Diracs framsetning

framsetning óháð hnitum eða grunni

grunnur	hnit $\psi(r)$
$u_i(r)$	c_i
$v_p(r)$	$\psi(p)$
$\delta(r-r_0)$	$\psi(r_0)$
$w_\alpha(r)$	$c(\alpha)$

$$\psi \in \mathcal{F} \subset L^2$$

→ tölum heldur um vektora í ástandarúminu $\mathcal{E}_r \subset$ Hilbertrúmið

„ástandsvektor" $|\psi\rangle$

$$\psi \in \mathcal{F} \iff |\psi\rangle \in \mathcal{E}_r$$

Innfeldi

$$\langle\varphi|\psi\rangle = (|\varphi\rangle, |\psi\rangle)$$

$$\langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^*$$

línulegir virkjar

$$|\psi'\rangle = A|\psi\rangle \qquad \underset{\mathcal{E}}{\underset{\in}{|\psi\rangle}} \xrightarrow{A} \underset{\mathcal{E}}{\underset{\in}{|\psi'\rangle}}$$

$$A\{\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle\} = \lambda_1 A|\psi_1\rangle + \lambda_2 A|\psi_2\rangle$$

$$AB|\psi\rangle = A(B|\psi\rangle)$$

$$\langle\varphi|(A|\psi\rangle) = \langle\varphi|\psi'\rangle$$ fylkisstak A

$|\psi\rangle\langle\varphi|$ er virki því

$$|\psi\rangle\langle\varphi|\chi\rangle = \lambda|\psi\rangle \qquad \lambda \in \mathbb{C}$$

$|\psi\rangle\langle\varphi|$ varpar $|\chi\rangle$ yfir í $|\psi\rangle$

$|\psi\rangle\lambda = \lambda|\psi\rangle$ sama fyrir bra

$$\langle\varphi|\lambda|\psi\rangle = \lambda\langle\varphi|\psi\rangle = \langle\varphi|\psi\rangle\lambda$$

Ofanvarpanir

$$P_\psi = |\psi\rangle\langle\psi|$$

$$P_\psi|\varphi\rangle = |\psi\rangle \underbrace{\langle\psi|\varphi\rangle}_{\in \mathbb{C}}$$

ofanvarp $|\varphi\rangle$ á $|\psi\rangle$, $P_\psi^2 = P_\psi$

$\langle\psi|\varphi\rangle$: hlutfall $|\psi\rangle$ í $|\varphi\rangle$

$|\varphi_i\rangle$ hornréttargrunnur í hlutrúmi $i = 1 \ldots q$

$$P_q = \sum_{i=1}^{q} |\varphi_i\rangle\langle\varphi_i|$$

er hornrétta ofanvörpunin á $|\varphi_i\rangle$

$$(\langle\varphi|A)|\psi\rangle = \langle\varphi|(A|\psi\rangle) \equiv \langle\varphi|A|\psi\rangle$$

Sjálfoka virkjar

til $|\psi\rangle$ samsvarar $\langle\psi|$

$|\psi'\rangle$ — || — $\langle\psi'|$

á sama hátt má skilgreina samoka virkja

$$|\psi'\rangle = A|\psi\rangle$$

þ.a. $\langle\psi'| = \langle\psi|A^+$

$$\langle\psi|A^+|\varphi\rangle = \langle\psi'|\varphi\rangle = \langle\varphi|\psi'\rangle^* = \langle\varphi|A|\psi\rangle^*$$

$$\rightarrow \boxed{\langle\psi|A^+|\varphi\rangle = \langle\varphi|A|\psi\rangle^*}$$

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

Virki er Hermískur „sjálfoka"

ef $A = A^+$

þ.e.

$$\langle\psi|A|\varphi\rangle = \langle\varphi|A|\psi\rangle^*$$

Athugasemd

Í raun þarf að skilja á milli sjálfoka og Hermísks virkja og fjalla um ódöl þeirra....
sjá Capri....

Velja grunn

$$\langle u_i|u_j\rangle = \delta_{ij} \qquad \langle w_\alpha|w_{\alpha'}\rangle = \delta(\alpha-\alpha')$$

$$|\psi\rangle = \sum_i c_i|u_i\rangle \longrightarrow \langle u_j|\psi\rangle = c_j$$

$$|\psi\rangle = \int d\alpha\, c(\alpha)|w_\alpha\rangle \qquad \langle w_{\alpha'}|\psi\rangle = c(\alpha')$$

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

fullkominn grunnur

$$\int d\alpha\, |w_\alpha\rangle\langle w_\alpha| = \mathbb{1}$$

Eigingildi

$$A|\psi\rangle = \lambda|\psi\rangle \qquad \lambda\in\mathbb{C}$$

ef fleiri $|\psi\rangle$ uppfylla þessa jöfnu

$$A|\psi^i\rangle = \lambda|\psi^i\rangle \qquad i=1,2,\dots g$$

þá er λ margfallt með margfeldnina g

Meginsetning

$\boxed{\text{Eigingildi sjálfoka virkja eru rauntölur}}$

Eiginvektorar mismunandi eigingilda eru hornréttir (sjálfoka virkjar)

