdinak, baina $B=0$ eginez antzera diratekegu berdinak izatea.

$\{\psi_k'\} = \{e^{ikx}, e^{-ikx}\} \neq \{\psi_k\} = \{e^{ikx}\}$ $k \in \mathbb{R}$

Bi eragile trukakorrak badira eta endakapenik ez badago haien autofuntzioak berdinak izan behar dira, baina endakapena bat badugu, endakapena, gerta daiteke autofuntzioak berdinak ez izatea, oinarriak ezberdinak izatea.

- $\hat{T}$ eragileak balioen multzo osoa osatzen du? Nahikoa da T neurtzea egoera orokorki zehaztuta egon dadin?

Ez, endakapena dagoelako. Momentu linealak, $\hat{p}$, ordea multzo osoa osatzen du, endakapenik ez duelako. Orduan $\hat{T}$-k berarekin bateragarria den beste eragile bat beharko luke multzo osoa zehazteko, $\hat{p}$ adibidez.

• $(\Delta\hat{A})_\psi^2 (\Delta\hat{B})_\psi^2 \geq -\frac{1}{4} \overline{[\hat{A},\hat{B}]}_\psi^2$

Izan daiteke $(\Delta\hat{A})_\psi = 0$? Edozein $\hat{A}$-rako, zein izan behar da ψ hori bete dadin?

$$(\Delta\hat{A})_\psi^2 = \overline{\hat{A}^2 - \bar{A}^2} = \overline{A^2} - (\bar{A})^2 = 0 \leftrightarrow \overline{A^2} = (\bar{A})^2 \leftrightarrow (\psi, \hat{A}^2\psi) = [(\psi, \hat{A}\psi)]^2$$

$$\int \psi^* \hat{A}^2 \psi \, dx = \left(\int \psi^* \hat{A} \psi \, dx \right)^2 \Rightarrow$$ Ziurgabetasuna 0 bada, A-ren balioa guztiz zehaztuta dago beraz ψ $\hat{A}$-ren autofuntzio bat izan behar da.

Froga:

* $\bar{A} = \int \psi^{a*} \hat{A} \psi^a \, dx = \int \psi^{a*} \cdot a \psi^a \, dx = a \int |\psi^a|^2 dx = a$

$\psi = \psi^a$; autobalioa $\hat{A}\psi^a = a\psi^a$

$$\overline{A^2} = \int \psi^{a*} \hat{A}^2 \psi^a \, dx = \int \psi^{a*} \hat{A} (\hat{A}\psi^a) \, dx = \int \psi^{a*} \hat{A}(a\psi^a) \, dx = a \int \psi^{a*} \hat{A} \psi^a \, dx =$$

$\hat{A}\psi^a = a\psi^a$

$$a^2 \int \psi^{a*} \psi^a \, dx = a^2 \int |\psi^a|^2 dx = a^2$$

Orduan, $(\Delta\hat{A})_\psi^2 = \overline{A^2} - (\bar{A})^2 = a^2 - a^2 = 0$

* $\hat{A}\psi_n = a_n \psi_n$ (ψ_n $\hat{A}$-ren autofuntzioak eta a_n autobalioak) ; $\hat{A}^2\psi_n = \hat{A}(\hat{A}\psi_n) = \hat{A}(a_n\psi_n) \overset{\text{lineala}}{=} a_n \hat{A}\psi_n = a_n^2 \psi_n \leftrightarrow \psi_n$ $\hat{A}^2$-ren autofuntzioa da eta autobalioak a_n^2

16-10-13

• $\Delta E \, \Delta t$ -k zer erlazio betetzen dute:

* Schrödingeren ekuaziotik

$$(\Delta\hat{A})^2 (\Delta\hat{B})^2 \geq -\frac{1}{4} (\overline{[\hat{A},\hat{B}]})^2$$

$$\hat{A} = \hat{E} = \hat{T} + \hat{V} = \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \overset{*}{=} i\hbar\frac{\partial}{\partial t}$$

$$\hat{B} = \hat{t} = t$$

$$\Rightarrow \left([\hat{A},\hat{B}] = \left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V, t\right] = \left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}, t\right] + \overset{0}{\cancel{[V, t]}} = \cancel{\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} t - t \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}} + 0 = \right.$$

$$\left(\cancel{\frac{\hbar^2}{2m} t \frac{\partial^2}{\partial x^2}} + \cancel{\frac{\hbar^2}{2m}\frac{\partial^2 t}{\partial x^2}} - \cancel{\frac{\hbar^2}{2m} t \frac{\partial^2}{\partial x^2}} = \cancel{\frac{\hbar^2}{2m}\frac{\partial^2 t}{\partial x^2}}\right)$$

$$[\hat{E}, t] = \left[i\hbar\frac{\partial}{\partial t}, t\right] = i\hbar\frac{\partial}{\partial t} t - t i\hbar\frac{\partial}{\partial t} = i\hbar + t i\hbar \cancel{\frac{\partial}{\partial t}} - t i\hbar\frac{\partial}{\partial t} = i\hbar$$

Berez ez dago eragilerik t → ez daukagu haren dentsitate probabilitatearik eta adierazteko, orduan erabili beharrean $\hat{H}$-ren adierazpen klasikoa $(\hat{T}+\hat{V})$ Schrödingeren ekuazioko berdintza bakarrik gara. $i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$

* Beraz ⇒ $(\Delta E)^2(\Delta t)^2 \geq -\frac{1}{4}(\langle i\hbar\rangle)^2 = -\frac{1}{4}(i\hbar)^2 = -\frac{1}{4}(-\hbar^2) = \frac{\hbar^2}{4} \leftrightarrow \boxed{(\Delta E)(\Delta t) \geq \hbar/2}$

px^2

$\parallel$

- SM (Super Momentum) magnitudea (Mekanika klasikoan erabiltzen den asmatutako magnitudea) → $SM = x^2 p$

Zein da magnitude horri dagokion eragilea?

Eragilea hermitikoa izan behar da, magnitude fisiko baten eragilea delako.

Errazago bat lehenengo, $A = xp$ magnitudea, $\hat{A}$?

Badakigu $\hat{A} = \hat{A}^+$ izan behar dela

Demagun $\hat{A} = \frac{x\hat{p} + \hat{p}x}{2} = \frac{1}{2}\left(x(-i\hbar)\frac{\partial}{\partial x} + (-i\hbar)\frac{\partial}{\partial x}x\right) = -\frac{i\hbar}{2}\left(x\frac{\partial}{\partial x} + \frac{\partial}{\partial x}x\right) = -\frac{i\hbar}{2}\left(x\frac{\partial}{\partial x} + 1 + x\frac{\partial}{\partial x}\right) =$

$-\frac{i\hbar}{2}\left(2x\frac{\partial}{\partial x} + 1\right)$

Adierazpen klasikoarekin bat egiteko → $xp = px$ → $\frac{xp + px}{2} = xp$

$\hat{A}^+ = \frac{1}{2}(x\hat{p})^+ + \frac{1}{2}(\hat{p}x)^+ = \frac{1}{2}(\hat{p}^+x^+) + \frac{1}{2}(x\hat{p}) = \frac{1}{2}(\hat{p}x + x\hat{p}) = \hat{A}$ Hermitikoa da.

$x^+ = x,\ \hat{p}^+ = \hat{p}$

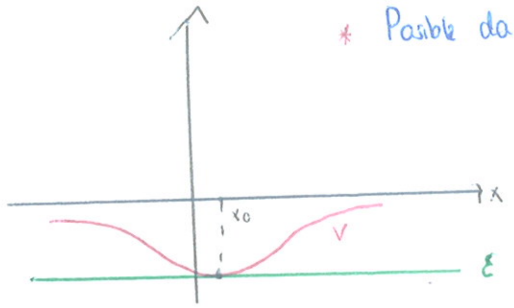
- Hamiltondarraren batazbestekoa beti da konstantea denborarekiko edozein egoeratarako?

Behagarrien denbora-garapenaren ekuazioa: $\frac{d}{dt}\langle\hat{A}\rangle_\psi = \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle_\psi + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle_\psi$

$\hat{A} = \hat{H}$ bada, $[\hat{H},\hat{H}]$ beti da 0, beraz $\frac{d}{dt}\langle\hat{H}\rangle_\psi = \left\langle\frac{\partial\hat{H}}{\partial t}\right\rangle_\psi$ ⇒ Hau 0 izango da, hau da $\langle\hat{H}\rangle_\psi = \text{kte}$ izango da ↔ $\left\langle\frac{\partial\hat{H}}{\partial t}\right\rangle_\psi = 0$ bada $\left(\frac{\partial\hat{H}}{\partial t} = \frac{\partial V}{\partial t}\right)$

Edozein ψ-rako bete dadin orduan $\frac{\partial\hat{H}}{\partial t} = 0$ izan beharko da; hau da, V t-ren independentea izan beharko da. ↔ $\frac{\partial V}{\partial t} = 0$

16-10-17



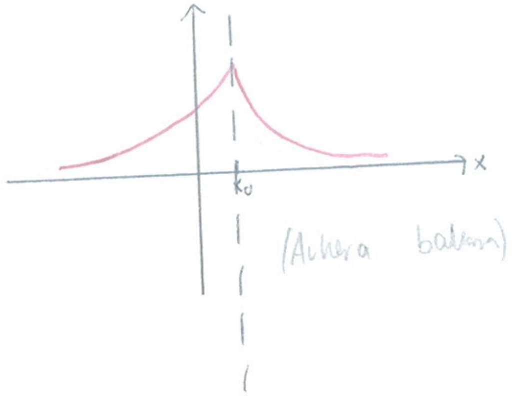
* Posible da egoera loti baten energia V_{min}-en berdina izatea →

$E = V_{min}$? ↔ $V \geq E$

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V-\mathcal{E})\psi \qquad \begin{cases} \psi > 0 \to \frac{d^2\psi}{dx^2} \geq 0 \\ \psi < 0 \to \frac{d^2\psi}{dx^2} \leq 0 \end{cases}$$

ψ-ren zuhu bero edo 0

$E = V_{min} = V(x_0) \to x_0$-n inflexio puntua



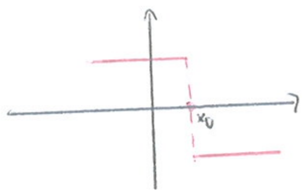
Aukera bakarra → $\psi \geq 0$ izatea $\forall x$ ⇒ Beti ahurra →

baina ez da deribagarria x_0-n ⇒ $\frac{\partial^2\psi}{\partial x^2}$-n

dirac-en delta agertzen da x_0-n → $\underset{\overset{\shortparallel}{K\cdot\delta(x-x_0)}}{\frac{d^2\psi}{dx^2}} \neq \frac{2m}{\hbar^2}(V-\mathcal{E})\psi$

Ezinezkoa

$\frac{\partial\psi}{\partial x}$



* $\psi = \delta(x-x_0)$ bada zein da $\langle T \rangle_\psi$?

$$\langle T \rangle_\psi = \langle \frac{\hat{p}^2}{2m} \rangle_\psi = \frac{1}{2m}\langle \hat{p}^2 \rangle_\psi$$

(ψ ezin da normalizatu)

$$A(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \psi(x) e^{-ikx}\,dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \delta(x-x_0)e^{-ikx}\,dx = \frac{1}{\sqrt{2\pi}}e^{-ikx_0} \to |A(k)|^2 = \frac{1}{2\pi} = \text{kte}$$

$$\langle T \rangle_\psi = \frac{1}{2m}\langle \hat{p}^2 \rangle_\psi = \frac{1}{2m}\int_{-\infty}^{\infty} \hbar^2 k^2 |A(k)|^2\,dk = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} k^2 \cdot \frac{1}{2\pi}\,dk = \frac{\hbar^2}{4\pi m}\left.\frac{k^3}{3}\right]_{-\infty}^{\infty} = \infty$$

⇒ egoera hori energia izatekotan $E = \infty$ izango litzateke ; ez da energia

16-10-18

• Partikula askea $(V=0)$ → $\hat{H}\psi_k = \mathcal{E}_k \psi_k$ → endakatua : $E_k = \frac{\hbar^2 k^2}{2m}$ $k \in \mathbb{R}$ energiari

bi autofuntzio dagozkio , $\psi_k = Ae^{ikx} + Be^{-ikx}$

Konstanteei balioak emanez ⇒

$A=0$ edo $B=0$ eginez e^{ikx} , e^{-ikx}

$A = B = 1/2$ edo $A = \frac{1}{2i} = -B$ $\sin kx$, $\cos kx$

* $e^{ikx} = \psi$ badugu, adibidez, $\hat{p}$-ren autofuntzioa denez p zehaztuta dago, $\hbar k$, beraz $\langle \hat{p} \rangle = \hbar k \neq 0$ izango da $\Rightarrow$ ψ $\hat{H}$-ren autofuntzio bat izateak ez du ziurtatzen $\langle \hat{p} \rangle = 0$ izatea, endekapena badugu ez da bete behar.

* Errealak badira beti betetzen da, eta $\hat{H}$-ren autofuntzioak beti bihur daitezke erreal baina ez dute zertan errealak izan. (ψ_n^* autofuntzio bat denez $\psi' = \frac{\psi + \psi^*}{2}$ hartuz)

Baina Ehrenfest-en erlazioarekin:

$$\frac{d\langle \hat{x} \rangle}{dt} = \frac{\langle \hat{p} \rangle}{m} \quad , \quad \psi = \psi_n \quad , \quad \Psi(x,t) = \psi_n(x)\, e^{-i\frac{E_n}{\hbar}t}$$

n jakin bat

$$\langle \hat{x} \rangle = (\Psi, x\Psi) = \cancel{e^{i\frac{E_n}{\hbar}t} \cdot e^{-i\frac{E_n}{\hbar}t}} (\psi_n, x\psi_n) = (\psi_n, x\psi_n)$$

izan daiteke endekatua eta $A\psi_n + B\psi_m$ eduki baina daukagun gorputza berdina denez emaitza da berdin

$$\frac{d\langle \hat{x} \rangle}{dt} = 0 \leftrightarrow \langle \hat{p} \rangle = 0$$

(Kontraesana, hemen endekapenak ez du zentzurik)

* $\hat{A}$ eta $\hat{B}$ trukakorrak badira baina endekatuak izango al dira bateragarriak?

$[\hat{A}, \hat{B}] = 0$, bateragarriak $\leftrightarrow$ bien aldiberako oinarria izatea

Ez du garantizatzen, beti aurki daitezke aldiberekoak diren oinarriak, beraz beti dira bateragarriak trukakorrak badira.

Endekatuak badira, beti daukagu askatasuna oinarria aukeratzeko.

Baina $\hat{A}$-ren edozein oinarri ez du zertan $\hat{B}$-ren oinarriaren berdina izan, baina aukera dezakegu bat berdinak izan daitezen.

$$\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}.$$

Partikula askean autofuntzio etorallo, $\langle x\rangle$ ez dagoenez ondo definitura (edozein izan daiteke), Ehrenfesten erlazioa ezin da aplikatu. Beraz, kasu honetan kasu singularra dugu.

* $\psi_k = K e^{ikx}$, $P(x) = |K|^2$ $\langle x\rangle = \int_{-\infty}^{\infty} x P(x)\, dx = |K|^2 \int_{-\infty}^{\infty} x\, dx = 0$ da. baina ez da

zgio, jatorria desplazatzen badugu, $x' = x - x_0$ jarriz, $\langle x'\rangle = 0$ da eta, beraz $\langle x\rangle = x_0 \to$

kontraesana

- Magnitude behagarrien eragilea ondoko eran jar daiteke beti? $\hat{A} = \frac{\hat{B} + \hat{B}^+}{2}$
  $(\hat{A})$

Hau da, aurkitu daiteke $\hat{B}$-rik beti non $\hat{A} = \frac{\hat{B} + \hat{B}^+}{2}$ den.

Magnitude behagarri bat denez, frogatu beharko dugu ea hermitikoa den:

$$\hat{A}^+ = \left(\frac{\hat{B} + \hat{B}^+}{2}\right) = \frac{\hat{B}^+}{2} + \left(\frac{\hat{B}^+}{2}\right)^+ = \frac{\hat{B}^+ + \hat{B}}{2} = \hat{A}$$ hermitikoa da $\Rightarrow$ onargarria da?

$\hat{B} = \hat{B}^+$ bada $\hat{B} = \hat{A}$ da.

Ad. $xp = S$ magnitude klasikoa $\to$ $\widehat{(xp)} = \frac{\hat{x}\hat{p} + \hat{p}\hat{x}}{2} = \frac{(\hat{x}\hat{p}) + (\hat{x}\hat{p})^+}{2}$

$\downarrow$ klasikoki $xp = px$, koherentzia mantentzeko.

- $S = xpx$ badugu $\Rightarrow$ Aurreko argudio bera aplikatuz, $\hat{B} = \hat{x}\hat{p}\hat{x}$, $\hat{B}^+ = (\hat{p}\hat{x})^+\hat{x}^+ = \hat{x}\hat{p}\hat{x}$

Orduan, $\widehat{(xpx)} = \frac{\hat{B}^+ + \hat{B}}{2} = \frac{2\hat{x}\hat{p}\hat{x}}{2} = \hat{x}\hat{p}\hat{x}$

Berez, $A = x^2p$-ren berdina izan behar da, $\hat{B} = \hat{x}^2\hat{p}$, $\hat{B}^+ = \hat{p}\,\hat{x}^2$

$$(\hat{A}) = \frac{x^2\hat{p} + \hat{p}x^2}{2}$$ $\Rightarrow$ Ondorioz gauza bera:

$*\ \hat{x}\hat{p}\hat{x} = -i\hbar x \frac{\partial}{\partial x} x = -i\hbar x\left(1 + x\frac{\partial}{\partial x}\right) = -i\hbar x \quad -i\hbar x^2 \frac{\partial}{\partial x}$, $*\ x^2\hat{p} + \hat{p}x^2 = -i\hbar x^2 \frac{\partial}{\partial x} - i\hbar \frac{\partial}{\partial x}(x^2) =$

$-i\hbar x^2 \frac{\partial}{\partial x} - i\hbar \cdot 2x - i\hbar x^2 \frac{\partial}{\partial x} =$

$\cdot 2$

$-2i\hbar x^2 \frac{\partial}{\partial x} - i\hbar 2x$

Printzipioz, onargarria dela dirudi

- Uhin-funtzio baten neurketa egiten ondoren kolapsatu egiten da eta neurketa horren autofuntzio bihurtzen da, $\Psi = \Psi_a$ (a, neurtutako magnitudea). Denbora pasa ahala posible al da beste neurketa batean balio ezberdina lortzea?

  - $\Psi = \Psi_{a_1}$ ($A = a_1$ neurtutako magnitudea) $t=0$-n. $*'$

    ↳ Denboran garatu → Ψ denborarekin aldatu, $P(a_1) = 1$ ez da zertan bete behar → beste balio batzuk lor daitezke

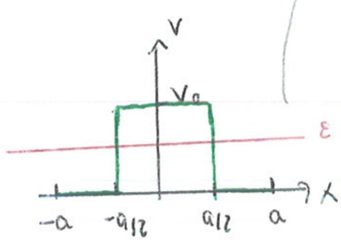
- Ad.: $\Psi = \frac{1}{\sqrt{2}}(\Psi_1 + \Psi_2)$ (Ψ_i $\hat{H}$-ren autofuntzioak → E_1 eta E_2 lortzeko probabilitatea berdina $P = 1/2$)

  Neurtu eta E_1 lortu dugu, Ψ aldatu, $\Psi = \Psi_1$ ⇒ denboraren garapena egin behar da, kasu honetan $\Psi = \Psi_1 e^{-\frac{E_1}{\hbar}t}$; kasu honetan ere, neurketa berriz egingo bagenu E_1 lortuko genuke. Hau Energiarekin pasatzen da bakarrik! Denboraren garapena $\hat{H}$-ren autofuntzioetan egin.

$*'$ $\hat{H}$-ren autofuntzioetan garatu ⇒ $\Psi = \sum c_n \Psi_n$; $c_n = (\Psi_n, \Psi_{a_1})$

Orduan $\Psi(x,t) = \sum c_n \Psi_n e^{-i\frac{E_n}{\hbar}t}$, egoera hau ez da hasierako egoeraren berdina → beste balio batzuk lortzea posiblea da.

16-10-23

- 

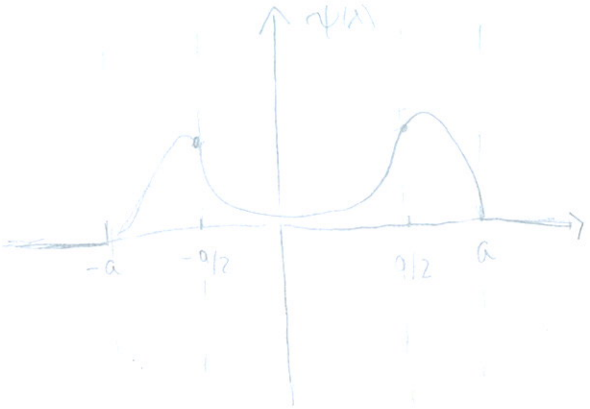
oinarrizko energia

$|x| > a$ → $V = \infty$ ⇔ $\Psi = 0$

$$\frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2}(V-E)\Psi$$

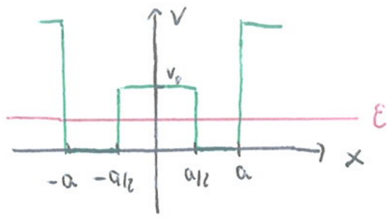
$$\begin{cases} -a/2 < x < a/2 & V-E \geq 0 \rightarrow \frac{d^2\Psi}{dx^2} = K^2\Psi \\ -a < x < -a/2 & V-E \leq 0 \rightarrow \frac{d^2\Psi}{dx^2} = -K^2\Psi \\ a/2 < x < a & V-E \leq 0 \rightarrow \frac{d^2\Psi}{dx^2} = -K^2\Psi \end{cases}$$

$x = \pm a/2$ inflexio puntuak

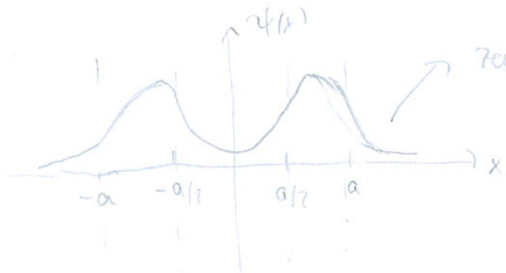


Simetrikoa da.

Bestalde, $|x|>a$ tartean orain potentziala, V, finitoa bada $\psi \neq 0$ izango da. Demagun finitua eta E baino handiagoa dela:

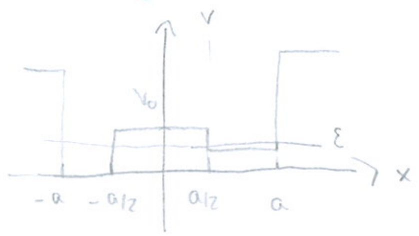


$\Rightarrow$

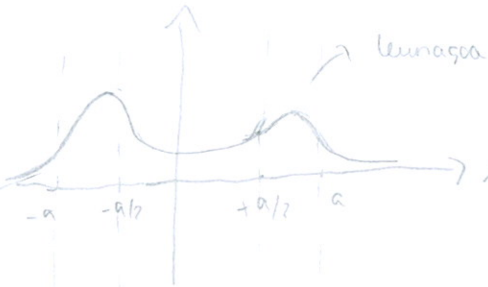


zerora joan, zerbait eta handiagoa izan V $|x|>a$ azkarrago joango da zerori

Putzua antisimetrikoa bada:



$\Rightarrow$

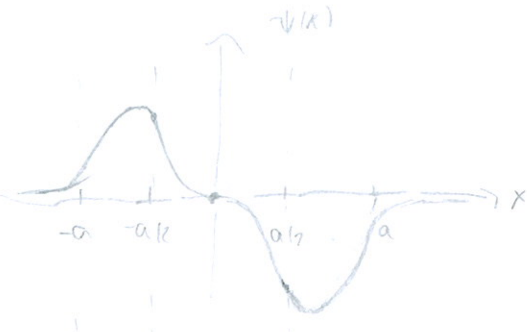


leunagoa V-E tartea txikiagoa delako

Probabilitate handiagoa ezkerrean egoteko

Lehenengo egoera kitzikatua (E handitu da):

$\Rightarrow$



Antisimetrikoa

lotutik eta oszilatuko gutxien izateko

$x=0$ inflexio puntua

Partikula bat daukagu, m masaduna, eta indar konstante bat aplikatzen zaio. Egoera $\Psi(x,t)$ izango da. Frogatu Δp t-ren independentea dela.

$$\langle F\rangle = We = F_0 = \frac{d\langle\hat{p}\rangle}{dt} \rightarrow \langle\hat{p}\rangle = F_0 t + A$$

↗ egoera iraunkorra izan behar da

$$\left[\cancel{\langle\hat{T}\rangle} = \langle\frac{\hat{p}^2}{2m}\rangle = \frac{1}{\cancel{2m}}\cancel{\langle\hat{p}^2\rangle} = -\frac{1}{2}\cancel{\langle xF\rangle} = -\frac{F_0}{\cancel{2}}\langle x\rangle \cancel{\rightarrow} \langle x\rangle = \cancel{-\frac{1}{F_0 m}}\cancel{\langle\hat{p}^2\rangle}\right)$$

$$\frac{d}{dt}\langle\hat{p}^2\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{p}^2]\rangle$$

$$[\hat{H},\hat{p}^2] = [\hat{T}+V,\hat{p}^2] = \cancel{[\hat{T},\hat{p}^2]} + \overset{[-Fx,\hat{p}^2]}{\overset{\parallel}{[V,\hat{p}^2]}} = \hat{p}[V,\hat{p}] + [V,\hat{p}]\hat{p} =$$

$$\hat{p}\left(i\hbar\frac{\partial V}{\partial x}\right) + \left(i\hbar\frac{\partial V}{\partial x}\right)\hat{p} = -2i\hbar\hat{p}F_0 \Rightarrow \frac{d}{dt}\langle\hat{p}^2\rangle = -2i\frac{\cancel{\hbar} i F_0\langle\hat{p}\rangle}{\cancel{\hbar}} = +2F_0\langle\hat{p}\rangle =$$

$$+2F_0^2 t + 2AF_0 \rightarrow \langle\hat{p}^2\rangle = F_0^2t^2 + 2AF_0t + B$$

$$\Delta p^2 = \langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2 = F_0^2t^2 + 2AF_0t + B - (F_0t+A)^2 = \cancel{F_0^2t^2} + \cancel{2AF_0t} + B - \cancel{F_0^2t^2} - A^2 - \cancel{2AF_0t} =$$

$$B - A^2 \rightarrow \Delta p = \sqrt{B-A^2}$$

16-10-25.

- $\{\psi_1, \psi_2\}$ oinarri ortonormala

$A = \begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix}$ → Beste oinarri batean $\{\varphi_1 = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2),\ \varphi_2 = \frac{1}{\sqrt{2}}(\psi_1 - \psi_2)\}$

Zein da A beste oinarrian? A' ? $T = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$ $T^{-1} = T^{t} = T$

ortogonala bada
$T^{-1} = T^{+} = (T^{t})^{*}$

$$A' = T^{-1} A T = TAT = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 1+\varepsilon & 0 \\ 0 & 1+\varepsilon \end{pmatrix}$$

Diagonala denez, horrek esan nahi du bere autofuntzioen oinarrian gaudela → φ_1 eta φ_2. Gainera, autobalioak $1+\varepsilon = \lambda_1$ eta $1-\varepsilon = \lambda_2$ dira.

Bestela → $A' = \begin{pmatrix} A'_{11} & A'_{12} \\ A'_{21} & A'_{22} \end{pmatrix}$ $A'_{11} = (\varphi_1, \hat{A}\varphi_1) = 1+\varepsilon, \ldots$

- A behagarria izanik $\varepsilon \in \mathbb{C}$ izan daiteke?

Ez → A hermitikoa izan behar da behagarria bada eta orduan autobalioak errealak → $\varepsilon^{*} = \varepsilon$

Gainera, adjuntua iraultzen konplexu konjokatua denez lortzen dugu $\varepsilon^{*} = \varepsilon$

Hala ere, matrizeak orokorrean konplexuak izan daitezke.

* Erregela orokorra → $B = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$; $B^{t} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$; $\underset{B^{+}}{\underset{\shortparallel}{B^{t*}}} = B$ → $a = a^{*}$, $c = b^{*}$ ⇒

Diagonaleko elementuak errealak dira eta $a_{ij} = a_{ji}^{*}$ bete behar da.

16-10-26

- Atomo baten momentu angeluarraren modulua konstantea da, baina osagaiak alda daitezke: $|\vec{L}| = \sqrt{2}\hbar$

$\hat{L}_z$ konstante duten $\{\varphi_1, \varphi_0, \varphi_{-1}\}$ oinarrian adierazten badugu $\hat{L}_x$ matrizea:
$$\begin{array}{ccc} \varphi_1 & \varphi_0 & \varphi_{-1} \\ \downarrow & \downarrow & \downarrow \\ \hbar & 0 & -\hbar \end{array}$$

$$\hat{L}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$ eta hamiltondarra: $$\hat{H} = \hbar\omega_0 \begin{pmatrix} 2 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 2 \end{pmatrix}$$

$\Psi(0)$ edozein izanik L_x neurtzen badugu zein da balorik txikiena? Beste aldiune batean atomoaren L_x neurtzen badugu beste balio bat lor dezakegu?

* $\hat{L}_x$-ren autobalioak:
$$|\hat{L}_x - \lambda I| = \begin{vmatrix} 0-\lambda & \hbar/\sqrt{2} & 0 \\ \hbar/\sqrt{2} & -\lambda & \hbar/\sqrt{2} \\ 0 & \hbar/\sqrt{2} & -\lambda \end{vmatrix} = -\lambda^3 + 2\lambda\frac{\hbar^2}{2} = \lambda(2\hbar^2 - \lambda^2) = 0$$

$\lambda_1 = 0$; $\hbar^2 - \lambda^2 = 0 \rightarrow \lambda_2 = -\hbar$, $\lambda_3 = \hbar$

- $\lambda_1 = 0 \rightarrow \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} b \\ a+c \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow b = 0,\ a = -c \rightarrow \phi_1 = \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_{-1})$

- $\lambda_3 = +\hbar \rightarrow \begin{pmatrix} -\hbar & \hbar/\sqrt{2} & 0 \\ \hbar/\sqrt{2} & -\hbar & \hbar/\sqrt{2} \\ 0 & \hbar/\sqrt{2} & -\hbar \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} -\hbar a + b\hbar/\sqrt{2} \\ \frac{\hbar}{\sqrt{2}}a - \hbar b + c\frac{\hbar}{\sqrt{2}} \\ \frac{\hbar}{\sqrt{2}}b - \hbar c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow$
$a = b/\sqrt{2} \rightarrow b = \sqrt{2}a$
$\frac{a}{\sqrt{2}} - b + \frac{c}{\sqrt{2}} = 0$
$\frac{b}{\sqrt{2}} = c \rightarrow a = c$

$$\phi_3 = \frac{1}{2}(\varphi_1 + \sqrt{2}\varphi_0 + \varphi_{-1})$$

- $\lambda_2 = -\hbar \rightarrow \begin{pmatrix} \hbar & \hbar/\sqrt{2} & 0 \\ \hbar/\sqrt{2} & \hbar & \hbar/\sqrt{2} \\ 0 & \hbar/\sqrt{2} & \hbar \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} \hbar a + b\hbar/\sqrt{2} \\ \frac{\hbar a}{\sqrt{2}} + \hbar b + c\frac{\hbar}{\sqrt{2}} \\ \frac{\hbar}{\sqrt{2}}b + \hbar c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow$
$b = -\sqrt{2}a$
$b = -\sqrt{2}c$ $\rightarrow a = c$

$$\phi_2 = \frac{1}{2}(\varphi_1 - \sqrt{2}\varphi_0 + \varphi_{-1})$$ $\Rightarrow$ Kalkulatu daitekeen L_x-ren balorik txikiena $-\hbar$ da. $\rightarrow \Psi(0) = \frac{1}{2}(\varphi_1 - \sqrt{2}\varphi_0 + \varphi_{-1})$

* $\hat{H}$-ren autofuntzioak eta autobalioak: $|\hat{H}-EI|=0$

$$|\hat{H}-EI| = \begin{pmatrix} 2\hbar\omega_0-E & 0 & \hbar\omega_0 \\ 0 & \hbar\omega_0-E & 0 \\ \hbar\omega_0 & 0 & 2\hbar\omega_0-E \end{pmatrix} = (2\hbar\omega_0-E)^2(\hbar\omega_0-E) - \hbar^2\omega_0^2(\hbar\omega_0-E) =$$

$$(\hbar\omega_0-E)\left((2\hbar\omega_0-E)^2-\hbar^2\omega_0^2\right)=0 \rightarrow$$

$$E_1=\hbar\omega_0 \quad ; \quad 4\hbar^2\omega_0^2+E^2-4\hbar\omega_0E-\hbar^2\omega_0^2 = E^2+3\hbar^2\omega_0^2-4\hbar\omega_0E=0 \rightarrow$$

$$E=\frac{4\hbar\omega_0 \pm \sqrt{16\hbar^2\omega_0^2-12\hbar^2\omega_0^2}}{2} = \frac{4\hbar\omega_0 \pm 2\hbar\omega_0}{2} = 2\hbar\omega_0 \pm \hbar\omega_0 = \begin{cases} 3\hbar\omega_0 \\ \hbar\omega_0 \ \text{(bikoitza)} \end{cases}$$

- $E_1=\hbar\omega_0 \rightarrow \begin{pmatrix} \hbar\omega_0 & 0 & \hbar\omega_0 \\ 0 & 0 & 0 \\ \hbar\omega_0 & 0 & \hbar\omega_0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \hbar\omega_0\begin{pmatrix} a+c \\ 0 \\ a+c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow a=-c \rightarrow$

$$\phi_1'=\varphi_0 \qquad \phi_2'=\frac{1}{\sqrt{2}}(\varphi_1-\varphi_{-1}) \qquad \text{(endekapena)}$$

- $E_2=3\hbar\omega_0 \rightarrow \begin{pmatrix} -\hbar\omega_0 & 0 & \hbar\omega_0 \\ 0 & -2\hbar\omega_0 & 0 \\ \hbar\omega_0 & 0 & -\hbar\omega_0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \hbar\omega_0\begin{pmatrix} -1 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \hbar\omega_0\begin{pmatrix} -a+c \\ -2b \\ a-c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$

$$a=c \ ; \ b=0 \rightarrow \qquad \phi_3'=\frac{1}{\sqrt{2}}(\varphi_1+\varphi_{-1})$$

* $\Psi(0)=\frac{1}{2}(\varphi_1-\sqrt{2}\varphi_0+\varphi_{-1})=\phi_2$ garatu $\hat{H}$-ren autofuntzioetan

$$\Psi(0)=-\frac{\sqrt{2}}{2}\varphi_0+\frac{1}{2}(\varphi_1+\varphi_{-1}) = -\frac{1}{\sqrt{2}}\phi_1'+\frac{\sqrt{2}}{2}\phi_3' \Rightarrow \Psi(x,t)=-\frac{1}{\sqrt{2}}\phi_1'e^{\frac{-iE_1t}{\hbar}}+\frac{1}{\sqrt{2}}\phi_3'e^{\frac{-iE_2t}{\hbar}}=$$

$$-\frac{1}{\sqrt{2}}\phi_1'e^{-i\omega_0t}+\frac{1}{\sqrt{2}}\phi_3'e^{-3\omega_0it} = \frac{1}{\sqrt{2}}\left(-\varphi_0e^{-i\omega_0t}+\frac{1}{\sqrt{2}}(\varphi_1+\varphi_{-1})e^{-3\omega_0it}\right) = a\phi_1+b\phi_2+$$

$$c\phi_3$$

* $b=\left(\phi_2, \Psi(x,t)\right) = \left(\frac{1}{2}\varphi_1-\frac{1}{\sqrt{2}}\varphi_0+\frac{1}{2}\varphi_{-1}, \frac{-1}{\sqrt{2}}\varphi_0e^{-i\omega_0t}+\frac{1}{2}\varphi_1e^{-3\omega_0it}+\frac{\varphi_{-1}}{2}e^{-3\omega_0it}\right)=$

$$\frac{1}{4}e^{-3\omega_0it}+\frac{1}{2}e^{-i\omega_0t}+\frac{1}{4}e^{-3\omega_0it} = \frac{1}{2}e^{-3i\omega_0t}+\frac{1}{2}e^{-i\omega_0t}$$

$$P(-\hbar)(t) = |b|^2 = b^* b = \left(\frac{1}{2}e^{3i\omega_0 t} + \frac{1}{2}e^{i\omega_0 t}\right)\left(\frac{1}{2}e^{-3i\omega_0 t} + \frac{1}{2}e^{-i\omega_0 t}\right) = \frac{1}{4} + \frac{1}{4}e^{2i\omega_0 t} +$$

$$\frac{1}{4}e^{-2i\omega_0 t} + \frac{1}{4} = \frac{1}{2} + \frac{1}{4}\left(e^{2i\omega_0 t} + e^{-2i\omega_0 t}\right) = \frac{1}{2} + \frac{1}{2}\cos(2\omega_0 t) = \cos^2 \omega_0 t$$

$$P(-\hbar)(t) = 1 \rightarrow \frac{1}{2} + \frac{1}{2}\cos(2\omega_0 t) = 1 \rightarrow \cos(2\omega_0 t) = 1 \rightarrow 2\omega_0 t = 2n\pi \rightarrow t = \frac{n\pi}{\omega_0} \quad n \in \mathbb{N}$$

16-11-2

$$\Psi(x,0) = \int_{-\infty}^{\infty} e^{-\alpha k^2} e^{ikx}\, dk = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \sqrt{2\pi}\, e^{-\alpha k^2} e^{ikx}\, dk$$

- $A(k) = \sqrt{2\pi}\, e^{-\alpha k^2}$ $*^1$ $\quad \langle x \rangle = \left(A(k), i\frac{\partial A(k)}{\partial k}\right) = \left(A(k), -2k\alpha i \sqrt{2\pi}\, e^{-\alpha k^2}\right) =$

$$\left(\sqrt{2\pi}\, e^{-\alpha k^2}, -2\sqrt{2\pi}\, k\alpha i\, e^{-\alpha k^2}\right) = -2 \cdot 2\pi\, \alpha i \left(e^{-\alpha k^2}, k e^{-\alpha k^2}\right) = -4\pi\, \alpha i \int_{-\infty}^{\infty} k e^{-2\alpha k^2}\, dk =$$

$$\frac{\cancel{-4}\pi \alpha i}{\cancel{4}\alpha}\, e^{-2\alpha k^2}\Big|_{-\infty}^{\infty} = 0$$

↳ baliotia, gainera erreala denez A(k), nulua [illegible] da

- $\langle x^2 \rangle = \left(A(k), -\frac{\partial^2 A(k)}{\partial k^2}\right) = \left(\left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha k^2}, -\left(\frac{2\alpha}{\pi}\right)^{1/4}\frac{\partial^2}{\partial k^2}\left(e^{-\alpha k^2}\right)\right) = -\sqrt{\frac{2\alpha}{\pi}}\left(e^{-\alpha k^2}, \frac{\partial^2}{\partial k^2}\left(e^{-\alpha k^2}\right)\right) =$

↳ normalizatua.

$$-\sqrt{\frac{2\alpha}{\pi}}\left(e^{-\alpha k^2}, \frac{\partial}{\partial k}\left(-2\alpha k e^{-\alpha k^2}\right)\right) = -\sqrt{\frac{2\alpha}{\pi}}\left(e^{-\alpha k^2}, (-2\alpha k)^2 e^{-\alpha k^2} - 2\alpha e^{-\alpha k^2}\right) \overset{*^2}{=}$$

$*^1$ Normalizatu $\rightarrow \quad \int_{-\infty}^{\infty} |A(k)|^2\, dk = 2\pi \int_{-\infty}^{\infty} e^{-2\alpha k^2}\, dk = 2\pi\sqrt{\frac{\pi}{2\alpha}} \rightarrow A(k) = \frac{(2\alpha)^{1/4}\cancel{\sqrt{2\pi}}}{(\pi)^{1/4}\cancel{\sqrt{2\pi}}}\, e^{-\alpha k^2} =$

$$\left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha k^2}$$

$$*^2 = -\sqrt{\frac{2\alpha}{\pi}}\left(e^{-\alpha k^2}, 4\alpha^2 k^2 e^{-\alpha k^2} - 2\alpha e^{-\alpha k^2}\right) = -\sqrt{\frac{2\alpha}{\pi}}\left(e^{-\alpha k^2}, 4\alpha^2 k^2 e^{-\alpha k^2}\right) + 2\alpha\sqrt{\frac{2\alpha}{\pi}}$$

$$\left(e^{-\alpha k^2}, e^{-\alpha k^2}\right) = -\sqrt{\frac{2\alpha}{\pi}}\left(e^{-\alpha k^2}, 4\alpha^2 k^2 e^{-\alpha k^2}\right) + 2\alpha\cancel{\sqrt{\frac{2\alpha}{\pi}}} \cdot \cancel{\sqrt{\frac{\pi}{2\alpha}}} =$$

$$-\sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} 4\alpha^2 K^2 e^{-2\alpha K^2} dK + 2\alpha = -4\alpha^2 \sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} K^2 e^{-2\alpha K^2} dK + 2\alpha =$$

$$-\cancel{4}\alpha^{\cancel{2}} \sqrt{\frac{\cancel{2\alpha}}{\cancel{\pi}}} \cdot \frac{\sqrt{\frac{\cancel{\pi}}{\cancel{2}}}}{\cancel{4\alpha\sqrt{\alpha}}} + 2\alpha = +\alpha \implies \Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\langle x^2\rangle} = \sqrt{\alpha}$$

neurketaren ezin gabe, aldaketaren ezin gabe

- Uhin-funtzioa behin normalizatuta betirako normalizatzen da?

$$\Psi(x,t) = \sum_n c_n \Psi_n(x,t) \implies \Psi(x,0) = \sum_n c_n \Psi_n(x,0)$$

Hamiltondarraren autofuntzioen garatuta

Normalizatu $\implies \int_{-\infty}^{\infty} \Psi(x,0) \cdot \Psi^*(x,0)\, dx = 1 = \int_{-\infty}^{\infty} \sum_n c_n \Psi_n(x,0) \sum_m c_m^* \Psi_m^*(x,0)\, dx =$

$$\int_{-\infty}^{\infty} \sum_{n,m} c_n c_m^* \Psi_n(x,0) \Psi_m^*(x,0)\, dx = 1 = \sum_{n,m} c_n c_m^* \int_{-\infty}^{\infty} \Psi_n(x,0)\Psi_m^*(x,0)\, dx = \sum_{n,m} c_n c_m^* \delta_{nm} = \sum_n |c_n|^2 \quad *'$$

$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)\, dx \rightarrow$ hau t-rekiko aldatzen den ikusteko $\implies \frac{\partial}{\partial t} \int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)\, dx =$

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial t} \left(\Psi^*(x,t)\Psi(x,t) \right) dx = 0$$

$$\Psi(x,t) = \sum_n c_n \Psi_n e^{-i\frac{E_n t}{\hbar}}$$

$$*' \quad \int_{-\infty}^{\infty} \Psi(x,t)\Psi^*(x,t)\, dx = \int_{-\infty}^{\infty} \sum_n c_n \Psi_n(x,t) \sum_m c_m^* \Psi_m(x,t)\, dx =$$

$$\int_{-\infty}^{\infty} \sum_{n,m} c_n c_m^* \Psi_n(x,t)\Psi_m^*(x,t)\, dx = \sum_{n,m} c_n c_m^* \int_{-\infty}^{\infty} \Psi_n(x,t)\Psi_m^*(x,t)\, dx \overset{\text{ortonormala}}{=}$$

$$\sum_{n,m} c_n c_m^* \delta_{nm} = \sum_n |c_n|^2 = 1$$

16-11-03

- Potentzial oso infinituan energia neurtuz: gero E_1 eta E_2 energia neurtzeko probabilitate bera dugu. Uhin funtzioa erreala da eta potentzial oso infinituan ezkerreen egon daiteke probabilitate handiagoarekin:

- Hamiltondarraren autofuntzioak: $\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$ $\quad E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$ $\quad n \in \mathbb{N}$

$$P(E_1) + P(E_2) = 1 \underset{\substack{\downarrow \\ P(E_1)+P(E_2)}}{=} 2P(E_1) \rightarrow P(E_1) = 1/2 = |c_1|^2 \rightarrow c_1 = \pm\sqrt{1/2} \rightarrow \text{uhin-funtzioa erreala delako}$$

$$c_2 = \pm\sqrt{1/2}$$

↳ bestela $c_1 = \frac{1}{\sqrt{2}} e^{i\alpha}$, $c_2 = \frac{1}{\sqrt{2}} e^{i\beta}$

- $\Psi(x) = c_1 \psi_1 + c_2 \psi_2$

* fase batura esanguragabea! $\psi \cdot e^{-i\alpha}$-gatik biderkatu! (edo $e^{-i\beta}$)

↳ uhina balioduna!

$$P(x \geq a/2) > P(x \leq a/2)$$

erreala

$$* \; P(x \geq a/2) = \int_{a/2}^{a} (c_1\psi_1 + c_2\psi_2)(c_1\psi_1 + c_2\psi_2)^* \, dx = \int_{a/2}^{a} (c_1\psi_1 + c_2\psi_2)^2 \, dx =$$

$$\int_{a/2}^{a} (c_1^2\psi_1^2 + c_2^2\psi_2^2 + 2c_1c_2\psi_2\psi_1)\, dx = \int_{a/2}^{a} c_1^2\psi_1^2\, dx + \int_{a/2}^{a} c_2^2\psi_2^2\, dx +$$

$$2c_1c_2 \int_{a/2}^{a} \psi_2\psi_1\, dx = \frac{1}{2}\int_{a/2}^{a} \psi_1^2\, dx + \frac{1}{2}\int_{a/2}^{a} \psi_2^2\, dx + 2c_1c_2 \int_{a/2}^{a} \psi_2\psi_1\, dx =$$

$$\frac{1}{\cancel{2}} \cdot \frac{\cancel{2}}{a} \int_{a/2}^{a} \sin^2\left(\frac{\pi}{a}x\right) dx + \frac{1}{\cancel{2}} \frac{\cancel{2}}{a} \int_{a/2}^{a} \sin^2\left(\frac{2\pi}{a}x\right) dx + 2c_1c_2 \int_{a/2}^{a} \frac{2}{a} \sin\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi x}{a}\right) dx =$$

$$\frac{1}{2a} \int_{a/2}^{a} \left(1 - \cos\left(\frac{2\pi}{a}x\right)\right) dx + \frac{1}{2a} \int_{a/2}^{a} \left(1 - \cos\left(\frac{4\pi}{a}x\right)\right) dx + \frac{4}{a}c_1c_2 \int_{a/2}^{a} \sin\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}x\right) dx =$$

$$\frac{1}{2a}\left(x - \frac{a}{2\pi}\sin\left(\frac{2\pi}{a}x\right)\right]_{a/2}^{a} + \frac{1}{2a}\left(x - \frac{a}{4\pi}\sin\left(\frac{4\pi}{a}x\right)\right)\Bigg]_{a/2}^{a} + \frac{4}{a}c_1c_2 \int_{a/2}^{a} \left[\frac{1}{2}\cos\left(+\frac{\pi}{a}x\right) - \frac{1}{2}\cos\left(\frac{3\pi}{a}x\right)\right] dx =$$

$$\frac{1}{2a}\left(a - \frac{a}{2}\right) + \frac{1}{2a}\left(a - \frac{a}{2}\right) + \frac{2}{a}c_1c_2\left[\frac{a}{\pi}\sin\left(\frac{\pi}{a}x\right)\Big]_{a/2}^{a} - \frac{a}{3\pi}\sin\left(\frac{3\pi}{a}x\right)\Big]_{a/2}^{a}\right] = \frac{1}{2} + \frac{2}{a}c_1c_2\left(\frac{-a}{\pi} - \frac{a}{3\pi}\right) =$$

$$\frac{1}{2} + 2c_1c_2\left(\frac{-4}{3\pi}\right) = \frac{1}{2} - \frac{8}{3\pi}c_1c_2$$

* $\frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\psi_2$ eta $\frac{1}{\sqrt{2}}\psi_1 + \frac{i}{\sqrt{2}}\psi_2$ ez dira baliokideak → $\langle x \rangle$ ezberdina!