$A|\psi_n^i\rangle = a_n|\psi_n^i\rangle \qquad i = 1, 2 \dots g$

Sjálfoka virki A er mælistærð ef eiginvektorarnir mynda grunn

∞-rúm $$\sum_{n=1}^{\infty}\sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i| = \mathbb{1}$$

Víxlandi mælistærðir

Ef $[A,B]=0$ (virkjar) og ef $|\psi\rangle$ er eiginvektor A þá er $B|\psi\rangle$ eiginvektor A með sama eigingildi

$$A|\psi\rangle = a|\psi\rangle$$

$$BA|\psi\rangle = aB|\psi\rangle$$

$$A(B|\psi\rangle) = a(B|\psi\rangle)$$

Ef $[A,B]=0$ þá er hvert eiginhlutrúm A óháð af B

Ef $[A,B]=0$ (mælistærðir) og $|\psi_1\rangle$ og $|\psi_2\rangle$ eru eiginvektorar A með mismunandi eigingildi $\longrightarrow \langle\psi_1|B|\psi_2\rangle = 0$

Ef (mælistærðir) $[A,B]=0$ þá má finna grunn í ástandarúminu með eiginvektorum A og B sameiginlegum

---

CSCO

$\{A, B, C \dots\}$ er CSCO ef

i) Allar mælistærðir A, B, C víxlast í pörum

ii) ákveðin eigingildi allra virkjanna A, B, C ákvarða einhlítt sameiginlegan vigur mælistærð með einföld eigingildi

er CSCO

í vetnis atómi

$$H, L^2, L_z \ (S)$$

Fullkomið safn víxlanlegra mælistærða

---

fyrir eðlisfræðilegt kerfi eru til nokkur slík söfn

$\{|r\rangle\}$ og $\{|p\rangle\}$ – framsetningar

höfum sagt að samsvörunin

$$\mathcal{F} \ni \psi(r) \longleftrightarrow |\psi\rangle \in \mathcal{E}_r$$

sé algild

sama um innfeldi

$$\langle\varphi|\psi\rangle = \int d\bar{r}\, \varphi^*(\bar{r})\, \psi(\bar{r})$$

---

athuga (Undirstrika notagildi)

$$|\bar{r}_0\rangle \longleftrightarrow \xi_{\bar{r}_0}(\bar{r}) = \delta(\bar{r}-\bar{r}_0)$$

$$|\bar{p}_0\rangle \longleftrightarrow v_{\bar{p}_0}(\bar{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\bar{p}_0\cdot\bar{r}}$$

1) Einingaréttir grunnar, því

$$\langle\bar{r}_0|\bar{r}_0'\rangle = \int d\bar{r}\, \xi^*_{\bar{r}_0}(\bar{r})\, \xi_{\bar{r}_0'}(\bar{r}) = \delta(\bar{r}_0-\bar{r}_0')$$

$$\langle\bar{p}_0|\bar{p}_0'\rangle = \int d\bar{r}\, v^*_{\bar{p}_0}(\bar{r})\, v_{\bar{p}_0'}(\bar{r}) = \delta(\bar{p}_0-\bar{p}_0')$$

Örsmáðar einoka virki

$U(\epsilon)$ er einoka ϵ : örsmátt

$U(\epsilon) \to \mathbb{1}$ þegar $\epsilon \to 0$

$$\to \begin{cases} U(\epsilon) = \mathbb{1} + i\epsilon F \\ U^{\dagger}(\epsilon) = \mathbb{1} - i\epsilon F^{\dagger} \end{cases}$$

$$U(\epsilon)U^{\dagger}(\epsilon) = \mathbb{1} + i\epsilon(F - F^{\dagger}) + \dots = \mathbb{1}$$

$$\to F = F^{\dagger}$$

og $$\tilde{A} - A = -i\epsilon[F, A]$$

F: er vaki (framleiðandi) ummyndunarinnar U

dæmi:

U	F
hliðrun	$\bar{P}$
snúningur	$\bar{L}$

Einoka ummyndanir virkja

$$\{|v_i\rangle\} \xrightarrow{U} \{|\tilde{v}_i\rangle\}$$

$$\langle v_i|A|v_j\rangle = \langle v_i|U^{\dagger}U A U^{\dagger}U|v_j\rangle$$
$$= \langle \tilde{v}_i|\tilde{A}|\tilde{v}_j\rangle$$

með $\tilde{A} = UAU^{\dagger}$

$\tilde{A}$ hefur sömu fylkisstök í $\{|\tilde{v}_i\rangle\}$ og A í $\{|v_i\rangle\}$

A og $\tilde{A}$ hafa sömu eigingildi

$$\tilde{F}(A) = F(\tilde{A})$$

Einoka ummyndanir varðveita norm

$$|\tilde{\Psi}_1\rangle = U|\Psi_1\rangle$$
$$|\tilde{\Psi}_2\rangle = U|\Psi_2\rangle \longrightarrow \langle\tilde{\Psi}_1|\tilde{\Psi}_2\rangle = \langle\Psi_1|U^{\dagger}U|\Psi_2\rangle = \langle\Psi_1|\Psi_2\rangle$$