* $P(x \le a/2) = \int_0^{a/2} (c_1\psi_1 + c_2\psi_2)(c_1\psi_1 + c_2\psi_2)^* \, dx = \int_0^{a/2} c_1^2 \psi_1^2 \, dx + \int_0^{a/2} c_2^2 \psi_2^2 \, dx +$

$\int_0^{a/2} 2c_1c_2 \psi_2 \psi_1 \, dx = \int_0^{a/2} \frac{1}{\cancel{2}} \sin^2\left(\frac{\pi}{a}x\right) dx \cdot \frac{\cancel{2}}{a} + \int_0^{a/2} \frac{1}{\cancel{2}} \sin^2\left(\frac{2\pi}{a}x\right) \frac{\cancel{2}}{a} + 2c_1c_2 \int_0^{a/2} \psi_2 \psi_1 \, dx =$

$\frac{1}{2a} \int_0^{a/2} \left(1 - \cos\left(\frac{2\pi}{a}x\right)\right) dx + \frac{1}{2a} \int_0^{a/2} \left(1 - \cos\left(\frac{4\pi}{a}x\right)\right) dx + \frac{4}{a} c_1 c_2 \int_0^{a/2} \sin\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}x\right) dx =$

$\frac{1}{2a} \left[x - \frac{a}{2\pi} \sin\left(\frac{2\pi}{a}x\right)\right]_0^{a/2} + \frac{1}{2a} \left[x - \frac{a}{4\pi} \sin\left(\frac{4\pi}{a}x\right)\right]_0^{a/2} + \frac{4}{a} \frac{c_1 c_2}{2} \int_0^{a/2} \left[\cos\left(\frac{\pi}{a}x\right) - \cos\left(\frac{3\pi}{a}x\right)\right] dx =$

$\frac{1}{2\cancel{a}} \cdot \frac{\cancel{a}}{2} + \frac{1}{2\cancel{a}} \cdot \frac{\cancel{a}}{2} + \frac{2}{a} c_1 c_2 \left[\frac{a}{\pi} \sin\left(\frac{\pi}{a}x\right) - \frac{a}{3\pi} \sin\left(\frac{3\pi}{a}x\right)\right]_0^{a/2} = \frac{1}{2} + \frac{2}{\cancel{a}} c_1 c_2 \left(\frac{\cancel{a}}{\pi} + \frac{\cancel{a}}{3\pi}\right) =$

$\frac{1}{2} + 2c_1c_2 \left(\frac{3+1}{3\pi}\right) = \frac{1}{2} + \frac{8c_1c_2}{3\pi}$

$\Rightarrow P(x \le a/2) < P(x \ge a/2) \Rightarrow \cancel{\frac{1}{2}} + \frac{8c_1c_2}{3\pi} < \cancel{\frac{1}{2}} - \frac{8c_1c_2}{3\pi} \rightarrow 2c_1c_2 < 0 \rightarrow$

$c_1 c_2 < 0 \Rightarrow c_1 = \frac{1}{\sqrt{2}}$ eta $c_2 = -\frac{1}{\sqrt{2}}$ edo $c_1 = -\frac{1}{\sqrt{2}}$ eta $c_2 = \frac{1}{\sqrt{2}}$

* $\Psi(x) = \frac{1}{\sqrt{2}} (\psi_1 - \psi_2)$ edo $\Psi(x) = \frac{1}{\sqrt{2}} (\psi_2 - \psi_1)$ $\Rightarrow$ baliokideak

FISIKA KUANTIKOA

DIMENTSIO BAKARREKO POTENTZIALAK:

16-11-08

∘ Hamiltondarra endekatuta ez badago zein da autofuntzioen $\vec{j}$?

Hamiltondarra endekatua ez bada beti aukeratu daitezke autofuntzio errealak,

beraz haien $\vec{j}=0$ izan beharko da ⇒ probabilitatea berdina izango da eskumara

edo ezkerrera joateko.

Gainera, momentuaren batezbestekoa 0 izango da eta p eta $-p$ lortzeko

probabilitatea berdina. $\left(|A(k)|^2 = |A(-k)|^2\right)$

16-11-09.

∘ $\psi \in \mathbb{R}$ $\quad A(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x)\,e^{-ikx}\,dx \quad ; \quad A^*(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x)\,e^{ikx}\,dx = A(-k)$

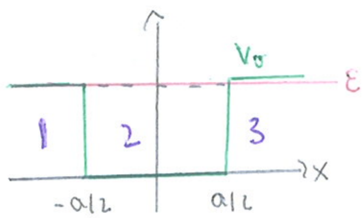
$A(-k)$ eta $A(k)$ $-k$ ez dute zertan berdinak izan.

$$P(k)=A(k)\cdot A^*(k) \quad ; \quad P(-k)=A(-k)\cdot A^*(-k) = A^*(k)\cdot\left(A(-k)\right)^* = A^*(k)\left(A^*(k)\right)^* = A^*(k)A(k)$$

$$\hookrightarrow \quad P(k)=P(-k)$$

Beraz, esan bezala, egoera geldikorretan adibidez, autofuntzio errealak aukera daitezke

(hamiltondarra endekatua ez bada) eta horregatik $P(k)=P(-k)$ denez $\langle p\rangle=0$ da.

∘ 

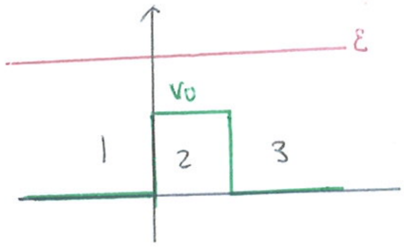
Izan ditzakegu $x\in(-a/2, a/2)$ tartean potentzial osin infinituan autofuntzioak (2. tartean), $E=V_0$ izanik?

$\psi_1 = A$ $\quad (k_1=0$ delako$)$

$\psi_2 = C\sin kx + D\cos kx \qquad k=\frac{\sqrt{2mV_0}}{\hbar}$

$\psi_3 = B$

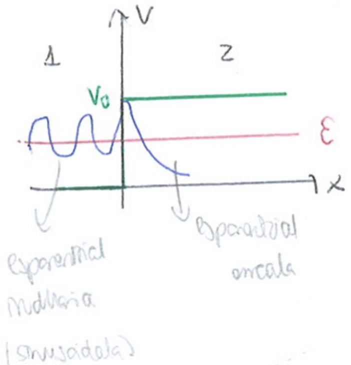
Ktea bada ez da normalizagarria baina ez du inporta, e^{ikx} ere ez delako normalizagarria.



Partikula ezkerretik eskuinera doanean 3. eremuan geratzen den uhin eluzioa $E e^{ik x} = \psi_3$ da, ezkerrerantza doan ekarpena kentzen dugulako. Baina zer gertatzen da 2. zonaldean?

2. zonaldea: $\psi_2 = Ce^{-ik_2 x} + De^{ik_2 x}$ $\quad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

2. eta 3. zonaldeen arteko mugan islatu egin daiteke eta beraz ezkerrerantzazko ekarpena ezin da anulatu, badago islatzeko probabilitatea, horregatik $C \neq 0 \Rightarrow$ bi fluxuak mantendu behar dira.



$T=0$ da, baina partikula 2. zonaldean egon daiteke?

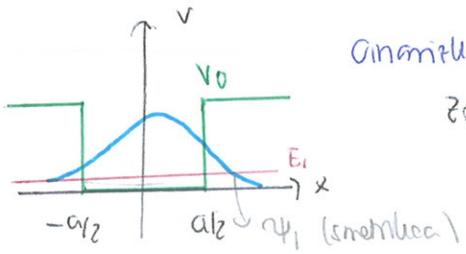
2. zonaldean $\Rightarrow$ $\psi_2 = e^{-kx}$ $\quad k = \frac{\sqrt{2m(V_0-E)}}{\hbar}$ (errezla $\Rightarrow j=0$)

$|\psi_2|^2 = P(x) = e^{-2kx} \neq 0$ $\Rightarrow$ beraz partikula egoteko probabilitatea badago, txikua bada ere.

R eta T energiaren independenteak dira. Kasu honetan $R=1$, $T=0$

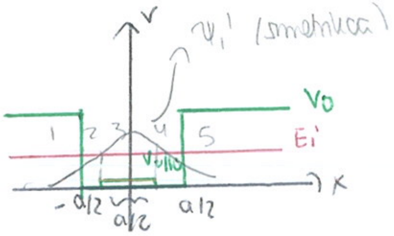
$R=1$ denez $|A|^2 = |B|^2$, beraz 1. zonaldean $j = \frac{\hbar k}{m}[|A|^2 - |B|^2] = 0$

↳ $\psi_1 = Ae^{ikx} + Be^{-ikx}$



Oinarrizko energia $\rightarrow E_1 = V_0/4$ (Egoera lotuak ditugu)

Zer gertatuko da $(-a/4, a/4)$ tartean eskaloi bat gehitzen badugu, $V_0/10$ altueradoa. Bere oinarrizko energia E_1', E_1 baino handiagoa ala txikiagoa izango da?



Konkabitatea txikiagoa izango da $x \in (-a/4, a/4)$ tartean

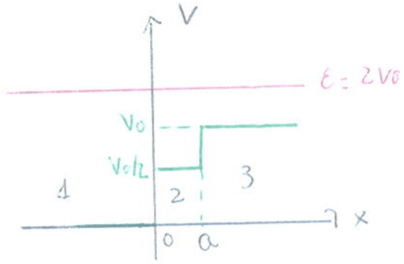
Eskalai bat gehitzean, potentziala handitzen denez tarte batean energia handituko da. (Konkabitateagatik ezin da ezer esateko, perturbazioen teoria behar da...)

↳ Mugalde baldintzekin kalkula daiteke baina oso da zeharra $\Rightarrow$ 5 zonalde $\Rightarrow$ baina egin daiteke

$$\psi = \begin{cases} \psi_1 = Ae^{k_1 x} & k_1 = \frac{\sqrt{2m(V_0-E)}}{\hbar}, \quad \psi_2 = Be^{ik_2 x} + Ce^{-ik_2 x} \quad k_2 = \frac{\sqrt{2mE_0'}}{\hbar} \\ \psi_3 = De^{ik_3 x} + Ee^{-ik_3 x} & k_3 = \frac{\sqrt{2m(E_1'-V_0)}}{\hbar}, \quad \psi_4 = Ge^{ik_2 x} + He^{-ik_2 x} \\ \psi_5 = Ie^{-k_1 x} & \end{cases}$$

simetrikoa

Simetria ; $[I = A,\ B = H,\ C = G,\ D = E]$ + Jarraitasuna



* 3 zonalde:

$$\psi_1 = A e^{ik_1 x} + B e^{-ik_1 x} \qquad k_1 = \frac{\sqrt{2m\,2V_0}}{\hbar} = \frac{\sqrt{4mV_0}}{\hbar}$$

$$\psi_2 = C e^{ik_2 x} + D e^{-ik_2 x} \qquad k_2 = \frac{\sqrt{2m(2V_0 - V_0/2)}}{\hbar} = \frac{\sqrt{3mV_0}}{\hbar}$$

$$\psi_3 = E e^{ik_3 x} \qquad k_3 = \frac{\sqrt{2mV_0}}{\hbar}$$

* Mugalde baldintzak:

- $x = 0 \rightarrow A + B = C + D$

  $k_1(A - B) = k_2(C - D)$

- $x = a \rightarrow C e^{ik_2 a} + D e^{-ik_2 a} = E e^{ik_3 a}$

  $k_2\left(C e^{ik_2 a} - D e^{-ik_2 a}\right) = k_3 E e^{ik_3 a}$

$$\Rightarrow C = \frac{1}{2}\left(1 + \frac{k_3}{k_2}\right) e^{i(k_3 - k_2)a} E \quad ; \quad D = \frac{1}{2}\left(1 - \frac{k_3}{k_2}\right) e^{i(k_3 - k_2)} E$$

↗ hauekin askatu A, B E-ren mepe

*

$$T = \frac{\frac{\hbar k_3}{m}|E|^2}{\frac{\hbar k_1}{m}|A|^2}$$

* hemen sartu.

- Potentzial osin infinitua $\Rightarrow$ bi egoera bakarrik $\psi_1, \psi_2 \Rightarrow P(E_1) = P(E_2) = 1/2$.

$\langle x \rangle (t=0) = 0$ $\qquad \psi(t=0) = \frac{e^{i\gamma}}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\psi_2 \quad (\gamma \in \mathbb{R}) \rightarrow \langle p \rangle (t)$?

↳ homogenoki zentroan zentratuta

$$\langle x \rangle = (\psi, x\psi) = \int_{-a/2}^{a/2} \left(\frac{e^{i\gamma}}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\psi_2\right)\left(\frac{e^{i\gamma}}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\psi_2\right)^* x\, dx =$$

$$\int_{-a/2}^{a/2}\left(\frac{1}{2}\psi_1^2 + \frac{e^{i\gamma}}{2}\psi_2\psi_1 + \frac{e^{-i\gamma}}{2}\psi_2\psi_1 + \frac{1}{2}\psi_2^2\right) x\, dx = \int_{-a/2}^{a/2}\left(\frac{1}{2}\psi_1^2 + \frac{1}{2}\psi_2^2 + \psi_2\psi_1 \cos\delta\right) x\, d$$

$$\frac{1}{\cancel{2}}\int_{-a/2}^{a/2} \frac{\cancel{2}}{a} \cancel{\cos^2\frac{\pi x}{a} \cdot x \, dx}^{\,0 \text{ (bakoitia)}} + \frac{1}{\cancel{2}}\int_{-a/2}^{a/2} \cancel{\frac{2}{a} \sin^2\frac{2\pi x}{a} \cdot x\, dx}^{\,0 \text{ (bakoitia)}} + \int_{-a/2}^{a/2} \cos\delta \cdot \frac{2}{a} \sin\frac{2\pi x}{a} \cos\frac{\pi x}{a} \cdot x\, dx =$$

$$0 + 0 + \frac{2}{a}\cos\delta \underbrace{\int_{-a/2}^{a/2} \sin\frac{2\pi x}{a}\cos\frac{\pi x}{a} \cdot x\, dx}_{\neq 0 \text{ (bikoitia)}} = 0 \Rightarrow \text{beraz } \cos\delta = 0 \rightarrow \delta = \frac{\pi}{2}, \frac{3\pi}{2}$$

$\delta = \pi/2$

$$\psi(t=0) = \frac{i}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\cdot\psi_2 \quad\Rightarrow\quad \psi(x,t) = \frac{i}{\sqrt{2}}\, e^{-\frac{iE_1}{\hbar}t}\psi_1 + \frac{1}{\sqrt{2}}\, e^{-\frac{iE_2}{\hbar}t}\psi_2$$

$$\langle p\rangle = \left(\psi, -i\hbar\frac{\partial}{\partial x}\psi\right) = \left(\frac{i}{\sqrt{2}}e^{-\frac{iE_1}{\hbar}t}\psi_1 + \frac{1}{\sqrt{2}}e^{-\frac{iE_2}{\hbar}t}\psi_2, -i\hbar\frac{\partial}{\partial x}\psi\right) = \dots$$

$$\left(\frac{i}{\sqrt{2}}e^{-\frac{iE_1}{\hbar}t}\psi_1 + \frac{1}{\sqrt{2}}e^{-\frac{iE_2}{\hbar}t}\psi_2, -i\hbar\left(\frac{i}{\sqrt{2}}e^{-\frac{iE_1}{\hbar}t}\frac{\partial\psi_1}{\partial x} + \frac{1}{\sqrt{2}}e^{-\frac{iE_2}{\hbar}t}\frac{\partial\psi_2}{\partial x}\right)\right) =$$

$$\frac{1}{2}\left(ie^{-\frac{iE_1}{\hbar}t}\psi_1 + e^{-\frac{iE_2}{\hbar}t}\psi_2, -i\hbar\left(ie^{-\frac{iE_1}{\hbar}t}\left(-\frac{\pi}{a}\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\right) + e^{-\frac{iE_2}{\hbar}t}\left(\sqrt{\frac{2}{a}}\frac{2\pi}{a}\cos\frac{2\pi}{a}x\right)\right)\right) =$$

$$\frac{1}{2}\cdot\sqrt{\frac{2}{a}}\,\frac{\pi}{a}\left(ie^{-\frac{iE_1}{\hbar}t}\psi_1 + e^{-\frac{iE_2}{\hbar}t}\psi_2, -\hbar e^{-\frac{iE_1}{\hbar}t}\sin\left(\frac{\pi x}{a}\right) - 2i\hbar e^{-\frac{iE_2}{\hbar}t}\cos\left(\frac{2\pi}{a}x\right)\right) =$$

Kompleks delalo

$$\frac{\pi}{a\sqrt{2a}}\left[\left(ie^{-\frac{iE_1}{\hbar}t}\psi_1, \cancel{-\hbar e^{-\frac{iE_1}{\hbar}t}}^{\,0}\sin\left(\frac{\pi x}{a}\right)\right) + \left(ie^{-\frac{iE_1}{\hbar}t}\psi_1, -2i\hbar e^{-\frac{iE_2}{\hbar}t}\cos\left(\frac{2\pi}{a}x\right)\right) +\right.$$

kompleksno delalo

$$\left.\left(e^{-\frac{iE_2}{\hbar}t}\psi_2, -\hbar e^{-\frac{iE_1}{\hbar}t}\sin\left(\frac{\pi x}{a}\right)\right) + \left(e^{-\frac{iE_2}{\hbar}t}\psi_2, \cancel{-2i\hbar e^{-\frac{iE_2}{\hbar}t}}^{\,0}\cos\left(\frac{2\pi}{a}x\right)\right)\right] =$$

$$\frac{\pi}{a\sqrt{2a}}\left[e^{+\frac{E_1-E_2}{\hbar}ti}\cdot 2\hbar\left(\psi_1, \cos\left(\frac{2\pi}{a}x\right)\right) + e^{-\frac{E_1-E_2}{\hbar}it}(-\hbar)\left(\psi_2, \sin\left(\frac{\pi}{a}x\right)\right)\right] =$$

$$\frac{\pi\hbar}{a\sqrt{2a}}\left[e^{i\frac{E_1-E_2}{\hbar}t}\cdot 2\left(\sqrt{\frac{2}{a}}\cos\frac{\pi x}{a}, \cos\left(\frac{2\pi}{a}x\right)\right) - e^{-\frac{E_1-E_2}{\hbar}it}\left(\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}, \sin\frac{\pi}{a}x\right)\right] \overset{*}{=} 0$$

Ortogonalni.

$$\sqrt{\frac{2}{a}}\,\frac{\pi\hbar}{a\sqrt{2a}}\left[e^{i\frac{E_1-E_2}{\hbar}t}\right.$$

4. GAIA: POTENTZIAL ZENTRALAK eta ELEKTROI BAKARREKO ATOMOAK

$\hat{L}_z$-ren autofuntzioak eta autobalioak:

1.)

Koordenatu esferikoetan $\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi} = -i\hbar\frac{\partial}{\partial\varphi}$ dela frogatu:

Kartesianoetan: $\hat{L}_z = -i\hbar(x\partial y - y\partial x)$

$*\ \partial y = \frac{\partial}{\partial y} = \frac{\partial}{\partial r}\frac{\partial r}{\partial y} + \frac{\partial}{\partial\theta}\frac{\partial\theta}{\partial y} + \frac{\partial}{\partial\varphi}\frac{\partial\varphi}{\partial y} = \frac{\partial}{\partial r}\left(\frac{1}{\frac{\partial y}{\partial r}}\right) + \frac{\partial}{\partial\theta}\left(\frac{1}{\frac{\partial y}{\partial\theta}}\right) + \frac{\partial}{\partial\varphi}\left(\frac{1}{\frac{\partial y}{\partial\varphi}}\right) = \frac{\partial}{\partial r}\left(\frac{1}{\sin\theta\sin\varphi}\right) +$

$\frac{\partial}{\partial\theta}\left(\frac{1}{r\cos\theta\sin\varphi}\right) + \frac{\partial}{\partial\varphi}\left(\frac{1}{r\sin\theta\cos\varphi}\right)$

$*\ \partial x = \frac{\partial}{\partial x} = \frac{\partial}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial}{\partial\theta}\frac{\partial\theta}{\partial x} + \frac{\partial}{\partial\varphi}\frac{\partial\varphi}{\partial x} = \frac{\partial}{\partial r}\left(\frac{1}{\frac{\partial x}{\partial r}}\right) + \frac{\partial}{\partial\theta}\left(\frac{1}{\frac{\partial x}{\partial\theta}}\right) + \frac{\partial}{\partial\varphi}\left(\frac{1}{\frac{\partial x}{\partial\varphi}}\right) = \frac{\partial}{\partial r}\left(\frac{1}{\sin\theta\cos\varphi}\right) +$

$\frac{\partial}{\partial\theta}\left(\frac{1}{r\cos\theta\cos\varphi}\right) + \frac{\partial}{\partial\varphi}\left(\frac{1}{-r\sin\varphi\sin\theta}\right)$

$\Rightarrow\ x\partial y - y\partial x = r\sin\theta\cos\varphi\left(\frac{1}{\sin\theta\sin\varphi}\frac{\partial}{\partial r} + \frac{1}{r\cos\theta\sin\varphi}\frac{\partial}{\partial\theta} + \frac{1}{r\sin\theta\cos\varphi}\frac{\partial}{\partial\varphi}\right) - r\sin\theta\sin\varphi\left(\frac{1}{\sin\theta\cos\varphi}\frac{\partial}{\partial r} +\right.$

$\left.\frac{1}{r\cos\theta\cos\varphi}\frac{\partial}{\partial\theta} - \frac{1}{r\sin\theta\sin\varphi}\frac{\partial}{\partial\varphi}\right) = \dots = \frac{\partial}{\partial\varphi}$

2.)

$\Psi(r,t) = \frac{e^{-\alpha r}}{r}(\cos\theta\, e^{2\phi i} + 1) \quad \alpha > 0 \Rightarrow L_z$ neurtu. $\Rightarrow \left\{\frac{e^{im\varphi}}{\sqrt{2\pi}}\right\}$

Normalizatu: $\int_0^{2\pi}\int_0^{\infty}\int_0^{\pi}\frac{e^{-2\alpha r}}{\cancel{r^2}}(\cos\theta e^{2\phi i}+1)(\cos\theta e^{-2\phi i}+1)\cancel{r^2}\sin\theta\, d\theta dr d\phi = \int_0^{2\pi}\int_0^{\infty}\int_0^{\pi} e^{-2\alpha r}(\cos^2\theta +$

$\cos\theta\cdot e^{2\phi i} + \cos\theta e^{2\phi i} + 1)\sin\theta\, d\theta dr d\phi = \int_0^{2\pi}\int_0^{\infty}\int_0^{\pi} e^{-2\alpha r}(\cos^2\theta + 1 + 2\cos\phi\cos\theta)\sin\theta\, d\theta\, dr d\phi =$

$\frac{1}{2\alpha}\int_0^{2\pi}\int_0^{\pi}(\cos^2\theta\sin\theta + \sin\theta + 2\cos\phi\cos\theta\sin\theta)\, d\theta d\phi = \frac{1}{2\alpha}\int_0^{2\pi}\left(\left[-\frac{\cos^3\theta}{3}\right]_0^{\pi} - \cos\theta + \cos\phi\sin^2\theta\right]_0^{\pi}\Big)d\phi =$

$$\frac{1}{2\alpha}\int_0^{2\pi}\left(\frac{2}{3}+2+\cancel{\cos\phi}\right)d\phi = \frac{1}{2\alpha}\left(\frac{8}{3}\phi\right)_0^{2\pi} = \frac{16\pi}{6\alpha} = \frac{1}{2\alpha}\cdot\frac{16\pi}{3} = \frac{8\pi}{3\alpha} \Rightarrow$$

$$\Psi(r,t) = \sqrt{\frac{3\alpha}{8\pi}}\cdot\frac{e^{-\alpha r}}{r}\left(\cos\theta e^{2\phi i}+1\right) = \sqrt{\frac{3\alpha}{8\pi}}\frac{e^{-\alpha r}}{r}\left(\cos\theta e^{2\phi i}+e^{0\phi i}\right) =$$

$$\sqrt{\frac{3\alpha}{8\pi}}\frac{e^{-\alpha r}}{r}\left(\sqrt{2\pi}\cos\theta\, Y_0^2+\sqrt{2\pi}\,Y_0^0\right) = \sqrt{\frac{3\alpha}{4}}\frac{e^{-\alpha r}}{r}\left(\cos\theta\, Y_0^2+Y_0^0\right)$$

- $l_z = 2\hbar$ eta $l_z = 0$ lor daitezke $\Rightarrow$ $\boxed{P(2\hbar) = \frac{3\alpha}{4}\int_0^{\pi}\int_0^{\infty}\frac{e^{-2\alpha r}}{\cancel{r^2}}\cancel{r^2}\cos^2\theta\sin\theta\, dr\, d\theta} =$

$$\frac{3\alpha}{4}\cdot\int_0^{\infty}e^{-2\alpha r}dr\int_0^{\pi}\sin\theta\cos^2\theta\, d\theta = -\frac{\cancel{3\alpha}}{2\cancel{\alpha}}\cdot\frac{1}{4}\cdot\frac{\cos^3\theta}{\cancel{3}}\Big]_0^{\pi} = -\frac{1}{8}\cdot(-2) = \boxed{\frac{1}{4}}$$

- $\boxed{P(0)} = \frac{3\alpha}{4}\int_0^{\pi}\int_0^{\infty}\frac{e^{-2\alpha r}}{\cancel{r^2}}\cancel{r^2}\,dr\sin\theta d\theta = \frac{3\cancel{\alpha}}{4\cdot2\cancel{\alpha}}\cdot(-\cos\theta)\Big]_0^{\pi} = \frac{3}{8}\cdot 2 = \boxed{\frac{3}{4}}$

3.)

$$\Psi(r,t=0) = e^{-\alpha r^2}\phi \qquad \alpha>0 \qquad \phi = \sum_{m=\infty}^{\infty} c_m\frac{e^{i\phi}}{\sqrt{2\pi}}$$

Aldibrean $r\in[a,b]$ eta $\hbar$ neurtu.

Normalizatu $\Rightarrow$ $\int_0^{\pi}\int_0^{\infty}\int_0^{\pi}e^{-2\alpha r^2}\phi^2 d\phi\, r^2\sin\theta\, dr\, d\theta = \int_0^{\pi}\sin\theta d\theta\int_0^{\infty}e^{-2\alpha r^2}r^2 dr\int_0^{2\pi}\phi^2 d\phi =$

$$-\cos\theta\Big]_0^{\pi}\;\frac{\sqrt{\frac{\pi}{2}}}{8\alpha^{3/2}}\cdot\frac{\phi^3}{3}\Big]_0^{2\pi} = \frac{2}{\cancel{8}\alpha^{3/2}}\sqrt{\frac{\pi}{2}}\cdot\frac{1}{3}\cdot 8\pi^3 = \frac{2}{3\alpha^{3/2}}\sqrt{\frac{\pi}{2}}\,\pi^3 = \frac{\sqrt{2\pi}\,\pi^3}{3\alpha^{3/2}}$$

$\hbar$ neurtu $\Rightarrow$ $l=1 \rightarrow \Psi = Ae^{-\alpha r^2}\cdot\sum_{m=0}^{\infty}c_m\frac{e^{im\phi}}{\sqrt{2\pi}}$; $c_1 = \left(\frac{e^{i\phi}}{\sqrt{2\pi}},\phi\right) = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi}e^{-i\phi}\phi\, d\phi = \frac{2i\pi}{\sqrt{2\pi}} = \sqrt{2\pi}i$

$$P(\hbar, r\in[a,b]) = 2\pi\left(\frac{3\alpha^{3/2}}{\pi^3\sqrt{2\pi}}\right)\cdot\int_a^b e^{-2\alpha r^2}r^2 dr\int_0^{\pi}\sin\theta d\theta = 4\pi\left(\frac{3\cancel{\alpha^{3/2}}}{\pi^2\sqrt{2\pi}}\right)\frac{1}{16\cancel{\alpha^{3/2}}}\cdot$$

$$\left(4\sqrt{\alpha}\left(ae^{-2\alpha a^2}-be^{-2\alpha b^2}\right)+\sqrt{2\pi}\left(\operatorname{erf}(\sqrt{2\alpha}b)-\operatorname{erf}(\sqrt{2\alpha}a)\right)\right)$$

Momentu angeluarraren trukatze-erlazioak:

1.)

kasu batzuk ezabatzen dira (?)

a) $[\hat{L}_x, \hat{L}_y] = [y\hat{p}_z - \hat{p}_y z, z\hat{p}_x - \hat{p}_z x] = [y\hat{p}_z, z\hat{p}_x] - [\cancel{\hat{p}_y z, z\hat{p}_x}]^{0} - [\cancel{y\hat{p}_z, \hat{p}_z x}]^{0} +$

$[\hat{p}_y z, \hat{p}_z x] = y[\hat{p}_z, z\hat{p}_x] + [\cancel{y, z\hat{p}_x}]^{0}\hat{p}_z + \hat{p}_y[z, \hat{p}_z x] + [\cancel{\hat{p}_y, \hat{p}_z x}]^{0}\hat{z}$ *

* $y\left(-i\hbar\frac{\partial}{\partial z}(z\hat{p}_x) + zi\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial}{\partial z}\right)\right) = y\left(-\hbar^2\left(\frac{\partial}{\partial x}\right) + \cancel{z\frac{\partial^2}{\partial z\partial x}}\right) + \cancel{\hbar^2 z\frac{\partial^2}{\partial z\partial x}}\Big) = -i\hbar y\,\hat{p}_x$

* $\hat{p}_y\left(z\left(-i\hbar\frac{\partial}{\partial z}(x)\right) + i\hbar x\frac{\partial}{\partial z}z\right)\Big) = \hat{p}_y x\left(\cancel{-i\hbar z\frac{\partial}{\partial z}} + i\hbar\left(1 + \cancel{\frac{\partial}{\partial z}}\right)\right) = i\hbar\,\hat{p}_y x$

$\Rightarrow \quad [\hat{L}_x, \hat{L}_y] = i\hbar(\hat{p}_y x - y\hat{p}_x) = i\hbar\hat{L}_z$

$[\hat{L}_y, \hat{L}_z] = [z\hat{p}_x - \hat{p}_z x, x\hat{p}_y - y\hat{p}_x] = [z\hat{p}_x, x\hat{p}_y] - [\cancel{z\hat{p}_x, y\hat{p}_x}]^{0} + [\hat{p}_z x, y\hat{p}_x] +$

$-[\cancel{\hat{p}_z x, x\hat{p}_y}]^{0}$ * $= i\hbar y\hat{p}_z - i\hbar z\hat{p}_y = \hat{L}_x\, i\hbar$

* $[z\hat{p}_x, x\hat{p}_y] = z[\hat{p}_x, x\hat{p}_y] + [\cancel{z, x\hat{p}_y}]^{0}\hat{p}_x = z\left(-i\hbar\frac{\partial}{\partial x}(x\hat{p}_y) + i\hbar x\frac{\partial}{\partial y}\left(-i\hbar\frac{\partial}{\partial x}\right)\right) = z\left(-i\hbar\hat{p}_y - \cancel{\hbar^2 x\frac{\partial^2}{\partial x\partial y}}\right. +$

$\left.+ \cancel{\hbar^2 x\frac{\partial^2}{\partial y\partial x}}\right) = -i\hbar z\hat{p}_y$

* $[\hat{p}_z x, y\hat{p}_x] = \hat{p}_z[x, y\hat{p}_x] + [\cancel{\hat{p}_z, y\hat{p}_x}]x = \hat{p}_z\left(-i\hbar xy\frac{\partial}{\partial x} + i\hbar y\frac{\partial x}{\partial x}\right) = \hat{p}_z\left(\cancel{-i\hbar xy\frac{\partial}{\partial x}}\right. +$

$\left. i\hbar y + \cancel{yi\hbar x\frac{\partial}{\partial x}}\right) = i\hbar y\hat{p}_z$

$[\hat{L}_z, \hat{L}_x] = [x\hat{p}_y - y\hat{p}_x, y\hat{p}_z - \hat{p}_y z] = [x\hat{p}_y, y\hat{p}_z] - [\cancel{x\hat{p}_y, \hat{p}_y z}]^{0} - [\cancel{y\hat{p}_x, y\hat{p}_z}]^{0} +$

$[y\hat{p}_x, \hat{p}_y z] = x[\hat{p}_y, y\hat{p}_z] + [\cancel{x, y\hat{p}_z}]^{0}\hat{p}_y + [\cancel{\hat{p}_x, \hat{p}_y z}]^{0}y + [y, \hat{p}_y z]\hat{p}_x =$

$x\left(\cancel{-\hbar^2 y\frac{\partial^2}{\partial y\partial z}} - i\hbar\hat{p}_z + \cancel{y\hbar^2\frac{\partial^2}{\partial y\partial z}}\right) + \left(\cancel{i\hbar yz\frac{\partial}{\partial y}} + \cancel{i\hbar zy\frac{\partial}{\partial y}} + i\hbar z\right)\hat{p}_x = -i\hbar x\hat{p}_z + i\hbar z\hat{p}_x =$

$i\hbar(z\hat{p}_x - x\hat{p}_z) = \hat{L}_y$

b) • $[\hat{L}^2, \hat{L}_x] = [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x] = \cancel{[\hat{L}_x^2, \hat{L}_x]}^{\,0} + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x] =$

$\hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y + \hat{L}_z[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z = -\cancel{\hat{L}_y}\hat{L}_z - \hat{L}_z\cancel{\hat{L}_y} + \cancel{\hat{L}_z}\hat{L}_y +$

$\cancel{\hat{L}_y}\hat{L}_z = 0$

• $[\hat{L}^2, \hat{L}_y] = [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_y] = [\hat{L}_x^2, \hat{L}_y] + \cancel{[\hat{L}_y^2, \hat{L}_y]}^{\,0} + [\hat{L}_z^2, \hat{L}_y] = \hat{L}_x[\hat{L}_x, \hat{L}_y] +$

$[\hat{L}_x, \hat{L}_y]\hat{L}_x + \hat{L}_z[\hat{L}_z, \hat{L}_y] + [\hat{L}_z, \hat{L}_y]\hat{L}_z = \cancel{\hat{L}_x}\hat{L}_z + \cancel{\hat{L}_z}\hat{L}_x - \cancel{\hat{L}_z}\hat{L}_x - \cancel{\hat{L}_x}\hat{L}_z = 0$

• $[\hat{L}^2, \hat{L}_z] = [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_z] = [\hat{L}_x^2, \hat{L}_z] + [\hat{L}_y^2, \hat{L}_z] + \cancel{[\hat{L}_z^2, \hat{L}_z]} =$

$\hat{L}_x[\hat{L}_x, \hat{L}_z] + [\hat{L}_x, \hat{L}_z]\hat{L}_x + [\hat{L}_y, \hat{L}_z]\hat{L}_y + \hat{L}_y[\hat{L}_y, \hat{L}_z] = \hat{L}_x \cancel{(-\hat{L}_y)} + (-\cancel{\hat{L}_y})\hat{L}_x +$

$\hat{L}_x\cancel{\hat{L}_y} + \cancel{\hat{L}_y}\hat{L}_x = 0$

2)

a) • $[\hat{L}_x, \hat{p}_x] = [y\hat{p}_z - z\hat{p}_y, \hat{p}_x] = 0$

• $[\hat{L}_x, \hat{p}_y] = [y\hat{p}_z - z\hat{p}_y, \hat{p}_y] = [y\hat{p}_z, \hat{p}_y] = y\cancel{[\hat{p}_z, \hat{p}_y]}^{\,0} + [y, \hat{p}_y]\hat{p}_z = i\hbar\hat{p}_z$

• $[\hat{L}_x, \hat{p}_z] = [y\hat{p}_z - z\hat{p}_y, \hat{p}_z] = \cancel{[y\hat{p}_z, \hat{p}_z]}^{\,0} - [z\hat{p}_y, \hat{p}_z] = -z\cancel{[\hat{p}_y, \hat{p}_z]} +$

$-[z, \hat{p}_z]\hat{p}_y = -i\hbar\hat{p}_y$

b) • $[\hat{L}_x, \hat{p}_x^2] = \hat{p}_x[\hat{L}_x, \hat{p}_x] + [\hat{L}_x, \hat{p}_x]\hat{p}_x = 0$

• $[\hat{L}_x, \hat{p}_y^2] = \hat{p}_y[\hat{L}_x, \hat{p}_y] + [\hat{L}_x, \hat{p}_y]\hat{p}_y = i\hbar\hat{p}_y\hat{p}_z + i\hbar\hat{p}_z\hat{p}_y = 2i\hbar\hat{p}_z\hat{p}_y$

• $[\hat{L}_x, \hat{p}_z^2] = \hat{p}_z[\hat{L}_x, \hat{p}_z] + [\hat{L}_x, \hat{p}_z]\hat{p}_z = -i\hbar\hat{p}_z\hat{p}_y - i\hbar\hat{p}_z\hat{p}_y = -2i\hbar\hat{p}_z\hat{p}_y$

$\hat{L}_x$ r-ren independentea da.

c) • $[\hat{H}, \hat{L}_x] = [\hat{T} + V(r), \hat{L}_x] = [\frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + V(r), \hat{L}_x] = 0$

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

• $[\hat{H}, \hat{L}^2] = [\hat{T} + V(r), \hat{L}^2] = [\frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr} + V(r), \hat{L}^2] = 0$

Momentu angeluarraren autofuntzioak eta autobalioak.

1.)

$Y_2^{\pm 2}(\theta,\phi)$, $Y_2^{\pm 1}(\theta,\phi)$

$$Y_2^{\pm 2}(\theta,\phi) = e^{\pm 2i\phi} \frac{1}{4}\sqrt{\frac{15}{2\pi}} \sin^2\theta \quad ; \quad Y_2^{\pm 1}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}} \sin\theta\cos\theta\, e^{\pm i\varphi}$$

2.)

a) • $Y_1^{-1}(\theta,\phi) = +\frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin\theta\, e^{-i\varphi} = +\frac{1}{2}\sqrt{\frac{3}{2\pi}}\left(\sin\theta\left(e^{-i\varphi} + e^{+i\varphi} - e^{+i\varphi}\right)\right) = +\frac{1}{2}\sqrt{\frac{3}{2\pi}}$

$\left(\sin\theta \cdot 2\cos\varphi - \sin\theta\, e^{-i\varphi}\right) = +\frac{1}{2}\sqrt{\frac{3}{2\pi}}\left(2\sin\theta\cos\varphi - \sin\theta\left(e^{+i\varphi} - e^{-i\varphi} + e^{-i\varphi}\right)\right) =$

$+\frac{1}{2}\sqrt{\frac{3}{2\pi}}\left(\frac{2x}{r} - \sin\theta\, e^{-i\varphi} - \sin\theta \cdot 2i\sin\varphi\right) = +\frac{x}{r}\sqrt{\frac{3}{2\pi}} - \frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{-i\varphi} - i\sin\theta\sin\varphi\sqrt{\frac{3}{2\pi}} =$

$+\frac{x}{r}\sqrt{\frac{3}{2\pi}} - \frac{i}{r}y\sqrt{\frac{3}{2\pi}} - Y_1^{-1} \Rightarrow \quad 2Y_1^{-1} = -\sqrt{\frac{3}{2\pi}} \cdot \frac{1}{r}(iy - x) \Rightarrow Y_1^{-1} = \frac{1}{2r}\sqrt{\frac{3}{2\pi}}(x - iy)$

• $Y_1^{1}(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{i\varphi} = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\left(e^{i\varphi} + e^{-i\varphi} - e^{-i\varphi}\right) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\,(2\cos\varphi +$

$-e^{-i\varphi}) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\left(2\cos\varphi - e^{-i\varphi} + e^{i\varphi} - e^{i\varphi}\right) = -\sqrt{\frac{3}{2\pi}}\sin\theta\cos\varphi + \frac{e^{i\varphi}}{2}\sqrt{\frac{3}{2\pi}}\sin\theta +$

$-\frac{1}{2}\sqrt{\frac{3}{2\pi}}\,2i\sin\theta\sin\varphi = -\sqrt{\frac{3}{2\pi}}\frac{x}{r} - \sqrt{\frac{3}{2\pi}}\frac{iy}{r} - Y_1^{1}(\theta,\varphi) \Rightarrow 2Y_1^{1} = -\sqrt{\frac{3}{2\pi}}\frac{1}{r}(x+iy) \Rightarrow$

$$Y_1^{1} = -\sqrt{\frac{3}{2\pi}} \cdot \frac{1}{2r}(x+iy)$$

• $Y_1^{0}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cdot \frac{z}{r}$

b) • $Y_2^{\pm 2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{\pm 2i\phi} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\left(e^{\pm i\varphi}\right)^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\left(\frac{e^{i\varphi}+e^{-i\varphi}}{2} \pm i\frac{e^{i\varphi}-e^{-i\varphi}}{2i}\right)^2$

$\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\left(\cos\phi \pm i\sin\phi\right)^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\frac{(x \pm iy)^2}{r^2}$

$$\circ\ Y_2^{\pm 1} = \sin\theta\cos\theta \cdot \frac{1}{2}\sqrt{\frac{15}{2\pi}}\, e^{\pm i\varphi} = \pm\sin\theta\cos\theta\frac{1}{2}\sqrt{\frac{15}{2\pi}}\left(\frac{e^{+i\varphi}+e^{-i\varphi}}{2} \pm \frac{e^{+i\varphi}-e^{-i\varphi}}{2}\right) = \mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}(\cos\varphi \pm i\sin\varphi).$$

$$\sin\theta\cos\theta = \mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}\,\frac{(xz \pm iyz)}{r^2}$$

$$\circ\ Y_2^0(\theta,\phi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1) = \frac{1}{4}\sqrt{\frac{5}{\pi}}(2\cos^2\theta + \cos^2\theta - 1) = \frac{1}{4}\sqrt{\frac{5}{\pi}}(2\cos^2\theta - \sin^2\theta) =$$

$$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(\frac{2z^2}{r^2} - \frac{(x^2+y^2)}{r^2}\right) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\,\frac{(2z^2-x^2-y^2)}{r^2}$$

3)

a) $$\langle \hat{L}_x\rangle_{Y_l^m} = (Y_l^m, \hat{L}_x Y_l^m) = \left(Y_l^m, \frac{\hat{L}_+Y_l^m}{2} + \frac{\hat{L}_-Y_l^m}{2}\right) = \frac{1}{2}\left[(Y_l^m, \hat{L}_+Y_l^m) + \right.$$

$$\left.(Y_l^m, \hat{L}_-Y_l^m)\right] = \frac{1}{2}\left[\underbrace{\cancel{(Y_l^m, \hbar\sqrt{l(l+1)-m(m+1)}\,Y_l^{m+1})}}_{\text{(ortogonales)}} + \underbrace{\cancel{(Y_l^m, \hbar\sqrt{l(l+1)-m(m-1)}\,Y_l^{m-1})}}_{\text{(ortogonales)}}\right] = 0$$

$$\langle \hat{L}_y\rangle_{Y_l^m} = (Y_l^m, \hat{L}_y Y_l^m) = \left(Y_l^m, \frac{\hat{L}_+ - \hat{L}_-}{2i} Y_l^m\right) = \frac{1}{2i}\left[(Y_l^m, \hat{L}_+Y_l^m) + \right.$$

$$\left. - (Y_l^m, \hat{L}_-Y_l^m)\right] = \frac{1}{2i}\left[\underbrace{\cancel{(Y_l^m, \hbar\sqrt{l(l+1)-m(m+1)}\,Y_l^{m+1})}}_{\text{(ortogonales)}} + \underbrace{\cancel{(Y_l^m, \hbar\sqrt{l(l+1)-m(m-1)}\,Y_l^{m-1})}}_{\text{(ortogonales)}}\right] = 0$$

b) $\Psi(x,0) = Y_l^m \Rightarrow \Delta\hat{L}_x\,?\quad \Delta\hat{L}_y?\qquad \langle\hat{L}_x\rangle_{Y_l^m} = \langle\hat{L}_y\rangle_{Y_l^m} = 0$

$$\circ\ \langle\hat{L}_x^2\rangle_{Y_l^m} = (Y_l^m, \hat{L}_x^2 Y_l^m) = \left(Y_l^m, \frac{(\hat{L}_+ + \hat{L}_-)^2}{4} Y_l^m\right) = \frac{1}{4}\cancel{(Y_l^m, \hat{L}_+^2 Y_l^m)} +$$

$$\frac{1}{4}\cancel{(Y_l^m, \hat{L}_-^2 Y_l^m)} + \frac{1}{4}(Y_l^m, \hat{L}_+\hat{L}_- Y_l^m) + \frac{1}{4}(Y_l^m, \hat{L}_-\hat{L}_+ Y_l^m) =$$

$$+\frac{1}{4}(Y_l^m, \hbar\sqrt{l(l+1)-m(m-1)}\,\hbar\sqrt{l(l+1)-(m-1)m}\,Y_l^m) + \frac{1}{4}(Y_l^m, \hbar^2(\sqrt{l(l+1)-m(m+1)})^2\,Y_l^m) =$$

$$\frac{1}{4}\hbar^2(l(l+1)-m(m-1)+l(l+1)-m(m+1)) = \frac{\hbar^2}{4}(2l(l+1) - m(m-1+m+1)) =$$

$$\frac{\hbar^2}{4}(2l(l+1)-2m^2) = \frac{\hbar^2}{2}(l(l+1)-m^2)$$

$$\Delta L_x = \sqrt{\langle L_x^2\rangle} = \hbar\frac{\sqrt{l(l+1)-m^2}}{\sqrt{2}}$$

- $\langle \hat{L}_y^2 \rangle_{lm} = (Y_l^m, \hat{L}_y^2 Y_l^m) = (Y_l^m, \frac{(\hat{L}_+ - \hat{L}_-)^2}{-4} Y_l^m) = -\frac{1}{4} \cancel{(Y_l^m, \hat{L}_+^2 Y_l^m)}^{0} +$

$- \frac{1}{4} \cancel{(Y_l^m, \hat{L}_-^2 Y_l^m)}^{0} + \frac{1}{4} (Y_l^m, \hat{L}_+ \hat{L}_- Y_l^m) + \frac{1}{4} (Y_l^m, \hat{L}_- \hat{L}_+ Y_l^m) =$

$\frac{1}{4}\left(\hbar \sqrt{l(l+1)-m(m-1)}\right)^2 + \frac{1}{4}\left(\hbar\sqrt{l(l+1)-m(m+1)}\right)^2 = \frac{\hbar^2}{4}(2l(l+1)-2m^2) = \frac{\hbar^2}{2}(l(l+1)-m^2)$

$$\Delta L_y = \sqrt{\langle L_y^2 \rangle} = \hbar \sqrt{\frac{l(l+1)-m^2}{2}}$$

4.)