Einoka virkjar eru því notaðir til þess að skipta um einingarétta grunna

---

Eigingildi einokavirkja eru tvinntölur z með $|z|^2=1$

$$\longrightarrow z = e^{ia}, \quad a \in \mathbb{R}$$

Eiginvektorar mismunandi eigingilda einoka virkja eru hornréttir

Viðvörun

$$\boxed{\frac{d}{dt}e^{A(t)} \neq \frac{dA}{dt}\cdot e^{A(t)} \quad \text{ef} \quad \left[A(t), \frac{dA}{dt}\right] \neq 0}$$

Viðbót um einokavirkja C11

Virki er einoka ef: $U^{-1} = U^{\dagger}$

$$\longrightarrow U^{\dagger}U = UU^{\dagger} = \mathbb{1}$$

---

t.d ef A er sjálfoka

$$\longrightarrow T = e^{iA} \text{ er einoka}$$

Margfeldi tveggja einoka virkja er einoka

(6)

Jafna Glaubers

$$e^{A} e^{B} = e^{A+B} e^{\frac{1}{2}[A,B]}$$

Sömmun bls 174-5

$$[\hat{X}, F(\hat{P})] = i\hbar F'(\hat{P})$$

$$[\hat{P}, G(\hat{X})] = -i\hbar G'(\hat{X})$$

Afleiða virkja

ekki endilega tími

$$\frac{dA}{dt} = \lim_{\Delta t \to 0} \frac{A(t+\Delta t) - A(t)}{\Delta t}$$

ef $\{|u_i\rangle\}$ er óháður t

og $\langle u_i | A | u_j \rangle = A_{ij}(t)$

$$\rightarrow \left(\frac{dA}{dt}\right)_{ij} = \frac{d}{dt} A_{ij}$$

(5)

Föll af virkjum

dæmi: ef ástand þróast í tíma

$$i\hbar \partial_t |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$

$$\rightarrow |\Psi(t)\rangle = \underbrace{e^{-i\hat{H}(t-t_0)/\hbar}} |\Psi(t_0)\rangle$$

hver er merking þessa ?

. . . . . .

Ef $f(z) = \sum_{n=0}^{\infty} f_n z^n$, $z \in \mathbb{C}$

$$\rightarrow f(A) = \sum_{n=0}^{\infty} f_n A^n$$

$$\rightarrow e^{A} = \sum_{n=0}^{\infty} \frac{A^n}{n!}$$

---

ef $A|\varphi_a\rangle = a|\varphi_a\rangle$

$$\rightarrow F(A)|\varphi_a\rangle = F(a)|\varphi_a\rangle$$

Viðbót B_{II} um virkja

hagnýtt gildi

Spor virkja

$$\mathrm{Tr}\,A = \sum_i \langle u_i|A|u_i\rangle \qquad \Big| \quad \mathrm{Tr}\,A = \int d\alpha \langle w_\alpha|A|w_\alpha\rangle$$

þ.s. $\{|u_i\rangle\}$ er einingaréttur grunnur

$\mathrm{Tr}\,A$ er óháður grunni

sama með svipaðri aðf.

$$\mathrm{Tr}\,AB = \mathrm{Tr}\,BA$$

$$\mathrm{Tr}\,ABC = \mathrm{Tr}\,BCA = \mathrm{Tr}\,CAB$$

$\longrightarrow$ notkun í safneðlisfræði (sjá síðar)

Víxlvirkja

$$[A,B] = -[B,A]$$

$$[A,(B+C)] = [A,B] + [A,C]$$

$$[A,BC] = [A,B]C + B[A,C]$$

$$[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$$

$$[A,B]^\dagger = [B^\dagger, A^\dagger]$$

Fourier staðreyndir

nota lokun

$$\langle \varphi|\psi\rangle = \int d\bar{r} \langle \varphi|\bar{r}\rangle\langle \bar{r}|\psi\rangle = \int d\bar{r}\, \varphi^*(\bar{r})\psi(\bar{r})$$

en einnig

$$\langle \varphi|\psi\rangle = \int d\bar{p} \langle \varphi|\bar{p}\rangle\langle \bar{p}|\psi\rangle = \int d\bar{p}\, \bar{\varphi}^*(\bar{p})\bar{\psi}(\bar{p})$$

skipta um grunn

$$\langle r|\psi\rangle = \int d\bar{p} \langle r|p\rangle\langle p|\psi\rangle$$

$$\psi(\bar{r}) = \frac{1}{(2\pi\hbar)^{3/2}}\int d\bar{p}\, e^{\frac{i}{\hbar}\bar{p}\cdot\bar{r}}\, \bar{\psi}(\bar{p})$$

$\hat{p}$ og $\hat{x}$ með eigin vektora $|\bar{x}\rangle$ og $|\bar{p}\rangle$ eru sjálfoka virkjar og mælistærðir

lesa sjálf 149–153

Geyma F hlutann bls 153

$$\sum_i \langle U_i | A | U_i \rangle = \sum_i \langle U_i | \left\{ \sum_l |t_l\rangle\langle t_l| \right\} A | U_i \rangle$$

$$= \sum_{i,l} \langle U_i | t_l \rangle \langle t_l | A | U_i \rangle$$

$$= \sum_{i,l} \langle t_l | A | U_i \rangle \langle U_i | t_l \rangle$$

$$= \sum_l \langle t_l | A | t_l \rangle$$

Fullkominn grunnar

$$\int d\bar{r}_0 \, |\bar{r}_0\rangle\langle \bar{r}_0| = \mathbb{1}$$

$$\int d\bar{p}_0 \, |\bar{p}_0\rangle\langle \bar{p}_0| = \mathbb{1}$$

---

tengsl

$$\langle \bar{r}_0 | \psi \rangle = \int d\bar{r} \, \xi^*_{\bar{r}_0}(\bar{r}) \psi(\bar{r}) = \psi(\bar{r}_0)$$