$(Y_l^{m'}, [\hat{L}_+, \hat{L}_-] Y_l^m)$? $\qquad [\hat{L}_+, \hat{L}_-] = [\hat{L}_x + i\hat{L}_y, \hat{L}_x - i\hat{L}_y] =$

$\cancel{[\hat{L}_x, \hat{L}_x]} + [\hat{L}_x, -i\hat{L}_y] = -i(i\hbar \hat{L}_z) + i[\hat{L}_y, \hat{L}_x] + \cancel{[\hat{L}_y, \hat{L}_y]} = 2\hbar \hat{L}_z$

$[\hat{L}_x, \hat{L}_y] = \hat{L}_z \cdot i\hbar$

$\hat{L}_z$-ren autob.

Beraz, $(Y_l^{m'}, 2\hbar \hat{L}_z Y_l^m) = 2\hbar (Y_l^{m'}, \hat{L}_z Y_l^m) = 2\hbar (Y_l^{m'}, \hbar m Y_l^m) =$

$2m\hbar^2 (Y_l^{m'}, Y_l^m) = 2m\hbar^2 \delta_{l'l} \delta_{m'm}$

5.)

$[\hat{A}, \hat{L}_x] = 0, \quad [\hat{A}, \hat{L}_y] = 0 \leftrightarrow \quad [\hat{A}, \hat{L}_z] = 0$

6.)

$\hat{L}_x, \hat{L}_y$ eta $\hat{L}_z$ eragileen aldibereko autofuntzioak.

$\hat{L}_x \psi(r) = l_x \psi(r)$ $\qquad$ $\hat{L}_z$-ren autofuntzioak: $\psi = F(\theta, r) e^{im\varphi}$ $\quad m \in \mathbb{Z}$

$\hat{L}_y \psi(r) = l_y \psi(r)$ $\qquad$ $\hat{L}_x, \hat{L}_y$-ren autofuntzioa ez dira beti ere.

$\hat{L}_z \psi(r) = l_z \psi(r)$

$\cdot\ \hat{L}_x \Psi = -i\hbar\left(-\sin\varphi\, e^{im\varphi}\frac{\partial F}{\partial\theta} - \frac{\cos\varphi}{\tan\theta}\, im\, e^{im\varphi} F\right) = i\hbar \sin\varphi\, \cancel{e^{im\varphi}}\frac{\partial F}{\partial\theta} - \frac{\hbar\cos\varphi}{\tan\theta}\, m\, \cancel{e^{im\varphi}} F =$

$l_x F \cancel{e^{im\varphi}}$ (1) $\Rightarrow \hat{l}_x = \frac{l_x}{\hbar}$

$\cdot\ \hat{L}_y \Psi = -i\hbar\left(\cos\varphi\, e^{im\varphi}\frac{\partial F}{\partial\theta} - \frac{\sin\varphi}{\tan\theta}\, im\, e^{im\varphi} F\right) = -i\hbar\cos\varphi\, \cancel{e^{im\varphi}}\frac{\partial F}{\partial\theta} - \frac{\sin\varphi}{\tan\theta}\hbar\, m\, \cancel{e^{im\varphi}} F =$

$l_y F \cancel{e^{im\varphi}}$ (2) $\Rightarrow \hat{l}_y = \frac{l_y}{\hbar}$

$$\Rightarrow \quad i\sin\varphi\frac{\partial F}{\partial\theta} - \frac{\cos\varphi}{\tan\theta} m F = \hat{l}_x F \Rightarrow i\sin\varphi\frac{\partial F}{\partial\theta} = F\left(\frac{\cos\varphi}{\tan\theta} m + \hat{l}_x\right) \qquad (1)$$

$$\Rightarrow \quad -i\cos\varphi\frac{\partial F}{\partial\theta} - \frac{\sin\varphi}{\tan\theta} m F = \tilde{l}_y F \Rightarrow -i\cos\varphi\frac{\partial F}{\partial\theta} = F\left(\frac{\sin\varphi}{\tan\theta} m + \tilde{l}_y\right) \qquad (2)$$

$$\frac{(1)}{(2)} = -\tan\varphi = \frac{\frac{\cos\varphi}{\tan\theta} m + \hat{l}_x}{\frac{\sin\varphi}{\tan\theta} m + \hat{l}_y} \Rightarrow -\tan\varphi\left(\frac{\sin\varphi}{\tan\theta} m + \hat{l}_y\right) = \frac{\cos\varphi}{\tan\theta} m + \hat{l}_x$$

Hau φ guztietarako bete behar denez aukera bakarra $m=0$ izatea da.

$\Rightarrow \Psi = A\cdot F,\ l_z = 0$

$\Rightarrow -i\hbar\left(-\sin\varphi A\frac{\partial F}{\partial\theta}\right) = F\cdot A\, l_x \Rightarrow$ gauza bera, F φ-ren independentea denez

aukera bakarra. $\frac{\partial F}{\partial\theta} = 0$ izatea da eta $l_x = 0$ orduan.

$\Rightarrow -i\hbar\left(\cos\varphi A\frac{\partial F}{\partial\theta}\right) = F\cdot A\, l_y \Rightarrow \frac{\partial F}{\partial\theta} = 0 \rightarrow l_y = 0$

Orduan: $\Psi = A f(r)$ da, $l_x = l_z = l_y = 0$ $f(r)$ edozein izan daiteke

7.)
$\{\phi(x) = x f(r),\quad \phi_y = y f(r)\}$ $\hat{L}_x$ eta $\hat{L}_y$-ren autofuntzioak.

• $\phi_x = x\,g(r) = r\sqrt{\frac{2\pi}{3}}\,(Y_1^{-1} - Y_1^{1})\,g(r)$ $\quad \phi_y = y\,g(r) = ri\sqrt{\frac{2\pi}{3}}\,(Y_1^{-1} + Y_1^{1})\,g(r)$

$$* \; \hat{L}_x \phi_x = \left(\frac{\hat{L}_+ + \hat{L}_-}{2}\right)\phi_x = \frac{1}{2}\, r\sqrt{\frac{2\pi}{3}}\,g(r)\left(\hat{L}_+ Y_1^{-1} - \hat{L}_+ Y_1^{1} + \hat{L}_- Y_1^{-1} - \hat{L}_- Y_1^{1}\right) =$$

$$g(r)\,\frac{r}{2}\sqrt{\frac{2\pi}{3}}\left(\hbar\sqrt{2+1\cdot 0}\; Y_1^0 - \cancel{\hbar\sqrt{2-2}\; Y_1^2} + \cancel{\hbar\sqrt{2-2}}^{\,0}\; Y_1^{-2} - \hbar\sqrt{2}\; Y_1^0\right) = 0$$

$l_x = 0$ da autobalioa

$$* \; \hat{L}_y \phi_y = \left(\frac{\hat{L}_+ - \hat{L}_-}{2i}\right)\phi_y = \frac{r}{2}\sqrt{\frac{2\pi}{3}}\,g(r)\left(\hat{L}_+ Y_1^{-1} + \hat{L}_+ Y_1^{1} - \hat{L}_- Y_1^{-1} +\right.$$

$$\left. - \hat{L}_- Y_1^{1}\right) = 0$$ $\quad l_y = 0$ da autobalioa

• $\hat{u}$ norabidea $\Rightarrow$ $\quad \hat{u} = \cos\alpha\,\hat{\imath} + \sin\alpha\,\hat{\jmath}$ $\quad \Rightarrow \hat{L}_u$ -ren autobalioa?

$$L_u = \vec{L}\cdot\hat{u} = L_x\cos\alpha + L_y \sin\alpha \;\Rightarrow\; \hat{L}_u = \hat{L}_x\cos\alpha + \hat{L}_y \sin\alpha$$

Bere autofuntzioak $\{\phi_x, \phi_y\}$ oinarrian garatuko ditugu: $\phi_u = a\phi_x + b\phi_y$

$$* \; \hat{L}_u\phi_u = \hat{L}_u(a\phi_x + b\phi_y) = (\hat{L}_x\cos\alpha + \hat{L}_y\sin\alpha)(a\phi_x + b\phi_y) = \cancel{a\cos\alpha\,\hat{L}_x\phi_x}^{\,0} +$$

$$b\cos\alpha\,\hat{L}_x\phi_y + a\sin\alpha\,\hat{L}_y\phi_x + \cancel{b\sin\alpha\,\hat{L}_y\phi_y}^{\,0} = a\sin\alpha\,\hat{L}_y\phi_x + b\cos\alpha\,\hat{L}_x\phi_y$$

$$* \; \hat{L}_y\phi_x = \left(\frac{\hat{L}_+ - \hat{L}_-}{2i}\right) r\sqrt{\frac{2\pi}{3}}\,g(r)\,(Y_1^{-1} - Y_1^{1}) = \frac{r}{2i}\,g(r)\sqrt{\frac{2\pi}{3}}\left(\hat{L}_+ Y_1^{-1} - \hat{L}_+ Y_1^{1} +\right.$$

$$\left. - \hat{L}_- Y_1^{-1} + \hat{L}_- Y_1^{1}\right) = \frac{r\,g(r)}{2i}\sqrt{\frac{2\pi}{3}}\left(\sqrt{2}\hbar Y_1^0 + \sqrt{2}\hbar Y_1^0\right) = \frac{\sqrt{2}\hbar}{i}\, Y_1^0\, r\, g(r)\sqrt{\frac{2\pi}{3}}$$

$$* \; \hat{L}_x\phi_y = \left(\frac{\hat{L}_+ + \hat{L}_-}{2}\right) ri\sqrt{\frac{2\pi}{3}}\,g(r)\,(Y_1^{-1} + Y_1^{1}) = \frac{r}{2}\, i\, g(r)\sqrt{\frac{2\pi}{3}}\left(\hat{L}_+ Y_1^{-1} + \hat{L}_+ Y_1^{1} + \hat{L}_- Y_1^{-1} +\right.$$

$$\left. \hat{L}_- Y_1^{1}\right) = \frac{i\,g(r)}{2}\sqrt{\frac{2\pi}{3}}\left(\sqrt{2}\hbar Y_1^0 + \sqrt{2}\hbar Y_1^0\right) = i\,g(r)\sqrt{2}\hbar\sqrt{\frac{2\pi}{3}}\, r\, Y_1^0$$

ezinbestekoa

$$\Rightarrow \hat{L}_u\phi_u = a\sin\alpha\; i\, g(r)\sqrt{2}\hbar\sqrt{\frac{2\pi}{3}}\, r\, Y_1^0 - i b\cos\alpha\, g(r)\sqrt{2}\hbar\sqrt{\frac{2\pi}{3}}\, r\, Y_1^0 = 0$$

$\longleftrightarrow \quad a\sin\alpha = b\cos\alpha \Rightarrow \quad b = a\,tg\,\alpha$

Orduan $\phi_u = a(\phi_x + tg\,\alpha\,\phi_y)$ non a normalizazio konstantea izango den.

8.)

Partikula aske baten ganean $\Rightarrow$ $\hat{L}^2$ eta $\hat{L}_z$ neurtu : $l = 1, m = 1$

$\psi = Y_1^1$ egoeran gaude.

$\hat{L}_y$ neurtu $\Rightarrow$ zeintzuk dira lor daitezkeen balioa eta haien probabilitateak?

• $l = 1$ denean L_y-ren autobalioak eta autofuntzioak hauek dira:

$l_y = 0 \quad \psi_1 = \frac{1}{\sqrt{2}}(Y_1^1 + Y_1^{-1})$; $\quad l_y = -\hbar \quad \psi_2 = \frac{1}{2}(Y_1^{-1} - Y_1^1 + \sqrt{2}\,i\,Y_1^0)$;

$l_y = \hbar \quad \psi_3 = \frac{1}{2}(Y_1^1 + \sqrt{2}\,i\,Y_1^0 - Y_1^{-1})$

Beraz $\psi = Y_1^1 = -(\psi_2 - \psi_3)\frac{1}{2} + \frac{1}{\sqrt{2}}\psi_1 = \left(\frac{\psi_1}{\sqrt{2}} - \frac{\psi_2 + \psi_3}{2}\right)$

$l_y = 0, \pm\hbar$ lor daiteke $\Rightarrow P(0) = \frac{1}{2}$, $P(\pm\hbar) = \frac{1}{4}$

9.)

$\hat{H} = \alpha \hat{L}_x^6 \quad (\alpha > 0) \qquad \psi(0,x) = \sqrt{\frac{1}{4}}\,Y_1^1(\theta,\phi) + \sqrt{\frac{1}{2}}\,Y_1^0(\theta,\phi) + \sqrt{\frac{1}{4}}\,Y_1^{-1}(\theta,\phi)$

$\langle L_x \rangle = \langle \psi(0,x), \hat{L}_x \psi(0,x) \rangle = (\psi, \frac{1}{2}(\hat{L}_+ + \hat{L}_-)\psi) = \frac{1}{2}(\psi, \hat{L}_+\psi) +$

$\frac{1}{2}(\psi, \hat{L}_-\psi) = \frac{1}{2}\left(\frac{1}{2}Y_1^1 + \frac{1}{\sqrt{2}}Y_1^0 + \frac{1}{2}Y_1^{-1}, \frac{\hbar}{\cancel{\sqrt{2}}}\cancel{\sqrt{2}}\,Y_1^1 + \frac{\hbar}{2}\sqrt{2}\,Y_1^0\right) +$

$\frac{1}{2}\left(\frac{1}{2}Y_1^1 + \frac{1}{\sqrt{2}}Y_1^0 + \frac{1}{2}Y_1^{-1}, \frac{\hbar}{2}\sqrt{2}\,Y_1^0 + \frac{\hbar}{\cancel{\sqrt{2}}}\cancel{\sqrt{2}}\,Y_1^{-1}\right) = \frac{\hbar}{4} + \frac{\hbar\sqrt{2}}{4\sqrt{2}} + \frac{\hbar\sqrt{2}}{4\sqrt{2}} + \frac{\hbar}{4} = \hbar$

$\hat{H}$-ren autobalioak $\hat{L}_x$-renak dira baina autofuntzioak: $E = \alpha\, l_x^6$

- $l=1$ denean $\hat{L}_x$-ren autobalio eta autofuntzioak hauek dira:

$$\lambda_1 = 0,\ \psi_1 = \frac{1}{\sqrt{2}}(Y_1^1 - Y_1^{-1})\ ;\ \psi_2 = \frac{1}{2}(Y_1^1 + \sqrt{2}Y_1^0 + Y_1^{-1})\quad \lambda_2 = \hbar\ ;$$

$$\psi_3 = \frac{1}{2}(Y_1^1 - \sqrt{2}Y_1^0 + Y_1^{-1})\qquad \lambda_3 = -\hbar$$

- Orduan Ψ L_x-ren oinarrian garatuz:

$$\Psi(x,0) = \psi_2 \xrightarrow{t} \Psi(x,t) = \psi_2\, e^{-i\alpha\hbar^5 t}$$ Geldikorra

Beraz denboran $\langle L_x\rangle(t) = \text{kte} = \hbar$ (guztira zehaztuta dago $l_x = \hbar$)

10.)

Sistema baten momentu angeluarra (zehatza) $\sqrt{2}\hbar$ da. $\Rightarrow$ $L^2 = 2\hbar^2$ ($l=1$ da)

- $\hat{H} = \frac{w_0}{\hbar}(\hat{L}_u^2 - \hat{L}_v^2)$ $\Rightarrow$ $\hat{L}_u = \hat{L}_x \cos 45 - \hat{L}_z \sin 45$ ($\hat{u} = (\hat{\imath}-\hat{k})/\sqrt{2}$

$$\hat{L}_v = \vec{\hat{L}}\cdot\hat{v} = \hat{L}_x \cos 45 + \hat{L}_z \sin 45 = \frac{1}{\sqrt{2}}(\hat{L}_x + \hat{L}_z)\ ;\ t=0\quad \langle \hat{L}^2\rangle = 2\hbar^2$$

- Beraz $\Rightarrow$ $$\hat{H} = \frac{w_0}{\hbar}\left(\cancel{\frac{\hat{L}_x^2}{2}} + \cancel{\frac{\hat{L}_z^2}{2}} - \frac{\hat{L}_x\hat{L}_z}{2} - \frac{\hat{L}_z\hat{L}_x}{2} - \cancel{\frac{\hat{L}_x^2}{2}} - \cancel{\frac{\hat{L}_z^2}{2}} - \frac{\hat{L}_x\hat{L}_z}{2} - \frac{\hat{L}_z\hat{L}_x}{2}\right) =$$

$$- \frac{w_0}{\hbar}(\hat{L}_x\hat{L}_z + \hat{L}_z\hat{L}_x)$$

- $$[\hat{H}, \hat{L}^2] = \left[-\frac{w_0}{\hbar}(\hat{L}_x\hat{L}_z + \hat{L}_z\hat{L}_x),\ \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2\right] = -\frac{w_0}{\hbar}\Big([\hat{L}_x\hat{L}_z, \hat{L}_x^2] + [\hat{L}_x\hat{L}_z, \hat{L}_y^2] +$$

$$[\hat{L}_x\hat{L}_z, \hat{L}_z^2] + [\hat{L}_z\hat{L}_x, \hat{L}_x^2] + [\hat{L}_z\hat{L}_x, \hat{L}_y^2] + [\hat{L}_z\hat{L}_x, \hat{L}_z^2]\Big) = -\frac{w_0}{\hbar}\big(\hat{L}_x[\hat{L}_z, \hat{L}_x^2] +$$

$$\cancel{[\hat{L}_x, \hat{L}_x^2]}\hat{L}_z + \hat{L}_x[\hat{L}_z, \hat{L}_y^2] + [\hat{L}_x, \hat{L}_y^2]\hat{L}_z + \cancel{\hat{L}_x[\hat{L}_z, \hat{L}_z^2]} + [\hat{L}_x, \hat{L}_z^2]\hat{L}_z +$$

$$\hat{L}_z\cancel{[\hat{L}_x, \hat{L}_x^2]} + [\hat{L}_z, \hat{L}_x^2]\hat{L}_x + \hat{L}_z[\hat{L}_x, \hat{L}_y^2] + [\hat{L}_z, \hat{L}_y^2]\hat{L}_x + \hat{L}_z[\hat{L}_x, \hat{L}_z^2] +$$

$$\cancel{[\hat L_z, \hat L_z^2]\hat L_x}) = -\frac{\omega_0}{\hbar}\Big(\hat L_x^2[\hat L_z,\hat L_x] + \hat L_x[\hat L_z,\hat L_x]\hat L_x + \hat L_x\hat L_y[\hat L_z,\hat L_y] + \hat L_x[\hat L_z,\hat L_y]\hat L_y +$$

$$\hat L_y[\hat L_x,\hat L_y]\hat L_z + [\hat L_x,\hat L_y]\hat L_y\hat L_z + \hat L_z[\hat L_x,\hat L_z]\hat L_z + [\hat L_x,\hat L_z]\hat L_z^2 + \hat L_x[\hat L_z,\hat L_x]\hat L_x +$$

$$[\hat L_z,\hat L_x]\hat L_x^2 + \hat L_z\hat L_y[\hat L_x,\hat L_y] + \hat L_z[\hat L_x,\hat L_y]\hat L_y + \hat L_y[\hat L_z,\hat L_y]\hat L_x + [\hat L_z,\hat L_y]\hat L_y\hat L_x +$$

$$\hat L_z^2[\hat L_x,\hat L_z] + \hat L_z[\hat L_x,\hat L_z]\hat L_z\Big) = -\frac{\omega_0}{\hbar}\Big(i\hbar\cancel{\hat L_x^2\hat L_y} + i\hbar\cancel{\hat L_x\hat L_y}\hat L_x - i\hbar\cancel{\hat L_x\hat L_y\hat L_x} - i\hbar\cancel{\hat L_x^2\hat L_y} +$$

$$+ i\hbar\cancel{\hat L_y\hat L_z^2} + i\hbar\hat L_z\cancel{\hat L_y}\hat L_z - i\hbar\cancel{\hat L_z}\hat L_y\hat L_z - i\hbar\cancel{\hat L_y\hat L_z^2} + i\hbar\hat L_x\cancel{\hat L_y}\hat L_x + i\hbar\cancel{\hat L_y\hat L_x^2} + i\hbar\cancel{\hat L_z}\hat L_y\hat L_z +$$

$$i\hbar\cancel{\hat L_z^2\hat L_y} - i\hbar\cancel{\hat L_y\hat L_x^2} - i\hbar\hat L_x\cancel{\hat L_y\hat L_x} - i\hbar\cancel{\hat L_z^2\hat L_y} - i\hbar\hat L_z\cancel{\hat L_y\hat L_z}\Big) = 0$$

Beraz $\frac{d\langle \hat L^2\rangle}{dt} = 0$ izango da, $\hat H$ eta $\hat L^2$ trukakorrak direlako,

ez da aldatuko $\langle \hat L^2\rangle = 2\hbar^2$

$l=1$ denez $\{Y_1^{-1}, Y_1^{1}, Y_1^{0}\}$ oinarrian garatuta egongo da egoera eta hala eta denboraren garapena egin $\hat H$ eta $\hat L^2$ oinarri komuna dutenez beti lortuko dugu $l=1$

- $\Psi(t=0) = \frac{1}{\sqrt2}[Y_1^1(\theta,\phi) - Y_1^{-1}(\theta,\phi)]$

Lehenengo ikusiko dugu ea $\hat L_x$ eta $\hat H$ trukakorrak diren:

$$[\hat L_x,\hat H] = [\hat L_x, -\frac{\omega_0}{\hbar}(\hat L_x\hat L_z + \hat L_z\hat L_x)] = -\frac{\omega_0}{\hbar}([\hat L_x,\hat L_x\hat L_z] + [\hat L_x,\hat L_z\hat L_x]) =$$

$$-\frac{\omega_0}{\hbar}(\hat L_x[\hat L_x,\hat L_z] + \cancel{[\hat L_x,\hat L_x]}\hat L_z + \hat L_z\cancel{[\hat L_x,\hat L_x]} + [\hat L_x,\hat L_z]\hat L_x) = -\frac{\omega_0}{\hbar}(-i\hbar\hat L_x\hat L_y - i\hbar\hat L_y\hat L_x) =$$

$\omega_0 i(\hat L_x\hat L_y + \hat L_y\hat L_x) \neq 0 \Rightarrow$ ez dira trukakorrak.

$$\langle \hat L_x\rangle_{t=0} = (\Psi, \hat L_x\Psi) = \frac{1}{\sqrt2}\Big(Y_1^1 - Y_1^{-1}, \frac{(\hat L_+ + \hat L_-)}{2}\cdot\frac{1}{\sqrt2}(Y_1^1 - Y_1^{-1})\Big) = \frac14(Y_1^1 - Y_1^{-1}, \hat L_+ Y_1^1) +$$

$$-\frac14(Y_1^1 - Y_1^{-1}, \hat L_+ Y_1^{-1}) + \frac14(Y_1^1 - Y_1^{-1}, \hat L_- Y_1^1) - \frac14(Y_1^1 - Y_1^{-1}, \hat L_- Y_1^{-1}) =$$

$$\frac14\cancel{(Y_1^1 - Y_1^{-1}, \hbar\cdot 0)} - \frac14(Y_1^1 - \cancel{Y_1^{-1}, \hbar\sqrt{l(l+1)}\,Y_1^0}) + \frac14(Y_1^1 - \cancel{Y_1^{-1}, \hbar\sqrt2\, Y_1^0}) +$$