$$\langle \bar{p}_0 | \psi \rangle = \int d\bar{r} \, v^*_{\bar{p}_0}(\bar{r}) \psi(\bar{r}) = \bar{\psi}(\bar{p}_0)$$

gildi ψ í punktinum $\bar{r}_0$ er þá hnit $|\psi\rangle$ í $|\bar{r}_0\rangle$ stefnuna í $\{|\bar{r}_0\rangle\}$ grunninum

Venja að nota ~~r~~ $\bar{r}$ í stað $\bar{r}_0$ ----

$$\sum_i |u_i\rangle\langle u_i| = \mathbb{1} \rightarrow \sum_i \langle \bar{r} | u_i \rangle \langle u_i | \bar{r}' \rangle = \langle \bar{r} | \bar{r}' \rangle$$

$$\rightarrow \sum_i u_i(\bar{r}) u_i^*(\bar{r}') = \delta(\bar{r} - \bar{r}')$$

Grunnur skammtafræðinnar

1. Á $t=t_0$ er ástand kerfisins ákveðið með $|\psi(t_0)\rangle \in \Sigma$

2. Mælistærðir eru virkjar A sem vinna á Σ

3. Mæliniðurstöður á A eru eitthvert eigingildi A

4. Þegar A er mælt eru líkindin $\mathcal{P}(a_n)$ fyrir a_n

$$\mathcal{P}(a_n)=\sum_{i=1}^{g_n}|\langle u_n^i|\psi\rangle|^2$$

þ.s. g_n er margfeldni a_n og $\{|u_n^i\rangle\}$ $i=1,2..g_n$ spannar Σ_n hlutrúm Σ ákveðið af a_n og A

$$\mathcal{P}(a_n)=|\langle u_n|\psi\rangle|^2$$

$d\mathcal{P}(\alpha)=|\langle w_\alpha|\psi\rangle|^2 d\alpha$

þ.s. u_n er eiginvektor A með a_n

5. Ef mæling á $\hat{A}$ gefur a_n þá er kerfið í

$$\frac{1}{\sqrt{\sum_{i=1}^{g_n}|c_n^i|^2}}\sum_{i=1}^{g_n} c_n^i|u_n^i\rangle$$

eftir mælingu. þ.s. $\{|u_n^i\rangle\}$ eru hlutrúm a_n

6. Tímaþróun $|\psi(t)\rangle$ er:

$$i\hbar\, d_t|\psi(t)\rangle=\hat{H}(t)|\psi(t)\rangle$$

þ.s. $\hat{H}$ er mælistærð fyrir heildarorkuna

Skömmtun

Hvernig er virkinn $\hat{A}$ búinn til sem samsvarar klassíska mælistærðinni $\mathcal{A}$?

Virkinn $\hat{A}$ er fenginn með því að $p \to \hat{p}$ og $r \to \hat{r}$ í $\mathcal{A}(p,r)$ eftir að röðun rapp hefur verið gerð samhverf í $\mathcal{A}(p,r)$ $[\hat{r},\hat{p}] = i\hbar$

t.d. $\frac{1}{2}(\hat{R}\cdot\hat{p} + \hat{p}\cdot\hat{R}) \leftarrow \bar{R}\cdot\bar{p}$

þ.s. $\hat{R}\cdot\hat{p}$ er ekki sjálfoka

$$\mathcal{H}(r,p) = \frac{\bar{p}^2}{2m} + V(\bar{r}) \to \hat{H} = \frac{\hat{p}^2}{2m} + V(\bar{r})$$

[Kör skömmtun] aðrar leiða til

meðalgildi virkja

$$\langle A \rangle_\psi \equiv \langle \psi | A | \psi \rangle$$

$$(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$$

Afleiðingar Schrödinger jöfnunnar

$$i\hbar d_t |\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$$

* norm breytist ekki í tíma

$$\frac{d}{dt}\langle \psi(t)|\psi(t)\rangle$$

$$= \{d_t\langle\psi(t)|\}|\psi(t)\rangle + \langle\psi(t)|\{d_t|\psi(t)\rangle\}$$

$$= -\frac{1}{i\hbar}\langle\psi|\hat{H}|\psi\rangle + \frac{1}{i\hbar}\langle\psi|H|\psi\rangle = 0$$

þ.s.

$$-i\hbar d_t\langle\psi(t)| = \langle\psi(t)|\hat{H}^\dagger(t) = \langle\psi(t)|\hat{H}(t)$$

$\to |\psi|^2$ má túlka með líkindadreifingu

staðbundin varðveisla líkinda

$$\rho(\bar r,t) = |\Psi(\bar r,t)|^2$$

höfum sýnt að heildar líkindin eru varðveitt staðbundið verður að bæta við, m.hliðsjón af t.d. varðveislu rafhl.

$$\partial_t \rho(\bar r,t) + \bar\nabla\cdot\bar j(\bar r,t) = 0$$

hvernig er líkindastraumurinn ?

ef $\hat H = \frac{\hat P^2}{2m} + V(\hat R,t)$

$$i\hbar\partial_t\Psi(r,t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\bar r,t) + V(\bar r,t)\Psi(r,t) \qquad (1)$$

$$-i\hbar\partial_t\Psi^*(r,t) = -\frac{\hbar^2}{2m}\nabla^2\Psi^*(r,t) + V(r,t)\Psi^*(r,t) \qquad (2)$$

$\Psi^*\cdot(1) + (2)\cdot\Psi$

$$\hookrightarrow i\hbar\partial_t\{\Psi^*(r,t)\Psi(r,t)\} = -\frac{\hbar^2}{2m}\{\Psi^*\nabla^2\Psi - (\nabla^2\Psi^*)\Psi\}$$

$\longrightarrow$

$$\partial_t\{\Psi^*\Psi\} = -\frac{\hbar}{2mi}\bar\nabla\cdot\{\Psi^*\bar\nabla\Psi - (\bar\nabla\Psi^*)\Psi\} -$$

$$\rightarrow \hat j(\bar r,t) = \frac{\hbar}{2mi}\{\Psi^*\bar\nabla\Psi - (\bar\nabla\Psi^*)\Psi\}$$

$$= \frac{\hbar}{2mi}\{\Psi^*\overleftrightarrow{\nabla}\Psi\}$$

í Rafsegulsviði fæst.

$$\bar j(r,t) = \frac{\hbar}{2mi}\{\Psi^*\overleftrightarrow{D}\Psi\}$$

þ.s. $-i\hbar\overleftrightarrow{D} = -i\hbar\overleftrightarrow{\nabla} - q\bar A$ ← vektormætti

tímaþróun væntingargildis

$$\langle A\rangle(t) = \langle\Psi(t)|\hat A|\Psi(t)\rangle$$

$$d_t \langle \Psi(t)| A(t) | \Psi(t)\rangle$$

$$= \left\{ d_t \langle \Psi(t)| \right\} A(t) |\Psi(t)\rangle + \langle \Psi(t)| A(t) \left\{ d_t |\Psi(t)\rangle \right\} + \langle \Psi(t)| \left\{ \partial_t A \right\} |\Psi(t)\rangle$$

$$\rightarrow d_t \langle A \rangle = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}(t)] \rangle + \langle \partial_t A \rangle$$

$\hat{R}$ og $\hat{P}$ eru óháð t, en ekki $|\Psi(t)\rangle$ munur frá klassískri eðl.

<u>Ehrenfest</u>

ef $\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{R})$

þá má sýna

$$\boxed{\begin{aligned} d_t \langle \hat{R} \rangle &= \frac{1}{m} \langle \hat{P} \rangle \\ d_t \langle \hat{P} \rangle &= - \langle \overline{\nabla} V(\hat{R}) \rangle \end{aligned}}$$

tengsl við klassíska eðlisfræði

$\hat{H}$ er óháð t

óháðar skammtatölum en n

finnum $|\Psi(t)\rangle$ ef $|\Psi(t_0)\rangle$ er þekkt

$$|\Psi(t_0)\rangle = \sum_{n,\tau} c_{n,\tau}(t_0) |\varphi_{n,\tau}\rangle$$

$$\rightarrow |\Psi(t)\rangle = \sum_{n,\tau} c_{n,\tau}(t_0) e^{-iE_n(t-t_0)/\hbar} |\varphi_{n,\tau}\rangle$$

<u>Safnvirkinn</u> (líkinda virki) E_{III}

<u>hreint ástand</u>

$$\rho(t) \equiv |\Psi(t)\rangle\langle\Psi(t)|$$

líkinda fylki $\rho_{nm}(t) = \langle u_n | \rho(t) | u_m \rangle$

$$= c_m^*(t) c_n(t)$$

$$\mathrm{tr}\,\rho(t) = \sum_n |c_n(t)|^2 = 1$$

A óháð tíma

$$\langle \hat{A} \rangle (t) = \langle \Psi(t)| A |\Psi(t)\rangle = \sum_{nm} c_n^*(t) c_m(t) A_{nm}$$

→

$$\langle \hat{A} \rangle (t) = \sum_{n,p} \langle u_p | \rho(t) | u_n \rangle \langle u_n | A | u_p \rangle$$

$$= \sum_p \langle u_p | \rho(t) A | u_p \rangle = tr\{\rho(t) A\}$$

$$d_t \hat{\rho}(t) = \frac{1}{i\hbar} [\hat{H}(t), \rho(t)]$$

$$\mathcal{P}(a_n) = \langle \psi(t) | P_n | \psi(t) \rangle = tr\{\rho(t) P_n\}$$

Í hreinu ástandi eru sömu upplýsingar í ρ og ψ

Blandað ástand

tölfræðileg blanda ástanda $|\psi_1\rangle, |\psi_2\rangle, \ldots$
með líkindum $p_1, p_2, \ldots$ ← ekki endilega þekkt
ástöndin þurfa ekki öll að vera hornrétt.

ekki rugla saman við $|\psi\rangle$ sem er línuleg samantekt ástanda

$$|\psi\rangle = \sum_k c_k |\psi_k\rangle$$ ← þá koma víxl liðir $c_k c_q^*$ í $|\psi|^2$