$l=1$

$$-\frac14(Y_1^1 - \cancel{Y_1^{-1}, \hbar\cdot 0)} = 0$$

Garatuko dugu $\Psi(t=0)$ denboran. Lehenago $\hat H$-ren autofuntzioak kalkulatuko ditugu.

$$\left(\frac{d\langle \hat{L}_x \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{L}_x] \rangle_\psi = \frac{-i}{\hbar^2} w_0 i \ \langle \hat{L}_x \hat{L}_y + \hat{L}_y \hat{L}_x \rangle_\psi = \frac{w_0}{\hbar^2} (\langle \hat{L}_x \hat{L}_y + \hat{L}_y \hat{L}_x \rangle_\psi) \right)$$

$$\hat{L}_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \hat{L}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad l=1 \quad \{ Y_1^1, Y_1^0, Y_1^{-1} \} \text{ ananian}$$

$$\hat{H} = -\frac{w_0}{\hbar} (\hat{L}_x \hat{L}_z + \hat{L}_z \hat{L}_x) = -\frac{w_0}{\cancel{\hbar}} \cancel{\hbar} \left(\frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right) =$$

$$-\frac{w_0 \hbar}{\sqrt{2}} \left(\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \right) = -\frac{w_0 \hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \cancel{= i \hbar w_0 i \hat{L}_y}$$

$$\tilde{\lambda} = \frac{\lambda}{w_0 \hbar / \sqrt{2}} \Rightarrow \begin{vmatrix} -\tilde{\lambda} & 1 & 0 \\ 1 & -\tilde{\lambda} & -1 \\ 0 & -1 & -\tilde{\lambda} \end{vmatrix} = -\tilde{\lambda}^3 + 2\tilde{\lambda} = \tilde{\lambda}(2 - \tilde{\lambda}^2) = 0 \Rightarrow \tilde{\lambda}_1 = 0 \ , \ \tilde{\lambda}_2 = \sqrt{2}, \ \tilde{\lambda}_3 = -\sqrt{2}$$

- $\tilde{\lambda}_1 = 0 \Rightarrow \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} b \\ a-c \\ -b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{matrix} b=0 \\ \cancel{a-b=0} \\ a=c \end{matrix} \qquad \varphi_1 = \frac{(Y_1^1 + Y_1^{-1})}{\sqrt{2}}$

  $(\lambda = 0)$

- $\tilde{\lambda}_2 = \sqrt{2} \quad (\lambda = w_0 \hbar \cdot 2) \Rightarrow \begin{pmatrix} -\sqrt{2} & 1 & 0 \\ 1 & -\sqrt{2} & -1 \\ 0 & -1 & -\sqrt{2} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} -\sqrt{2}a + b \\ a - \sqrt{2}b - c \\ -b - \sqrt{2}c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{matrix} b = \sqrt{2}a \\ b = -\sqrt{2}c \\ a = -c \end{matrix}$

$$\varphi_2 = \frac{(Y_1^1 + \sqrt{2} Y_1^0 - Y_1^{-1})}{2}$$

- $\tilde{\lambda}_3 = -\sqrt{2} \quad (\lambda = -2 w_0 \hbar) \Rightarrow \begin{pmatrix} \sqrt{2} & 1 & 0 \\ 1 & \sqrt{2} & -1 \\ 0 & -1 & \sqrt{2} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} \sqrt{2}a + b \\ a + \sqrt{2}b - c \\ -b + \sqrt{2}c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{matrix} b = -\sqrt{2}a \\ b = \sqrt{2}c \\ a = -c \end{matrix}$

$$\varphi_3 = \frac{1}{2} (Y_1^1 - \sqrt{2} Y_1^0 - Y_1^{-1})$$

$$\Rightarrow \psi(0) = \frac{1}{\sqrt{2}} (\varphi_2 + \varphi_3) \Rightarrow \psi(t) = \frac{1}{\sqrt{2}} (\varphi_2 e^{-2w_0 i t} + \varphi_3 e^{2w_0 i t}) =$$

$$\frac{1}{\sqrt{2}} \left(\frac{e^{-2w_0 i t}}{2} (Y_1^1 + \sqrt{2} Y_1^0 - Y_1^{-1}) + \frac{e^{2w_0 i t}}{2} (Y_1^1 + \sqrt{2} Y_1^0 - Y_1^{-1}) \right) =$$

$\frac{1}{\sqrt{2}}(Y_1^1\cos 2w_0t - Y_1^{-1}\cos 2w_0t - \sqrt{2}i\, Y_1^0 \sin 2w_0t)$

$\boxed{\langle \hat{L}_x\rangle_\Psi} = (\Psi, \hat{L}_x\Psi) = \cancel{\tfrac{1}{2}}(\Psi, (\frac{\hat{L}_+ + \hat{L}_-}{2})\Psi) = \frac{1}{4}(Y_1^1\cos 2w_0t - Y_1^{-1}\cos 2w_0t +$

$-\sqrt{2}i\sin 2w_0t\, Y_1^0, \cos \cancel{2w_0t}\cdot 0 - \cos 2w_0t\, \hbar\sqrt{2}\, Y_1^0 - \sqrt{2}i\sin 2w_0t\, \hbar\sqrt{2}Y_1^1) +$

$\frac{1}{4}(Y_1^1\cos 2w_0t - Y_1^{-1}\cos 2w_0t - \sqrt{2}i\sin 2w_0t\, Y_1^0, \hbar\sqrt{2}\cos 2w_0t\, Y_1^0 - \sqrt{2}i\sqrt{2}\hbar\sin 2w_0t\, Y_1^{-1}) =$

$\frac{1}{4}(-2i\hbar\sin \cancel{2w_0t}\cos 2w_0t + 2i\hbar\sin\cancel{2w_0t\cos}\, 2w_0t - \sqrt{2}\sqrt{2}\hbar i\sin 2w_0t\cos 2w_0t +$

$2i\hbar\sin 2w_0t\cos 2w_0t) = \boxed{0}$

11)

$\hat{L}^2$ eta $\hat{L}_z$ behagarriak neurtu: $l=1$ eta $m=1$ lortu.

$\Psi(t=0) = Y_1^1$

Gero $\hat{L}_y$ neurtu $\Rightarrow$ Garatu $\Psi(t=0)$ $\hat{L}_y$-ren autofuntzioetan eta ikusi

autobalio bakoitzaren probabilitatea:

- $l=1 \Rightarrow L_y = \frac{i\hbar}{\sqrt{2}}\begin{pmatrix}0 & -1 & 0\\ 1 & 0 & -1\\ 0 & 1 & 0\end{pmatrix} \Rightarrow \varphi_1 = \frac{1}{\sqrt{2}}(Y_1^1 + Y_1^{-1}) \quad \lambda_1 = 0$

$\varphi_2 = \frac{1}{2}(-Y_1^1 + \sqrt{2}i\, Y_1^0 + Y_1^{-1}) \quad \lambda_2 = -\hbar, \quad \varphi_3 = \frac{1}{2}(Y_1^1 + \sqrt{2}i\, Y_1^0 - Y_1^{-1}) \quad \lambda_3 = \hbar$

- $\lambda = 0$ lortzeko probabilitatea $\Rightarrow$ $P(\lambda=0) = |c_0|^2$; $c_0 = (\varphi_1, Y_1^1) = (\frac{Y_1^1}{\sqrt{2}} + \frac{Y_1^{-1}}{\sqrt{2}}, Y_1^1) =$

$\frac{1}{\sqrt{2}} \Rightarrow P(\lambda=0) = \frac{1}{2}$

- $P(\lambda=\hbar) = |c_3|^2$; $c_3 = (\varphi_3, Y_1^1) = \frac{1}{2}(Y_1^1 + \sqrt{2}i\, Y_1^0 - Y_1^{-1}, Y_1^1) = \frac{1}{2} \Rightarrow P(\hbar) = \frac{1}{4}$

- $P(\lambda=-\hbar) = |c_2|^2$; $c_2 = (\varphi_2, Y_1^1) = \frac{1}{2}(-Y_1^1 + \sqrt{2}i\, Y_1^0 + Y_1^{-1}, Y_1^1) = -\frac{1}{2} \Rightarrow P(-\hbar) = \frac{1}{4}$

12)

$\hat{L}^2, \hat{L}_y \Rightarrow 2\hbar^2$ eta $\hbar \Rightarrow l=1, m=1 \Rightarrow \Psi(t=0) = Y_1^1$

$\hat{L}_x$ neurtu $\Rightarrow l=1 \Rightarrow L_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \Rightarrow \varphi_1 = \frac{1}{\sqrt{2}}(Y_1^1 - Y_1^{-1}) \quad \lambda_1 = 0$

$\varphi_2 = \frac{1}{2}(Y_1^1 + \sqrt{2}Y_1^0 + Y_1^{-1}) \quad \lambda_2 = \hbar \; ; \quad \varphi_3 = \frac{1}{2}(Y_1^1 - \sqrt{2}Y_1^0 + Y_1^{-1}) \quad \lambda_3 = -\hbar$

$P(\hbar) = |c_2|^2 \; ; \quad c_2 = (\varphi_2, \Psi) = \frac{1}{2}(Y_1^1 + \sqrt{2}Y_1^0 + Y_1^{-1}, Y_1^1) = \frac{1}{2} \Rightarrow P(\hbar) = \frac{1}{4}$

13)

- $\hat{L} = \sqrt{2}\hbar \Rightarrow \hat{L}^2 = 2\hbar^2 \Leftrightarrow l = 1 \Rightarrow \phi = \alpha\phi_{+1} + \beta\phi_0 + \gamma\phi_{-1} = \alpha Y_1^1 + \beta Y_1^0 + \gamma Y_1^{-1}$ $(\alpha, \beta, \gamma \in \mathbb{C})$ (Kontuan hartuz $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$)

- $\langle \hat{L}_x^2 \rangle = \langle \phi, \hat{L}_x^2 \phi \rangle = \langle \alpha Y_1^1 + \beta Y_1^0 + \gamma Y_1^{-1}, \frac{(\hat{L}_+ + \hat{L}_-)^2}{4}(\alpha Y_1^1 + \beta Y_1^0 + \gamma Y_1^{-1}) \rangle =$

$\frac{1}{4}\langle \alpha Y_1^1 + \beta Y_1^0 + \gamma Y_1^{-1}, \hat{L}_+^2\phi + \hat{L}_-^2\phi + \hat{L}_+\hat{L}_-\phi + \hat{L}_-\hat{L}_+\phi \rangle = \frac{1}{4}\langle \alpha Y_1^1 + \beta Y_1^0 + \gamma Y_1^{-1},$

$\underbrace{\cancel{\alpha \hat{L}_+^2 Y_1^1}}_{=0} + \underbrace{\cancel{\beta \hat{L}_+^2 Y_1^0}}_{=0} + \gamma \hat{L}_+^2 Y_1^{-1} + \alpha \hat{L}_-^2 Y_1^1 + \underbrace{\cancel{\beta \hat{L}_-^2 Y_1^0}}_{=0} + \underbrace{\cancel{\gamma \hat{L}_-^2 Y_1^{-1}}}_{=0} + \hat{L}_+\hat{L}_-\alpha Y_1^1 +$

$\beta \hat{L}_+\hat{L}_- Y_1^0 + \gamma \underbrace{\cancel{\hat{L}_+\hat{L}_- Y_1^{-1}}}_{=0} + \alpha \underbrace{\cancel{\hat{L}_-\hat{L}_+ Y_1^1}}_{=0} + \beta \hat{L}_-\hat{L}_+ Y_1^0 + \gamma \hat{L}_-\hat{L}_+ Y_1^{-1} \rangle =$

$\frac{1}{4}\langle \alpha Y_1^1 + \beta Y_1^0 + \gamma Y_1^{-1}, \gamma\hbar^2 2 Y_1^1 + \alpha\hbar^2 2 Y_1^{-1} + \alpha\hbar^2 \cdot 2 Y_1^1 + \beta\hbar^2 2 Y_1^0 + \beta\hbar^2 \cdot 2 Y_1^0 +$

$\gamma\hbar^2 2 Y_1^{-1} \rangle = \frac{1}{4}(\gamma^* 2\hbar^2\alpha + 2\hbar^2|\alpha|^2 + 2\hbar^2|\beta|^2 + 2|\beta|^2\hbar^2 + 2|\gamma|^2\hbar^2 + 2\hbar^2\alpha^*\gamma) =$

$\frac{1}{4}(2\hbar^2\alpha^*\gamma + 2\hbar^2|\alpha|^2 + 2|\gamma|^2\hbar^2 + 4\hbar^2|\beta|^2 + 2\hbar\gamma^*\alpha) = \frac{\hbar^2}{2}(|\alpha|^2 + |\gamma|^2 + 2|\beta|^2 + \alpha^*\gamma + \gamma^*\alpha)$

- $\langle \hat{L}_y^2 \rangle = \langle \phi, \hat{L}_y^2 \phi \rangle = \langle \phi, \frac{(\hat{L}_+ - \hat{L}_-)^2}{-4}\phi \rangle = \langle \phi, \left(-\frac{\hat{L}_+^2}{4} - \frac{\hat{L}_-^2}{4} + \frac{\hat{L}_+\hat{L}_-}{4} + \frac{\hat{L}_-\hat{L}_+}{4}\right)\phi \rangle =$

$\frac{1}{4}\langle \phi, -\gamma\hat{L}_+^2 Y_1^{-1} - \alpha\hat{L}_-^2 Y_1^1 + \hat{L}_+\hat{L}_-\alpha Y_1^1 + \beta\hat{L}_+\hat{L}_- Y_1^0 + \beta\hat{L}_-\hat{L}_+ Y_1^0 + \gamma\hat{L}_-\hat{L}_+ Y_1^{-1} \rangle =$

$$\frac{1}{4}\left(4|\beta|^2\hbar^2+2|\gamma|^2\hbar^2+|\alpha|^2\hbar^2\cdot 2-2\hbar^2\alpha^*\gamma-2\alpha\hbar^2\gamma^*\right)=\frac{\hbar^2}{2}\left(2|\beta|^2+|\gamma|^2+|\alpha|^2+\right.$$

$$\left.-\alpha^*\gamma-\gamma^*\alpha\right)$$

- $$\langle\hat{L}_z^2\rangle=(\phi,\ \hat{L}_z^2\,\phi)=\left(\alpha Y_1^1+\beta Y_1^0+\gamma Y_1^{-1},\ \hat{L}_z(\hat{L}_z(\alpha Y_1^1+\beta Y_1^0+\gamma Y_1^{-1}))\right)=$$

$$\left(\alpha Y_1^1+\beta Y_1^0+\gamma Y_1^{-1},\ \alpha\hbar^2 Y_1^1+\beta\cdot 0\,Y_1^0+\gamma\hbar^2(-1)^2 Y_1^{-1}\right)=|\alpha|^2\hbar^2+|\gamma|^2\hbar^2=\hbar^2\left(|\alpha|^2+|\gamma|^2\right)$$

- $$\langle\hat{L}\rangle=\langle\hat{L}_x\rangle\hat{i}+\langle\hat{L}_y\rangle\hat{j}+\langle\hat{L}_z\rangle\hat{k}$$

* $$\langle\hat{L}_x\rangle=\left(\alpha\phi_{+1}+\beta\phi_0+\gamma\phi_{-1},\ \frac{(\hat{L}_++\hat{L}_-)}{2}\,\phi\right)=\frac{1}{2}\left(\alpha Y_1^1+\beta Y_1^0+\gamma Y_1^{-1},\right.$$

$$\left.\hat{L}_+\alpha Y_1^1+\beta\hat{L}_+Y_1^0+\gamma\hat{L}_+Y_1^{-1}+\hat{L}_-\alpha Y_1^1+\beta\hat{L}_-Y_1^0+\gamma\hat{L}_-Y_1^{-1}\right)=$$

$$\frac{1}{2}\left(\alpha Y_1^1+\beta Y_1^0+\gamma Y_1^{-1},\ \alpha\cdot 0+\beta\hbar\sqrt{2}\,Y_1^1+\gamma\hbar\sqrt{2}\,Y_1^0+\alpha\hbar\sqrt{2}\,Y_1^0+\beta\hbar\sqrt{2}\,Y_1^{-1}+0\right)=$$

$$\frac{1}{2}\left(\hbar\beta\sqrt{2}\,\alpha^*+\beta^*\hbar\sqrt{2}\,(\alpha+\gamma)+\gamma^*\beta\hbar\sqrt{2}\right)=\frac{\hbar}{\sqrt{2}}\left(\beta\alpha^*+\beta^*\alpha+\beta^*\gamma+\gamma^*\beta\right)$$

* $$\langle\hat{L}_y\rangle=\left(\alpha\phi_{+1}+\beta\phi_0+\gamma\phi_{-1},\ \frac{\hat{L}_+-\hat{L}_-}{2i}\,\phi\right)=\frac{1}{2i}\left(\alpha Y_1^1+\beta Y_1^0+\gamma Y_1^{-1},\right.$$

$$\left.\hat{L}_+\alpha Y_1^1+\beta\hat{L}_+Y_1^0+\gamma\hat{L}_+Y_1^{-1}-\alpha\hat{L}_-Y_1^1-\beta\hat{L}_-Y_1^0-\gamma\hat{L}_-Y_1^{-1}\right)=$$

$$\frac{1}{2i}\left(\alpha Y_1^1+\beta Y_1^0+\gamma Y_1^{-1},\ \alpha\cdot 0+\beta\hbar\sqrt{2}\,Y_1^1+\gamma\hbar\sqrt{2}\,Y_1^0-\alpha\hbar\sqrt{2}\,Y_1^0-\beta\hbar\sqrt{2}\,Y_1^{-1}\right)=$$

$$\frac{1}{2i}\left(\alpha^*\beta\hbar\sqrt{2}+\hbar\sqrt{2}\,\beta^*(\gamma-\alpha)-\gamma^*\hbar\sqrt{2}\,\beta\right)=\frac{-i\hbar}{\sqrt{2}}\left(\alpha^*\beta+\beta^*\gamma-\beta^*\alpha-\gamma^*\beta\right)$$

* $$\langle\hat{L}_z\rangle=\left(\alpha Y_1^1+\beta Y_1^0+\gamma Y_1^{-1},\ \hat{L}_z\,\phi\right)=\left(\alpha Y_1^1+\beta Y_1^0+\gamma Y_1^0,\ \hbar\alpha Y_1^1+0-\hbar\gamma Y_1^{-1}\right)=$$

$$\hbar\left(|\alpha|^2-|\gamma|^2\right)$$

14)

$$\psi(r,\theta,\phi) = \frac{1}{4}\left(e^{i\varphi}\sin\theta + \cos\theta\right)R(r) \Rightarrow \int_0^{\infty} |R(r)|^2 r^2 dr = 1$$

$\hat{L}_x$?

$$\psi(r,\theta,\phi) = \frac{R(r)}{4}\left(-2\sqrt{\frac{2\pi}{3}}\, Y_1^1 + 2\sqrt{\frac{\pi}{3}}\, Y_1^0\right) = \frac{R(r)}{2}\sqrt{\frac{\pi}{3}}\left(Y_1^0 - \sqrt{2}\,Y_1^1\right)$$

Normalizatu $\Rightarrow \psi = \sqrt{\frac{12}{3\cancel{\pi}}} \cdot \frac{R(r)}{2}\sqrt{\frac{\cancel{\pi}}{3}}\left(Y_1^0 - \sqrt{2}\,Y_1^1\right) = \frac{1}{\sqrt{3}} R(r)\left(Y_1^0 - \sqrt{2}\,Y_1^1\right)$

$l=1$ denean $\Rightarrow$ $\hat{L}_x$-ren autobalioak eta autofuntzioak hauek dira:

$\lambda_1 = 0$, $\varphi_1 = \frac{1}{\sqrt{2}}\left(Y_1^1 - Y_1^{-1}\right)$; $\lambda_2 = \hbar$, $\varphi_2 = \frac{1}{2}\left(Y_1^1 + \sqrt{2}\,Y_1^0 + Y_1^{-1}\right)$

$\lambda_3 = -\hbar$, $\varphi_3 = \frac{1}{2}\left(Y_1^1 - \sqrt{2}\,Y_1^0 + Y_1^{-1}\right)$

r-rekiko (θ, φ)

- $P(0) = \int |C_0|^2 dr \rightarrow C_0 = (\varphi_1, \psi) = \frac{1}{\sqrt{2}}\left(Y_1^1 - Y_1^{-1}, \frac{1}{\sqrt{3}}\left(Y_1^0 - \sqrt{2}\,Y_1^1\right)\right) = \frac{1}{\sqrt{6}}(-\sqrt{2}) = -\frac{1}{\sqrt{3}}$

$$P(0) = \int_{-\infty}^{\infty} \left|\frac{1}{\sqrt{3}}\right|^2 |R(r)|^2 dr\, r^2 = \frac{1}{3}$$

- $P(\hbar) = \int |C_1|^2 dr \rightarrow C_1 = (\varphi_2, \psi) = \frac{1}{2}\left(Y_1^1 + \sqrt{2}\,Y_1^0 + Y_1^{-1}, \frac{1}{\sqrt{3}}\left(Y_1^0 - \sqrt{2}\,Y_1^1\right)\right) = \frac{1}{2\sqrt{3}}\left(\sqrt{2} - \sqrt{2}\right) = 0$

$P(\hbar) = 0$

- $P(-\hbar) = \int |C_2|^2 dr \rightarrow C_2 = (\varphi_3, \psi) = \frac{1}{2}\left(Y_1^1 - \sqrt{2}\,Y_1^0 + Y_1^{-1}, \frac{1}{\sqrt{3}}\left(Y_1^0 - \sqrt{2}\,Y_1^1\right)\right) =$

$$\frac{1}{2\sqrt{3}}\left(-\sqrt{2} - \sqrt{2}\right) = -\frac{2\sqrt{2}}{2\sqrt{3}} = -\frac{\sqrt{2}}{\sqrt{3}} \Rightarrow P(-\hbar) = \int_0^{\infty} |C_2|^2 |R(r)|^2 r^2 dr = \frac{2}{3}$$

15)

$$\psi(r,\theta,\phi) = \frac{e^{-2r}}{r^2}(x+r)$$

L_x^{23} neurtu $\Rightarrow$ $\hat{L}_x^{23}$ eta $\hat{L}_x$-ren autofuntzioak berdinak ($L_x^{23} = (L_x)^{23}$)

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

$\frac{e^{-2r}}{r}\left(\sqrt{4\pi}\,Y_0^0+\sqrt{\frac{2\pi}{3}}\,(Y_1^{-1}-Y_1^1)\right) \rightarrow$ Normalizatu $(\Psi,\Psi)=\left(4\pi+2\cdot\frac{2\pi}{3}\right)\int_0^\infty e^{-4r}dr=$

$\frac{16\pi}{3}\cdot\frac{1}{4}=\frac{4\pi}{3} \Rightarrow \qquad \Psi=\sqrt{\frac{3}{4\pi}}\,\frac{e^{-2r}}{r}\left(\sqrt{4\pi}\,Y_0^0+\sqrt{\frac{2\pi}{3}}\,(Y_1^{-1}-Y_1^1)\right)=$

$\sqrt{3}\,\frac{e^{-2r}}{r}\left(Y_0^0+\frac{1}{\sqrt{6}}(Y_1^{-1}-Y_1^1)\right)$

Y_0^0 $\hat{L}_x$-ren autofuntzioa da $\rightarrow l_x=0$: $P(l_x=0)=(\sqrt{3})^2\int_0^\infty \frac{e^{-4r}}{r^2}r^2dr=\frac{3}{4}$

$l=1$ denean $\frac{1}{\sqrt{2}}(Y_1^1-Y_1^{-1})$ $\hat{L}_x$-ren autofuntzioa da $\lambda=0 \Rightarrow$

Beraz hau datekean $L_x{}^{23}$-ren balio bakarra 0 da, %100-eko probabilitatearekin.