Hvað er nú $\mathcal{P}(a_n)$

P_n er ofanvarp á hlutrúmið fy $= a_n$

$$P_n = \sum_{i=1}^{g_n} |u_n^i\rangle\langle u_n^i|$$

$$\mathcal{P}_k(a_n) = \langle \psi_k | P_n | \psi_k \rangle$$

$$\mathcal{P}(a_n) = \sum_k p_k \mathcal{P}_k(a_n)$$

$\langle P_n \rangle (t)$

eins og áður → $\mathcal{P}_k(a_n) = Tr\{\rho_k P_n\}$

ef $\rho_k = |\psi_k\rangle\langle\psi_k|$

$$\rightarrow \mathcal{P}(a_n) = \sum_k p_k Tr\{\rho_k P_n\}$$

$$= Tr\{\underbrace{\textstyle\sum_k p_k \rho_k}\, P_n\} = Tr\{\rho P_n\}$$

Skilgr. á ρ

og eins og áður

$$\langle \hat{A} \rangle = \mathrm{Tr}\{\rho \hat{A}\}$$

$$i\hbar \, d_t \, \hat{\rho}_k(t) = [\hat{H}(t), \hat{\rho}_k(t)]$$

---

dæmi um notkun

Safneðlisfræði

$$\rho = Z^{-1} e^{-\hat{H}/kT}$$

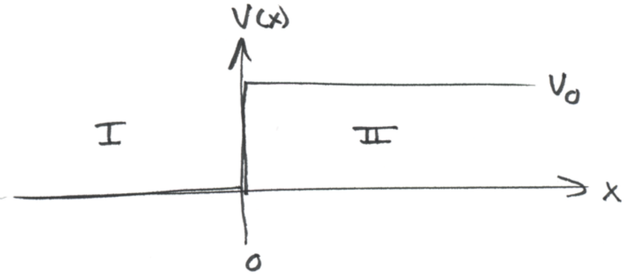
⋮

Myndir Heisenbergs
Schrödingers

....

Viðbót B

Straumur við mættisþrep



(I) $$\psi(x) = A e^{ikx} + A' e^{-ikx} \qquad E = \frac{\hbar^2 k^2}{2m}$$

Ef $E < V_0$

(II) $$\psi(x) = B e^{\kappa x} + B' e^{-\kappa x}$$

Þar sem $B' = 0$ ef mættisþrepið er óendanlega langt, annars $B' \neq 0$

$$J(\vec{r},t) = \frac{\hbar}{2mi}\left\{ \psi^*(\vec{r},t)\, \vec{\nabla}\psi(\vec{r},t) - \text{c.c.} \right\}$$

á svæði (I) fyrst:

$$J_x = \frac{\hbar k}{m}\left\{|A|^2 - |A'|^2\right\}$$

→ tvær bylgjur með $p = \pm \hbar k$
og líkindaþéttleika $|A|^2$ og $|A'|^2$

á svæði (II)

$$J_x = \frac{\hbar k}{2mi}\left\{(B^* e^{kx} + B'^* e^{-kx})(B e^{kx} - B' e^{-kx}) - (B^* e^{kx} - B'^* e^{-kx})(B e^{kx} + B' e^{-kx})\right\}$$

$$= \frac{\hbar k}{2mi}\left\{-B^* B' + B^{*\prime} B - B^* B' + B^{*\prime} B\right\}$$

$$= \frac{\hbar k}{m}\left\{ i B^* B' + c.c.\right\}$$

$= 0$ ef $B' = 0$ þegar þrepið
er óendanlegt.

<u>líkindi speglunar</u> er hlutfall
út og inn straums á svæði (I)

$$R = \left|\frac{A'}{A}\right|^2$$

<u>líkindi framferðar</u> um þrepið
er hlutfall inn straums og
gegnflæðis <u>finnast aðeins þegar $E > V_0$</u>

$$T = \frac{k_2}{k}\left|\frac{B}{A}\right|^2$$

Viðbót G

Schrödinger, Heisenberg-myndir

Schrödinger mynd
(notuð hingað til)

$$i\hbar d_t |\Psi_s(t)\rangle = \hat{H}_s |\Psi_s(t)\rangle$$

→ ástand þróast í tíma

$$|\Psi_s(t)\rangle = U(t,t_0)|\Psi_s(t_0)\rangle$$

með
$$U(t,t_0) = e^{-iH_s(t-t_0)/\hbar}$$
ef $H_s \neq H(t)$

meðan virkjar eins og $\hat{p}$ og $\hat{x}$ o.s.fr. ...
eru tímaóháðir!