16)

$l>2 \rightarrow \qquad |m|\leq l \qquad \psi(r)=\frac{e^{-\alpha r}}{r}\left(Y_l^l+2iY_l^{l-1}-Y_l^{l-2}\right)$

$(\alpha>0) \qquad \Delta L_x\,? \qquad \Delta L_x^2=\langle L_x^2\rangle-\langle L_x\rangle$

Normalizatu $\Rightarrow \quad (\psi,\psi)=(1+4+1)\int_0^\infty \frac{e^{-2\alpha r}}{\cancel{r^2}}\cancel{r^2}dr=\frac{6}{2\alpha}=\frac{3}{\alpha}$

Orduan $\Rightarrow \quad \psi(r)=\sqrt{\frac{\alpha}{3}}\,\frac{e^{-\alpha r}}{r}\left(Y_l^l+2iY_l^{l-1}-Y_l^{l-2}\right)$

$\langle\hat{L}_x\rangle=\frac{\alpha}{3}\left(\frac{e^{-\alpha r}}{r}(Y_l^l+2iY_l^{l-1}-Y_l^{l-2}),\ \frac{e^{-\alpha r}}{r}\cdot\frac{(\hat{L}_++\hat{L}_-)}{2}(Y_l^l+2iY_l^{l-1}-Y_l^{l-2})\right)=$

$\frac{1}{2}\cdot\frac{\cancel{\alpha}}{3}\cdot\frac{1}{2\cancel{\alpha}}\Big(Y_l^l+2iY_l^{l-1}-Y_l^{l-2},\ 0+2i\hbar\sqrt{l(l+1)-l(l-1)}\,Y_l^l-\hbar\sqrt{l(l+1)-(l-2)(l-1)}\,Y_l^{l-1}+$

$\hbar\sqrt{l(l+1)-l(l-1)}\,Y_l^{l-1}+2i\hbar\sqrt{l(l+1)-(l-1)(l-2)}\,Y_l^{l-2}-\hbar\sqrt{l(l+1)-(l-2)(l-3)}\,Y_l^{l-3}\Big)=$

$\frac{1}{12}\left(2i\hbar\cancel{\sqrt{l(l+1)-l(l-1)}}+2i\hbar\sqrt{l(l+1)-(l-2)(l-1)}-2i\hbar\cancel{\sqrt{l(l+1)-l(l-1)}}-2i\hbar\sqrt{l(l+1)-(l-1)(l-2)}\right)=0$

$$\langle \hat{L}_x^2 \rangle = \frac{\alpha}{3}\left(\frac{e^{-\alpha r}}{r}(Y_\lambda^\lambda + 2i Y_\lambda^{\lambda-1} - Y_\lambda^{\lambda-2}), \frac{e^{-\alpha r}}{r} \frac{(\hat{L}_+ + \hat{L}_-)^2}{4}(Y_\lambda^\lambda + 2iY_\lambda^{\lambda-1} - Y_\lambda^{\lambda-2})\right) =$$

$$\frac{1}{4}\cdot\frac{1}{6}\Big(Y_\lambda^\lambda + 2iY_\lambda^{\lambda-1} - Y_\lambda^{\lambda-2}, \cancel{\hat{L}_+^2 Y_\lambda^\lambda + 2i\hat{L}_+^2 Y_\lambda^{\lambda-1}} - \hat{L}_+^2 Y_\lambda^{\lambda-2} + \hat{L}_-^2 Y_\lambda^\lambda +$$

$$2i\hat{L}_-^2 Y_\lambda^{\lambda-1} - \hat{L}_-^2 Y_\lambda^{\lambda-2} + \hat{L}_+\hat{L}_- Y_\lambda^\lambda + 2i\hat{L}_+\hat{L}_- Y_\lambda^{\lambda-1} - \hat{L}_+\hat{L}_- Y_\lambda^{\lambda-2} + \hat{L}_-\cancel{\hat{L}_+ Y_\lambda^\lambda} +$$

$$2i\hat{L}_-\hat{L}_+ Y_\lambda^{\lambda-1} - \hat{L}_-\hat{L}_+ Y_\lambda^{\lambda-2}\Big) = \frac{1}{24}\Big(Y_\lambda^\lambda + 2iY_\lambda^{\lambda-1} - Y_\lambda^{\lambda-2}, -\hbar\sqrt{\lambda(\lambda+1)-(\lambda-2)(\lambda-3)}\,\hbar\sqrt{\lambda(\lambda+1)-\lambda(\lambda-1)}\,Y_\lambda^\lambda +$$

$$\hbar^2\sqrt{\lambda(\lambda+1)-\lambda(\lambda-1)}\sqrt{\lambda(\lambda+1)-(\lambda-1)(\lambda-2)}\,Y_\lambda^{\lambda-2} + 2i\hbar^2\sqrt{\lambda(\lambda+1)-(\lambda-1)(\lambda-2)}\sqrt{\lambda(\lambda+1)-(\lambda-2)(\lambda-3)}\,Y_\lambda^{\lambda-3} +$$

$$-\hbar^2\sqrt{\lambda(\lambda+1)-(\lambda-2)(\lambda-3)}\sqrt{\lambda(\lambda+1)-(\lambda-3)(\lambda-4)}\,Y_\lambda^{\lambda-4} + \hbar^2\left(\sqrt{\lambda(\lambda+1)-\lambda(\lambda-1)}\right)^2 Y_\lambda^\lambda + 2i\hbar^2\left(\sqrt{\lambda(\lambda+1)-(\lambda-1)(\lambda-2)}\right)^2 Y_\lambda^{\lambda-1} +$$

$$-\hbar^2\left(\sqrt{\lambda(\lambda+1)-(\lambda-2)(\lambda-3)}\right)^2 Y_\lambda^{\lambda-2} + 2i\hbar^2\left(\sqrt{\lambda(\lambda+1)-\lambda(\lambda-1)}\right)^2 Y_\lambda^{\lambda-1} - \hbar^2\left(\sqrt{\lambda(\lambda+1)-(\lambda-1)(\lambda-2)}\right)Y_\lambda^{\lambda-2}\Big) =$$

$$\frac{1}{24}\Big(-\hbar^2\sqrt{\lambda(\lambda+1)-(\lambda-2)(\lambda-3)}\sqrt{\lambda(\lambda+1)-\lambda(\lambda-1)} + \hbar^2(\lambda(\lambda+1)-\lambda(\lambda-1)) - 4\hbar^2(\lambda(\lambda+1)-(\lambda-1)(\lambda-2)) - 4\hbar^2(\lambda(\lambda+1)-\lambda(\lambda-1)) +$$

$$-\hbar^2\sqrt{\lambda(\lambda+1)-\lambda(\lambda-1)}\sqrt{\lambda(\lambda+1)-(\lambda-1)(\lambda-2)} + \hbar^2(\lambda(\lambda+1)-(\lambda-2)(\lambda-3)) + \hbar^2(\lambda(\lambda+1)-(\lambda-1)(\lambda-2))\Big) = \hbar^2\left(\sqrt{\frac{9\lambda-4}{6}}\right)^2$$

$$\Delta x = \sqrt{\langle \hat{L}_x^2 \rangle} = \hbar\sqrt{\frac{9\lambda-4}{6}}$$

17.)

$$\psi(r) = \frac{e^{-\alpha r}}{r^2}(x+y+2z+r) = \frac{e^{-\alpha r}}{r^2}\left(r\sqrt{\frac{2\pi}{3}}(Y_1^{-1}-Y_1^1) + r\sqrt{\frac{2\pi}{3}}\,i(Y_1^{-1}+Y_1^1) + 2r\sqrt{\frac{4\pi}{3}}Y_1^0 +\right.$$

$$\left. r\right) = \frac{e^{-\alpha r}}{r}\left(\sqrt{\frac{2\pi}{3}}\left(Y_1^{-1}(1+i) + Y_1^1(i-1)\right) + 2\sqrt{\frac{4\pi}{3}}Y_1^0 + \sqrt{4\pi}\,Y_0^0\right)$$

Normalizatu $\Rightarrow \int_0^\infty \frac{e^{-2\alpha r}}{\cancel{r^2}}\cancel{r^2}\,dr = \frac{1}{2\alpha} \Rightarrow \psi = \sqrt{2\alpha}\,\frac{e^{-\alpha r}}{r}\left(\frac{(1+i)}{\sqrt{18}}Y_1^{-1} + \frac{(i-1)}{\sqrt{18}}Y_1^1 + \frac{2}{3}Y_1^0 + \right.$

$\left.\frac{1}{\sqrt{3}}Y_0^0\right)$

Y_0^0 $\hat{L}_x$-ren autofuntzioa da eta bere autobalioa $l_x = 0$

$l=1$ denean $\hat{L}_x$-ren autobalio eta autofuntzioak $\psi_1 = \frac{1}{\sqrt{2}}(Y_1^1 - Y_1^{-1})$ $\lambda_1 = 0$;

$\lambda_2 = \hbar \quad \varphi_2 = \frac{1}{2}(Y_1^1 + \sqrt{2}Y_1^0 + Y_1^{-1})$; $\varphi_3 = \frac{1}{2}(Y_1^1 - \sqrt{2}Y_1^0 + Y_1^{-1}) \quad \lambda_3 = -\hbar$

$$\boxed{P(0) = \overset{Y_0^0\text{-ms}}{\frac{1}{3}} + |C_1|^2 = \frac{1}{3} + \frac{1}{9} = \frac{4}{9}}$$

$$C_1 = \frac{1}{\sqrt{2}}\left(Y_1^1 - Y_1^{-1}, \frac{(1+i)}{\sqrt{18}}Y_1^{-1} + \frac{(i-1)}{\sqrt{18}}Y_1^1 + \frac{2}{3}Y_1^0 + \frac{1}{\sqrt{3}}Y_0^0\right) = \frac{-1}{\sqrt{2}\sqrt{18}}(1+\cancel{i}-\cancel{i}+1) = \frac{-\sqrt{2}}{\sqrt{18}} = \frac{-1}{3}$$

18.)

$$\psi(r) = Axy\frac{e^{-\alpha r}}{r^3} = \frac{Ae^{-\alpha r}}{r^3}\cdot r^2\sin^2\theta\sin\varphi\cos\varphi = \frac{Ae^{-\alpha r}}{r}\sin^2\theta\cdot 2\sin 2\varphi =$$

$$\cancel{2}\frac{Ae^{-\alpha r}}{r}\sin^2\theta\left(\frac{e^{2i\varphi}-e^{-2i\varphi}}{\cancel{2}i}\right) = \frac{Ae^{-\alpha r}}{r}\left(\sin^2\theta\, i e^{-2i\varphi} - i\sin^2\theta e^{2i\varphi}\right) =$$

$$\frac{Ae^{-\alpha r}}{r}\left(4i\sqrt{\frac{2\pi}{15}}Y_2^{-2} - i4\sqrt{\frac{2\pi}{15}}Y_2^2\right) = 4i\sqrt{\frac{2\pi}{15}}\frac{Ae^{-\alpha r}}{r}(Y_2^{-2} - Y_2^2)$$

$$\langle\hat{L}_x\rangle = \overset{\text{nenormalizirat.}}{\frac{1}{2}}(\langle\hat{L}_+\rangle + \langle\hat{L}_-\rangle) = 0$$

$$\langle\hat{L}_+\rangle = \frac{1}{2}(Y_2^{-2} - Y_2^2, \hat{L}_+Y_2^{-2} - \hat{L}_+Y_2^2) = 0$$

$$\langle\hat{L}_-\rangle = \frac{1}{2}(Y_2^{-2} - Y_2^2, \hat{L}_-Y_2^{-2} - \hat{L}_-Y_2^2) = 0$$

FISIKA KUANTIKA: HIDROGENO ATOMOAREN AUTOFUNTZIOAK eta AUTOBALIOAK.

1.)

Hidrogeno-atomoaren oinarrizko egoera: $\Psi = \psi_{1,0,0} = Y_0^0 R_{10} = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0} \frac{1}{\sqrt{4\pi}}$

- $\langle V \rangle = (\Psi, V\Psi) = \left(\frac{2}{\sqrt{4\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}, -\frac{Ze^2}{4\pi\varepsilon_0} \cdot 2\left(\frac{Z}{a_0}\right)^{3/2} \cdot \frac{1}{\sqrt{4\pi}} \frac{e^{-Zr/a_0}}{r} \right) =$

$-\frac{2^2}{\cancel{4\pi}} \left(\frac{Z}{a_0}\right)^3 \frac{Ze^2}{\cancel{4}\pi\varepsilon_0} \cdot \cancel{4\pi} \int_0^\infty e^{-2Zr/a_0} r \, dr = -\left(\frac{Z}{a_0}\right)^3 \frac{Ze^2}{\pi\varepsilon_0} \cdot \frac{a_0^2}{4Z^2} = \frac{-Z^2 e^2}{4\pi\varepsilon_0 a_0}$

$\nearrow$ Ψ $\hat{H}$-ren autofuntzioa delako.

- $\langle T \rangle + \langle V \rangle = \langle \hat{H} \rangle = \varepsilon_{100} \Rightarrow \langle T \rangle = \varepsilon_{100} - \langle V \rangle = \frac{-me^2}{(4\pi\varepsilon_0)^2 \cdot 2\hbar^2} + \underbrace{\frac{e^2}{4\pi\varepsilon_0 a_0}}_{-2\varepsilon_{100}} =$

(Virialaren teorema)

$13'6 \, eV$

2.)

H-atomoa $\rightarrow$ 2s e^-, nukleoan zentratutako $4a_0$ erradioko gainazal esferiko baten barnealdean aurkitzeko probabilitatea $\Rightarrow$ $P(0<r<4a)$

- 2s $\Rightarrow$ $l=0$, $n=2$, $m=0$ $\Rightarrow$ $P(0<r<4a) = \int_0^{4a} r^2 dr \, |R_{20}(r)|^2 =$

$\left(2\left(\frac{1}{2a_0}\right)^{3/2}\right)^2 \int_0^{4a} r^2 \left(1-\frac{r}{2a_0}\right)^2 e^{-\cancel{2}r/\cancel{2}a_0} dr = 4 \left(\frac{1}{2a_0}\right)^3 \int_0^{4a} r^2 \left(1-\frac{r}{2a_0}\right)^2 e^{-r/a_0} dr =$

$\frac{4}{8\cancel{a_0^3}} \frac{2(e^4-45)\cancel{a_0^3}}{e^4} = \frac{e^4-45}{e^4} \Rightarrow \% \, 17'57$

- 2p $\Rightarrow$ $n=2$, $l=1$ $\Rightarrow$ $P(0<r<4a) = \int_0^{4a} r^2 dr \, |R_{21}(r)|^2 = \frac{1}{3} \cdot \frac{1}{8a_0^3} \int_0^{4a} \frac{r^2 \cdot r^2}{a_0^2} e^{-r/a_0} dr =$

$\frac{1}{24a_0^5} \int_0^{4a} r^4 e^{-r/a_0} dr = \frac{1}{24\cancel{a_0^5}} \cdot 8\left(3-\frac{103}{e^4}\right)\cancel{a_0^5} = \frac{1}{3}\left(3-\frac{103}{e^4}\right) \Rightarrow \% \, 37'116$

3.)

H atomoa $\Rightarrow$ ψ_{100} $\Rightarrow$ $\langle r \rangle$? $\langle r \rangle = (\psi_{100}, r\psi_{100}) =$

$$\int_0^\infty |R_{10}|^2 r^3 dr = \frac{4}{a_0^3}\int_0^\infty r^3 e^{-2r/a_0} dr = \frac{4}{\cancel{a_0^3}}\cdot\frac{3a_0^4}{8} = \frac{3a_0}{2}$$

$$\langle r^2 \rangle = (\psi_{100}, r^2\psi_{100}) = \frac{4}{a_0^3}\int_0^\infty r^4 e^{-2r/a_0} dr = \frac{4}{a_0^3}\frac{3a_0^5}{4} = 3a_0^2$$

$$\Delta r = \sqrt{\langle r^2\rangle - \langle r\rangle^2} = a_0\sqrt{9-\frac{9}{4}} = \frac{a_0}{2}\sqrt{27} > \langle r \rangle$$

4.)

$\langle r^{-1} \rangle$ egoera geldikorretan: $\langle r^{-1}\rangle_{\psi_n} = \int_0^\infty r|R_{nl}|^2 dr$

Virialaren teorema $\langle \hat{T}\rangle_{\psi_E} = \frac{1}{2}\langle \vec{r}\cdot\vec{\nabla}V\rangle_{\psi_E} = \frac{1}{2}\langle r\frac{\partial V}{\partial r}\rangle_{\psi_E} = \frac{+e^2}{8\pi\varepsilon_0}\langle +\frac{r}{r^2}\rangle =$

$-\frac{1}{2}\langle V\rangle_{\psi_E}$ $\Rightarrow$ $\langle \hat{H}\rangle = E_n = \langle \hat{T}\rangle + \langle V\rangle = -\frac{1}{2}\langle V\rangle_{\psi_E} + \langle V\rangle_{\psi_E} = \frac{1}{2}\langle V\rangle_{\psi_E}$

$$\langle V\rangle_{\psi_E} = 2\cdot E_n = \frac{-e^2}{4\pi\varepsilon_0}\left\langle\frac{1}{r}\right\rangle_{\psi_E} \leftrightarrow \left\langle\frac{1}{r}\right\rangle_{\psi_E} = -\frac{8\pi\varepsilon_0\cdot E_n}{e^2} = \frac{13'6\,eV\cdot 8\pi\varepsilon_0}{n^2\;e^2}$$

5.)

$$\psi(r) = R_{21}(r)\left[\sqrt{\tfrac{1}{3}}Y_1^0(\theta,\phi) + \sqrt{\tfrac{2}{3}}Y_1^1(\theta,\phi)\right] = \sqrt{\tfrac{1}{3}}\underbrace{R_{21}Y_1^0(\theta,\phi)}_{\psi_{210}} + \sqrt{\tfrac{2}{3}}\underbrace{R_{21}Y_1^1(\theta,\phi)}_{\psi_{211}}$$

E_2 neurtuko dugu beti, 1-eko probabilitatearekin. $E_2 = -\frac{13'6}{4}eV = -3'4\,eV$

L_z neurtean $l_z = 0, \hbar$ lor genezake: $P(0) = \frac{1}{3}$, $P(\hbar) = \frac{2}{3}$

6.)

E, L^2, L_z aldi berean neurtu $\Rightarrow$ $(E, L^2, L_z) = (E_2, 0, 0) \neq (E_3, 6\hbar^2, 2\hbar), (E_3, 2\hbar^2, -\hbar)$

$\downarrow$ $P = 1/2$ $\qquad$ $\downarrow$ $P = 1/4$ $\qquad$ $\downarrow$ $P = 1/4$

$$\psi_1 = \frac{1}{\sqrt{2}} R_{20} Y_0^0 + \frac{1}{2} R_{32} Y_2^2 + \frac{1}{2} R_{31} Y_1^{-1} \Rightarrow \psi_1(t) = \frac{1}{\sqrt{2}} R_{20} Y_0^0 e^{\frac{-iE_2 t}{\hbar}} + \frac{1}{2} e^{-\frac{iE_3 t}{\hbar}} (R_{32} Y_2^2 + R_{31} Y_1^{-1})$$

$$\psi_2 = \frac{1}{\sqrt{2}} R_{20} Y_0^0 - \frac{1}{2} R_{32} Y_2^2 + \frac{1}{2} R_{31} Y_1^{-1} \Rightarrow \psi_2(t) = \frac{1}{\sqrt{2}} R_{20} Y_0^0 e^{-\frac{iE_2 t}{\hbar}} - \frac{1}{2} e^{-\frac{iE_3 t}{\hbar}} (R_{32} Y_2^2 - R_{31} Y_1^{-1})$$

7.)

$$\Psi(r, t=0) = A[\phi_{100}(r) - \phi_{210}(r)] \Rightarrow \quad \langle (\hat{L}_x^2 + \hat{L}_y^2)^2 \rangle (t)$$

$$\hookrightarrow \Psi(r,t) = \frac{1}{\sqrt{2}} (\phi_{100} e^{-\frac{iE_1 t}{\hbar}} - \phi_{210} e^{-\frac{iE_2 t}{\hbar}})$$

- $\hat{L}_x^2 + \hat{L}_y^2 = \left(\frac{\hat{L}_+ + \hat{L}_-}{2}\right)^2 + \left(\frac{\hat{L}_+ - \hat{L}_-}{2i}\right)^2 = \frac{1}{4} [\cancel{\hat{L}_+^2} + \cancel{\hat{L}_-^2} + \hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+ \cancel{- \hat{L}_+^2} \cancel{- \hat{L}_-^2} + \hat{L}_+\hat{L}_- +$

$+ \hat{L}_-\hat{L}_+] = \frac{1}{2} (\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+) \Rightarrow \quad (\hat{L}_x^2 + \hat{L}_y^2)^2 = \frac{1}{4} (\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+)^2 =$

$\frac{1}{4} (\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+)(\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+) = \frac{1}{4} (\hat{L}_+\hat{L}_-\hat{L}_+\hat{L}_- + \hat{L}_+\hat{L}_-^2\hat{L}_+ + \hat{L}_-\hat{L}_+^2\hat{L}_- +$

$\hat{L}_-\hat{L}_+\hat{L}_-\hat{L}_+)$

- $\langle (\hat{L}_x^2 + \hat{L}_y^2)^2 \rangle = \frac{1}{4} \langle \hat{L}_+\hat{L}_-\hat{L}_+\hat{L}_- \rangle + \frac{1}{4} \cancel{\langle \hat{L}_+\hat{L}_-^2\hat{L}_+ \rangle} + \frac{1}{4} \langle \hat{L}_- \cancel{\hat{L}_+^2 \hat{L}_-} \rangle +$

$\frac{1}{4} \langle \hat{L}_-\hat{L}_+\hat{L}_-\hat{L}_+ \rangle = \frac{2\hbar^4}{4} + \frac{2\hbar^4}{4} = \hbar^4$

$*$ $\langle \hat{L}_+\hat{L}_-\hat{L}_+\hat{L}_- \rangle = \left(\frac{1}{\sqrt{2}}\right)^2 \left(Y_0^0 e^{-\frac{iE_1 t}{\hbar}} - Y_1^0 e^{-\frac{iE_2 t}{\hbar}}, e^{-\frac{iE_1 t}{\hbar}} \hat{L}_+\hat{L}_-\hat{L}_+\hat{L}_- Y_0^0 - e^{-\frac{iE_2 t}{\hbar}} \hat{L}_+\hat{L}_-\hat{L}_+\hat{L}_- Y_1^0 \right) =$

$\left(\frac{1}{\sqrt{2}}\right)^2 \left(Y_0^0 e^{-\frac{iE_1 t}{\hbar}} - Y_1^0 e^{-\frac{iE_2 t}{\hbar}}, e^{-\frac{iE_1 t}{\hbar}} \cdot 0 - e^{-\frac{iE_2 t}{\hbar}} 4\hbar^4 Y_1^0 \right) = \frac{4\hbar^4}{2} = 2\hbar^4$