Skilgreinum Heisenberg mynd

Einota umvörpun

ástand þróast ekki í tíma

$$\boxed{|\Psi_H\rangle \equiv U^+(t,t_0)|\Psi_s(t)\rangle}$$

$$= U^+(t,t_0)U(t,t_0)|\Psi_s(t_0)\rangle$$

$$= |\Psi_s(t_0)\rangle$$

fylgja stök óbreytt

$$\boxed{A_H(t) \equiv U^+(t,t_0)A_s(t)U(t,t_0)}$$

Svo Heisenberg virki er tímaháður jafnvel þó Schrödingervirkinn sé það ekki!

og í stað Schrödinger jöfnunnar kemur

$$\boxed{i\hbar d_t A_H(t) = [A_H(t), H_H(t)] + i\hbar\left(d_t A_s(t)\right)_H}$$

Sjá bók

Hreintóna sveifill V

(1)

$$H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 X^2$$

þ.s. H, P og X eru virkjar, $[X, P] = i\hbar$

Eigingildi H

til einföldunar, nota víddarlausu virkjana

$$\hat{X} = \sqrt{\frac{m\omega}{\hbar}}\, X \quad \text{og} \quad \hat{P} = \sqrt{\frac{1}{m\hbar\omega}}\, P$$

þá fæst

$$[\hat{X}, \hat{P}] = i$$

og

$$H = \frac{m\hbar\omega}{2m} \hat{P}^2 + \frac{1}{2} \frac{m\omega^2\hbar}{m\omega} \hat{X}^2$$

$$= \hbar\omega \left\{ \frac{1}{2}\left(\hat{P}^2 + \hat{X}^2 \right) \right\} = \hbar\omega \hat{H}$$

leitum því lausna á

$$\hat{H} |\varphi_\nu^i\rangle = \varepsilon\, |\varphi_\nu^i\rangle$$

(2)

Veljum nýja virkja

$$\hat{X} = \frac{1}{\sqrt{2}}(a^+ + a)$$

$$\hat{P} = \frac{i}{\sqrt{2}}(a^+ - a)$$

a og a^+ eru ekki sjálfoka virkjar

hvers vegna a^+ og a .... hornalínuform $\hat{H}$

$$[a, a^+] = \frac{1}{2}[\hat{X} + i\hat{P}, \hat{X} - i\hat{P}] = \frac{i}{2}[\hat{P}, \hat{X}] - \frac{i}{2}[\hat{X}, \hat{P}]$$

$$= 1$$

$$a^+ a = \frac{1}{2}(\hat{X} - i\hat{P})(\hat{X} + i\hat{P})$$

$$= \frac{1}{2}(\hat{X}^2 + \hat{P}^2 + i\hat{X}\hat{P} - i\hat{P}\hat{X})$$

$$= \frac{1}{2}(\hat{X}^2 + \hat{P}^2 - 1)$$

$$\rightarrow \boxed{\hat{H} = a^+ a + \frac{1}{2}}$$

3

Skilgreinum $N = a^\dagger a \qquad N^\dagger = a^\dagger a = N$

$\longrightarrow \hat{H} = N + \frac{1}{2}$

$\longrightarrow$ $\boxed{\text{eiginvektorar } \hat{H} \text{ og } N \text{ eru sameiginlegir}}$ — $[\hat{H}, N] = 0$

$[N,a] = [a^\dagger a, a] = a^\dagger [a,a] + [a^\dagger, a] a = -a$

$[N,a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger [a,a^\dagger] + [a^\dagger, a^\dagger] a = a^\dagger$

~~Ākvörđ~~

~~Lítum á róf N~~

$\cancel{\| a |\varphi_\nu^i\rangle \|^2 \geq 0}$

$\cancel{\hookrightarrow \langle \varphi_\nu^i | a^\dagger a | \varphi_\nu^i \rangle \geq 0}$

$\cancel{= \langle \varphi_\nu^i | N | \varphi_\nu^i \rangle \geq 0}$

$\cancel{= f(\nu) \langle \varphi_\nu^i | \varphi_\nu^i \rangle \geq 0}$

$\cancel{\rightarrow f(\nu) \geq 0}$

ef $\hat{H} = N + \frac{1}{2}$ hefur eigingildi

$\hat{H} |\varphi_\nu^i\rangle = (\nu + \frac{1}{2}) |\varphi_\nu^i\rangle$

$N |\varphi_\nu^i\rangle = \nu |\varphi_\nu^i\rangle$

$\| a |\varphi_\nu^i\rangle \|^2 \geq 0$

$\hookrightarrow \langle \varphi_\nu^i | a^\dagger a | \varphi_\nu^i \rangle \geq 0$

$\parallel$

$\langle \varphi_\nu^i | N | \varphi_\nu^i \rangle \geq 0$

$\nu \langle \varphi_\nu^i | \varphi_\nu^i \rangle = \nu \geq 0$

4

Orkuróf

$\hat{P}$ og $\hat{X}$ eru sjálfoka → eigingildi þeirra eru rauntölur

$$\hat{H} = \frac{1}{2}(\hat{P}^2 + \hat{X}^2)$$

→ eigingildi $\hat{H}$ ~~og þar með~~ eru pósitíf

sjá ← $\hat{H}|\varphi_\nu^i\rangle = \varepsilon_\nu|\varphi_\nu^i\rangle \quad , \quad \varepsilon_\nu \geq 0$