$*$ $\langle \hat{L}_-\hat{L}_+\hat{L}_-\hat{L}_+ \rangle = \frac{1}{2} \left(Y_0^0 e^{-\frac{iE_1 t}{\hbar}} - Y_1^0 e^{-\frac{iE_2 t}{\hbar}}, e^{-\frac{iE_1 t}{\hbar}} \hat{L}_-\hat{L}_+\hat{L}_-\hat{L}_+ Y_0^0 - e^{-\frac{iE_2 t}{\hbar}} \hat{L}_-\hat{L}_+\hat{L}_-\hat{L}_+ Y_1^0 \right) =$

$\frac{1}{2} \left(Y_0^0 e^{-\frac{iE_1 t}{\hbar}} - Y_1^0 e^{-\frac{iE_2 t}{\hbar}}, e^{-\frac{iE_1 t}{\hbar}} \cdot 0 - e^{-\frac{iE_2 t}{\hbar}} 4\hbar^4 Y_1^0 \right) = 2\hbar^4$

$$|\Psi(r,t)|^2 = \frac{1}{2}\left(\phi_{100}\, e^{-i\frac{E_1}{\hbar}t} - \phi_{210}\, e^{-i\frac{E_2}{\hbar}t}\right)\left(\phi_{100}^*\, e^{i\frac{E_1}{\hbar}t} - \phi_{210}^*\, e^{i\frac{E_2}{\hbar}t}\right) =$$

$$\frac{1}{2}\left(|\phi_{100}|^2 + |\phi_{210}|^2 - \phi_{100}\phi_{210}^*\, e^{i\frac{E_2-E_1}{\hbar}t} - \phi_{210}\phi_{100}^*\, e^{-i\frac{E_2-E_1}{\hbar}t}\right) =$$

$$\frac{1}{2}\left(|\phi_{100}|^2 + |\phi_{210}|^2 - 2\,\mathrm{Re}\left(\phi_{100}\phi_{210}^*\, e^{i\frac{E_2-E_1}{\hbar}t}\right)\right) \Rightarrow T = \frac{2\pi}{\omega} = \frac{2\pi}{E_2-E_1}\hbar$$

8.)

$$n=2,\ l=1,\ m_l=1 \Rightarrow \Psi = \phi_{211} = R_{21}Y_1^1$$

Nukleotik r distantziora egoteko probabilitatea: $P_{n,l}(r) = r^2|R_{n,l}(r)|^2$

- $$P_{n,l}(r) = r^2|R_{21}|^2 = \frac{r^2}{3}\cdot\frac{1}{(2a_0)^3}\cdot\frac{r^2}{a_0^2}e^{-r/a_0} = \frac{r^4}{24a_0^5}e^{-r/a_0}$$

- $$\frac{\partial P_{n,l}(r)}{\partial r} = \frac{1}{24a_0^5}\cdot\left(4r^3e^{-r/a_0} - \frac{1}{a_0}r^4e^{-r/a_0}\right) = \frac{e^{-r/a_0}r^3}{24a_0^5}\left(4 - \frac{r}{a_0}\right) = 0 \Rightarrow$$

$r=0$ edo $r = 4a_0$ $\rightarrow$ $P(r=0) = 0$, $P(r=4a_0) = P_{max}$.

$$r = 4a_0 = 2'116\ \text{Å}$$

- $$\langle V\rangle_{\Psi_{211}} + \langle T\rangle_{\Psi_{211}} = E_2 = \frac{-13'6}{4}\ eV = -3'4\ eV$$

Virialaren teorema: $\langle T\rangle_{\Psi_{211}} = \frac{1}{2}\langle r\frac{\partial V}{\partial r}\rangle_{\Psi_{211}} = \frac{1}{2}\langle r\frac{Ze^2}{4\pi\varepsilon_0 r^2}\rangle_{\Psi_{211}} = -\frac{1}{2}\langle V\rangle_{\Psi_{211}}$

$$\underbrace{\langle E\rangle_{\Psi_{211}}}_{\text{egoera geldikorra}} = E_2 = \langle T\rangle_{\Psi_{211}} + \langle V\rangle_{\Psi_{211}} = \frac{1}{2}\langle V\rangle_{\Psi_{211}} \Rightarrow \langle V\rangle_{\Psi_{211}} = -2\cdot 3'4\ eV = -6'8\ eV$$

$$\langle T\rangle_{\Psi_{211}} = -\frac{1}{2}\langle V\rangle_{\Psi_{211}} = 3'4\ eV$$

9.)

H atomoa $\Rightarrow$ 4d egoeran $n=4$, $l=2$; $R_{42}(r) \propto \left(6 - \frac{r}{2a_0}\right)r^2e^{-r/4a_0}$

$\psi_{321} \propto r^2 e^{-r/3a_0} \sin\theta\cos\theta e^{i\phi}$; ψ_{42-1} ? $\quad l=2, m=1 \Rightarrow \sin\theta\cos\theta e^{i\phi}$ bada $\rightarrow m=-1$ $e^{-i\phi}$

$$\psi_{42-1} = R_{42} Y_2^{-1} \propto \left(6-\frac{r}{2a_0}\right) r^2 e^{-r/4a_0} \sin\theta\cos\theta e^{-i\phi}$$

- $R_{42} \propto \underbrace{\left(6-\frac{r}{2a_0}\right)}_{\text{Laguerren polinomio elkartua}} \underbrace{r^2}_{r^l} \underbrace{e^{-r/4a_0}}_{e^{-r/na_0}}$ $\qquad L_1^5\left(\frac{2r}{4a_0}\right) \propto \left(6-\frac{r}{2a_0}\right)$

(10.)

$$E_n = -0'85\,eV = \frac{-13'6\,eV}{n^2} \Rightarrow n = \sqrt{\frac{13'6}{0'85}} = 4 \rightarrow l = 0,1,2,3$$

Uhin-funtzioa bakoitia da, $\langle \hat{L}^2 \rangle = 6\hbar^2$

Egoera geldikorra: $\psi = \sum_{l=0}^{3} \sum_{m=-l}^{l} C_{lm} \psi_{4lm} = \sum_{m=-3}^{3} C_m \psi_{43m} + \cancel{\sum_{m=-2}^{2} D_m \psi_{42m}} +$

$\sum_{m=-1}^{1} E_m \psi_{41m} + \cancel{A\psi_{400}}$ (bakoitia delako)

l bakoitia $\Rightarrow$ harmoniko esferiko bakoitia
l bikoitia $\Rightarrow$ harmoniko esferiko bikoitia

$$\langle \hat{L}^2 \rangle = (\psi, \hat{L}^2 \psi) = \left(\sum_{m=-3}^{3} C_m \psi_{43m} + \sum_{m=-1}^{1} E_m \psi_{41m} ; \sum_{m=-3}^{3} C_m \hat{L}^2 \psi_{43m} + \right.$$

$$\left. \sum_{m=-1}^{1} E_m \hat{L}^2 \psi_{41m} \right) = \left(\sum_{m=-3}^{3} C_m \psi_{43m} + \sum_{m=-1}^{1} E_m \psi_{41m}, \sum_{m=-3}^{3} C_m \hbar^2 12 \psi_{43m} + \sum_{m=-1}^{1} E_m 2\hbar^2 \psi_{41m} \right) =$$

$$\left(\sum_{m=-3}^{3} C_m \psi_{43m}, 12\hbar^2 \sum_{m=-3}^{3} C_m \psi_{43m} \right) + \left(\sum_{m=-1}^{1} E_m \psi_{41m}, 2\hbar^2 \sum_{m=-1}^{1} E_m \psi_{41m} \right) =$$

$$12\cancel{\hbar^2} \underbrace{\sum_{m=-3}^{3} |C_m|^2}_{\hat{L}^2 = 12\hbar^2 \text{ izateko probabilitatea } (l=3)} + 2\cancel{\hbar^2} \underbrace{\sum_{m=-1}^{1} |E_m|^2}_{\hat{L}^2 = 2\hbar^2 \text{ izateko probabilitatea } (l=1)} = 6\cancel{\hbar^2} \Rightarrow 2\sum_{m=-3}^{3} |C_m|^2 + \frac{1}{3}\sum_{m=-1}^{1} |E_m|^2 = 1 \quad (1)$$

Gainera $\sum_{m=-3}^{3} |C_m|^2 + \sum_{m=-1}^{1} |E_m|^2 = 1 \quad (2)$ (Normalizazio baldintza)

(1) eta (2) konbinatuz $\Rightarrow$ $\quad 2(2)-(1) \Rightarrow \cancel{2\sum_{m=-3}^{3} |C_m|^2} + 2\sum_{m=-1}^{1} |E_m|^2 - \cancel{2\sum_{m=-3}^{3} |C_m|^2} - \frac{1}{3}\sum_{m=-1}^{1} |E_m|^2 =$

$$\frac{5}{3}\sum_{m=-1}^{1} |E_m|^2 = 1 \Rightarrow \sum_{m=-1}^{1} |E_m|^2 = 3/5 \Rightarrow \sum_{m=-3}^{3} |C_m|^2 = 1 - 3/5 = 2/5$$

Berat, $\hat{L}^2$ $2\hbar^2$ izateko probabilitatea $\sum_{m=-1}^{1} |E_m|^2 = 3/5$ da.

11.)

$$\Psi(r, t=0) = A\,[\psi_{100} - \psi_{210}] = \frac{1}{\sqrt{2}}(\underset{\substack{\downarrow \\ n=1}}{\psi_{100}} - \underset{\substack{\downarrow \\ n=2}}{\psi_{210}}) \rightarrow \langle \hat{L}^4\rangle(t),\ \langle z\rangle(t)?$$

Denboran garatu $\rightarrow$ $\Psi(r,t) = \frac{1}{\sqrt{2}}\left(\psi_{100}\, e^{-i\frac{E_1}{\hbar}t} - \psi_{210}\, e^{-i\frac{E_2}{\hbar}t}\right)$ $\quad E_n = \frac{-13'6\,eV}{n^2}$

- $\langle \hat{L}^4 \rangle = (\Psi(t), \hat{L}^4\Psi(t)) = (\hat{L}^2\Psi, \hat{L}^2\Psi) = \left(\frac{1}{\sqrt{2}}\hat{L}^2(\psi_{100}e^{-i\frac{E_1}{\hbar}t} - \psi_{210}e^{-i\frac{E_2}{\hbar}t}),\right.$

$$\left.\frac{1}{\sqrt{2}}\hat{L}^2(\psi_{100}e^{-i\frac{E_1}{\hbar}t} - \psi_{210}e^{-i\frac{E_2}{\hbar}t})\right) = \frac{1}{2}4\hbar^4 = 2\hbar^4$$

- $\langle z\rangle(t) = (\Psi, r\cos\theta\,\Psi) = \frac{1}{2}(\psi_{100} - \psi_{210},\ r\cos\theta\,\psi_{100} - r\cos\theta\,\psi_{210}) =$

$$\frac{1}{2}\int_0^\infty\int_0^{2\pi}\int_0^\pi (\psi_{100} - \psi_{210})^* (r\cos\theta\,\psi_{100} - r\cos\theta\,\psi_{210})\, r^2 d\theta \sin\theta\, d\varphi\, dr =$$

$$\frac{1}{2}\int_0^\infty\int_0^\pi (R_{10}P_0^0 - R_{21}P_1^0)^*(r\cos\theta\, R_{10}P_0^0 - R_{21}P_1^0\, r\cos\theta)\, r^2 d\theta \sin\theta\, dr =$$

$$\frac{1}{2}\int_0^\infty\int_0^\pi (R_{10}^2 P_0^{02}\, r^3\cos\theta\sin\theta + R_{21}^2 P_1^0\, r^3\cos\theta\sin\theta - 2R_{21}P_0^0\, r^3\cos\theta\sin\theta\, R_{10}P_1^0)\, d\theta\, dr =$$

$$\frac{1}{2}\int_0^\infty\int_0^\pi \left(\cancel{\frac{2}{a_0^3}e^{-2r/a_0} r^3\cos\theta\sin\theta} + \cancel{\frac{1}{16a_0^5} r^5 \cos^3\theta\sin\theta\, e^{-r/a_0}} - \frac{1}{\sqrt{2}}\frac{r^4}{a_0^4}e^{-r/a_0}\cos^2\theta\sin\theta\right)d\theta\, dr$$

$$\frac{1}{2}\int_0^\infty dr\left(+\frac{1}{\sqrt{2}}\frac{r^4}{a_0^4}e^{-r/a_0}\frac{\cos^3\theta}{3}\right)\Big]_0^\pi = \frac{1}{6\sqrt{2}}\cdot\frac{1}{a_0^4}(-2)\int_0^\infty r^4 e^{-r/a_0}dr = -\frac{1}{3\sqrt{2}}\cdot\frac{1}{a_0^4}\cdot 24a_0^5 =$$

$$-\frac{8a_0}{\sqrt{2}}$$

12.)

$Z=1$, momentu dipolarra $\Rightarrow d=-er$ (r: e^--ak nukleoarekiko duen posizioa) $\rightarrow$ ezaguna (?) etik.

Egoera egonkorrak $\Rightarrow$ egoera geldikorrak: $\langle d\rangle_{\psi_E}=0$

$$\Psi(r,t)=\frac{1}{\sqrt{1+\gamma^2}}\left[\underbrace{\psi_{1s}}_{n=1,\,l=0,\,m=0}e^{-i\frac{E_1t}{\hbar}}+\gamma\underbrace{\Psi_{2p0}}_{n=2,\,l=1,\,m=0}e^{-i\frac{E_2t}{\hbar}}\right]$$

Normalizatuta dago baldin eta $\gamma\in\mathbb{R}$ den ($|\gamma|^2=\gamma^2$)

* $\langle\hat{H}\rangle=\frac{E_1}{1+\gamma^2}+\frac{\gamma^2E_2}{1+\gamma^2}=\frac{E_1+\gamma^2E_2}{1+\gamma^2}$, $\langle\hat{L}^2\rangle=0+\frac{2\hbar^2\gamma^2}{1+\gamma^2}=\frac{2\hbar^2\gamma^2}{1+\gamma^2}$

$\langle\hat{L}_z\rangle=0$

* $$\langle d\rangle=\langle -re\rangle=\frac{-e}{1+\gamma^2}\left(\Psi_{100}e^{-i\frac{E_1t}{\hbar}}+\gamma\Psi_{210}e^{-i\frac{E_2t}{\hbar}},\ r\Psi_{100}e^{-i\frac{E_1t}{\hbar}}+\gamma r\Psi_{210}e^{-i\frac{E_2t}{\hbar}}\right)=$$

$$-\frac{e}{1+\gamma^2}\left(R_{10}e^{-i\frac{E_1t}{\hbar}}+\gamma R_{21}e^{-i\frac{E_2t}{\hbar}},\ rR_{10}e^{-i\frac{E_1t}{\hbar}}+\gamma rR_{21}e^{-i\frac{E_2t}{\hbar}}\right)=$$

$$\frac{-e}{1+\gamma^2}\left[(R_{10},rR_{10})+e^{-i\frac{(E_2-E_1)t}{\hbar}}(R_{10},\gamma rR_{21})+\gamma e^{i\frac{(E_2-E_1)t}{\hbar}}(R_{21},rR_{10})+\right.$$

$$\left.(R_{21},rR_{21})\right]=-\frac{e}{1+\gamma^2}\left[(R_{10},rR_{10})+(R_{21},rR_{21})+2\gamma\cos\left(\frac{E_2-E_1}{\hbar}t\right)(R_{10},rR_{21})\right]=$$

$$-\frac{e}{1+\gamma^2}\left(\frac{3a_0}{2}+5a_0+\frac{512}{81\sqrt6}a_0\cos\left(\frac{E_2-E_1}{\hbar}t\right)\right)\Rightarrow\nu=\frac{E_2-E_1}{h}$$

* $(R_{10},rR_{10})=\frac{4}{a_0^3}\int_0^\infty r^3e^{-2r/a_0}dr=\frac{3a_0}{2}$

$(R_{10},rR_{21})=\frac{1}{\sqrt6}\cdot\frac{1}{a_0^4}\int_0^\infty e^{-3r/2a_0}r^4dr=\frac{1}{\sqrt6}\cdot\frac{1}{a_0^4}\cdot\frac{256}{81}a^5=\frac{256}{81\sqrt6}a_0$

$(R_{21},rR_{21})=\frac{1}{24a_0^5}\int_0^\infty r^5e^{-r/a_0}dr=5a_0$

(Beste partea egin gabe)

13)

$\Psi(r) = \left[\frac{1}{2} R_{32} Y_2^{1} - i\frac{\sqrt{3}}{2} R_{42} Y_2^{-1} \right]$ ez da autofuntzioa n ezberdinak

dituelako (baita l eta m)

Bai da L_z^2-ren autofuntzioa m ezberdinak badira ere ($\hat{L}_z$-ren autofuntzio

berdinak dira) $\hat{l}_z = \hbar^2$ duguelako bi autofuntzioekin.

$$\langle L_z \rangle = \frac{1}{4} \cdot \hbar + \frac{3}{4}(-\hbar) = -\frac{\hbar}{2}$$

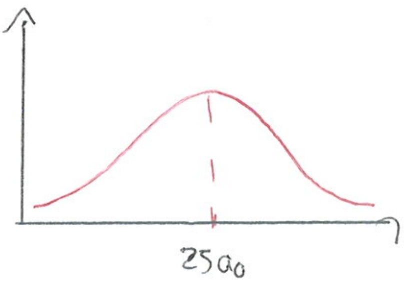
14)

$n=5,\ l=4,\ m_l=-4 \Rightarrow R_{nl}(r) = R_{54}(r) \Rightarrow P_{54}(r) = r^2 |R_{54}(r)|^2$

$$R_{54}(r) = \underbrace{N_{54}\left(\frac{a_0}{Z}\right)^{3/2}}_{kte} \left(\frac{2Zr}{5a_0}\right)^4 e^{-\frac{Zr}{5a_0}} \underbrace{L_0^9\left(\frac{2Zr}{5a_0}\right)}_{kte} \Rightarrow P_{54} = kte\, r^2 e^{-\frac{2Zr}{5a_0}} r^8 =$$

$$A r^{10} e^{-\frac{2Zr}{5a_0}} \Rightarrow \frac{dP_{54}}{dr} = 10Ar^9 e^{-2Zr/5a_0} - \frac{2Z}{5a_0} A r^{10} e^{-2Zr/5a_0} =$$

$$A e^{-2Zr/5a_0} r^9 \left(10 - \frac{2Z}{5a_0} r\right) = 0 \rightarrow \underset{\text{minimo}}{r=0} \text{ edo } \underset{\text{maximo}}{r = \frac{25a_0}{Z}} \overset{Z=1}{=} 25a_0$$



Ez du nodorik

Nodo kopurua : $n-l-1=0$

15)

$\psi(r,t=0) = \frac{1}{\sqrt{3}} \phi_{200}(r) + \frac{2}{\sqrt{3}} \phi_{320}(r)$ $\langle r \rangle(t)$? $\langle L_x \rangle(t)$?

Garatu denboran: $\psi(r,t) = \left(\frac{1}{\sqrt{3}} \phi_{200} e^{-i\frac{E_2}{\hbar}t} + \frac{2}{\sqrt{3}} \phi_{320} e^{-i\frac{E_3}{\hbar}t} \right) \sqrt{\frac{3}{5}}$

$$E_n = \frac{-13'6\,eV}{n^2} \Rightarrow \quad E_2 = -3'4\,eV, \quad E_3 = -1'51\,eV$$

- $\frac{d\langle L_x\rangle(t)}{dt} = 0$ da $[\hat{H}, \hat{L}_x] = 0$ delako.

$$\langle L_x\rangle(t=0) = \frac{1}{2}\langle\hat{L}_+\rangle + \frac{1}{2}\langle\hat{L}_-\rangle = \frac{1}{10}\left(Y_0^0 + 2Y_2^0, \hat{L}_+(Y_0^0 + 2Y_2^0)\right) +$$

$$\frac{1}{10}\left(Y_0^0 + 2Y_2^0, \hat{L}_-(Y_0^0 + 2Y_2^0)\right) = 0 \Rightarrow \langle L_x\rangle(t) = 0$$

- $\langle\vec{r}\rangle = \langle x\rangle\hat{i} + \langle y\rangle\hat{j} + \langle z\rangle\hat{k}$

$$\langle\vec{r}\rangle = 0 \quad \begin{cases} \langle x\rangle = (\Psi, x\Psi) = \int_{-\infty}^{\infty}|\Psi|^2 x\,dx = 0 \\ \langle y\rangle = (\Psi, y\Psi) = \int_{-\infty}^{\infty}|\Psi|^2 y\,dy = 0 \\ \langle z\rangle = (\Psi, z\Psi) = \int_{-\infty}^{\infty}|\Psi|^2 z\,dz = 0 \end{cases}$$

(bakoitiak direlako) *

* l bakoitia $\rightarrow$ Y_l^m bakoitia ; l bikoitia $\rightarrow$ Y_l^m bikoitia

$$\Psi_{nlm} = R_{nl}\,Y_l^m$$

$$\Psi = \underbrace{\frac{1}{\sqrt{5}}Y_0^0}_{\text{bikoitia}} R_{20} + \frac{2}{\sqrt{5}}R_{32}\underbrace{Y_2^0}_{\text{bikoitia}} \Rightarrow |\Psi|^2 \text{ bikoitia}$$

16.)

$$\psi(r, t=0) = \frac{1}{2}\psi_{321}(r) - i\frac{\sqrt{3}}{2}\psi_{42-1}(r)$$

- n ezberdina dutenez egoera ez da iraunkorra $\Rightarrow$ $\psi(r,t) = \frac{1}{2}\psi_{321} e^{-i\frac{E_3}{\hbar}t} + -i\frac{\sqrt{3}}{2}\psi_{42-1} e^{-i\frac{E_4}{\hbar}t}$

- $$\hat{L}_x^2 + \hat{L}_y^2 = \left(\frac{\hat{L}_+ + \hat{L}_-}{2}\right)^2 + \left(\frac{\hat{L}_+ - \hat{L}_-}{2i}\right)^2 = \cancel{\frac{\hat{L}_+^2}{4}} + \cancel{\frac{\hat{L}_-^2}{4}} + \frac{\hat{L}_+\hat{L}_-}{4} + \frac{\hat{L}_-\hat{L}_+}{4} - \cancel{\frac{\hat{L}_+^2}{4}} + -\cancel{\frac{\hat{L}_-^2}{4}} + \frac{\hat{L}_-\hat{L}_+}{4} + \frac{\hat{L}_+\hat{L}_-}{4} = \frac{\hat{L}_+\hat{L}_-}{2} + \frac{\hat{L}_-\hat{L}_+}{2}$$

zati erradialen gainean eraginik ez

$$\langle \hat{L}_x^2 + \hat{L}_y^2 \rangle = \frac{1}{2}\langle \hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+ \rangle = \frac{1}{2}\left(\frac{1}{2}Y_2^1 - i\frac{\sqrt{3}}{2}Y_2^{-1}, \frac{\hat{L}_+\hat{L}_-}{2}Y_2^1\right) + -\frac{1}{2}\left(\frac{1}{2}Y_2^1 - i\frac{\sqrt{3}}{2}Y_2^{-1}, \frac{\hat{L}_-\hat{L}_+}{2} i\sqrt{3}\, Y_2^{-1}\right) = \frac{1}{2}\left(\frac{1}{2}Y_2^1 - i\frac{\sqrt{3}}{2}, 3\hbar^2 Y_2^1\right) + -\frac{1}{2}\left(\frac{1}{2}Y_2^1 - i\frac{\sqrt{3}}{2}Y_2^{-1}, i\frac{\sqrt{3}}{2}6\hbar^2 Y_2^{-1}\right) = \frac{3\hbar^2}{4} + \frac{9\hbar^2}{4} = 3\hbar^2$$