Veljum $|\varphi_0^i\rangle$ sem lægstu eiginástönd $\hat{H}$

$$\hat{H}|\varphi_0^i\rangle = \varepsilon_0|\varphi_0^i\rangle$$

$$a\hat{H}|\varphi_0^i\rangle = \varepsilon_0 a|\varphi_0^i\rangle$$

$$a\hat{H} = \hat{H}a + [a,\hat{H}] = \hat{H}a + [a,N]$$
$$= \hat{H}a + a$$

→ $(\hat{H}a + a)|\varphi_0^i\rangle = E_0 a|\varphi_0^i\rangle$

→ $\hat{H}(a|\varphi_0^i\rangle) = (\varepsilon_0 - 1)a|\varphi_0^i\rangle$

ef $\nu > 0$ þá er $a|\varphi_\nu^i\rangle$ eiginvigur N með eigingildi $\nu - 1$

ef $\nu > 0$ þá er $a^+|\varphi_\nu^i\rangle$ eiginvigur N með eigingildi $\nu + 1$

síðan þarf að sanna að $\nu = n$

5

en $|\varphi_0^i\rangle$ vora\ orka lægstu eiginástöndin

$$\rightarrow \quad a|\varphi_0^i\rangle = 0$$

$$\rightarrow \quad a^+a|\varphi_0^i\rangle = N|\varphi_0^i\rangle = 0$$

$$\rightarrow \quad \hat{H}|\varphi_0^i\rangle = \frac{1}{2}|\varphi_0^i\rangle$$

með þá $\quad \Sigma_0^i = \frac{1}{2}$ núllpunktsorka kom vegna $[a,a^+] \neq 0$

---

athugum

$$a^+\hat{H}|\varphi_0^i\rangle = \frac{1}{2}a^+|\varphi_0^i\rangle$$

$$\rightarrow \quad (\hat{H}a^+ - a^+)|\varphi_0^i\rangle = \frac{1}{2}a^+|\varphi_0^i\rangle$$

$$\rightarrow \quad \hat{H}(a^+|\varphi_0^i\rangle) = (1+\frac{1}{2})(a^+|\varphi_0^i\rangle)$$

ítra

$$\hat{H}((a^+)^n|\varphi_0^i\rangle) = (n+\frac{1}{2})((a^+)^n|\varphi_0^i\rangle)$$

$$a^+|\varphi_n\rangle = \sqrt{n+1}\,|\varphi_{n+1}\rangle$$

$$a|\varphi_n\rangle = \sqrt{n}\,|\varphi_{n-1}\rangle$$

$$\langle\varphi_{n'}|a|\varphi_n\rangle = \sqrt{n}\,\delta_{n';n-1}$$

$$\langle\varphi_{n'}|a^+|\varphi_n\rangle = \sqrt{n+1}\,\delta_{n';n+1}$$

(6)

a^+ : skapar orkuskammt 1

a : eyðir orkuskammti 1

$$\mathcal{E}_n^i = (n + 1/2)$$

og eigingildi N er n

N : telur orkuskammta
(eða ákvarðar # ástands)

---

finnum $\langle x | \varphi_0^i \rangle$

$$a | \varphi_0^i \rangle = 0$$

$$\to \frac{1}{\sqrt{2}} \left\{ \sqrt{\frac{m\omega}{\hbar}}\, x + \frac{i}{\sqrt{m\hbar\omega}}\, p \right\} | \varphi_0^i \rangle = 0$$

eða
$$\left(\frac{m\omega}{\hbar} x + d_x \right) \varphi_0^i(x) = 0$$

$$\to \varphi_0^i(x) = c\, e^{-\frac{1}{2}\frac{m\omega}{\hbar} x^2}$$

(7)

i : er óþarfur vísir þ.s. $\varphi_0(x)$ er einkvæmt (aðeins mism. c mögul sem við festum með normun)

$$E_n = \hbar\omega(n + \tfrac{1}{2})$$

sýnt er fram á að öll ástöndin eru einkvæm ⟺ engin margfeldni

með ítrun fæst:

$$|\varphi_n\rangle = \frac{1}{\sqrt{n!}} (a^+)^n |\varphi_0\rangle$$

full komin $\{|\varphi_n\rangle\}$ einingarettur grunnur

$$\varphi_n(x) = \left[\frac{1}{2^n n!} \left(\frac{\hbar}{m\omega} \right)^n \right]^{1/2} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \left\{ \frac{m\omega}{\hbar} x - \frac{d}{dx} \right\}^n e^{-\frac{m\omega x^2}{2\hbar}}$$

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

↑ Hermite fleirliður

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n e^{-x^2}}{dx^n}$$

$$e^{2xt - t^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n \qquad |t| < \infty$$

$\vdots$

Ef

$$|\Psi(0)\rangle = \sum_{n=0}^{\infty} C_n(0) |\varphi_n\rangle$$

$$\rightarrow |\Psi(t)\rangle = \sum_{n=0}^{\infty} C_n(0) e^{-iE_n t/\hbar} |\varphi_n\rangle$$

$$\rightarrow \langle\Psi(t)| A |\Psi(t)\rangle = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} C_m^*(0) C_n(0) A_{nm} \cdot e^{i(m-n)\omega t}$$

Viðbætur Hv

tveir tengdir hreintóna sveiflar

$$H = H_1 + H_2 + H_{int}$$

$$H_1 = \frac{P_1^2}{2m} + \frac{1}{2} m\omega^2 (x_1 - a)^2$$

$$H_2 = \frac{P_2}{2m} + \frac{1}{2} m\omega^2 (x_2 + a)^2$$

$$H_{int} = \lambda m\omega^2 (x_1 - x_2)^2$$

lítum á tilfellið með 2 eins sveifla

$\omega_1 = \omega_2 = \omega$

$\uparrow$

margfeldni orkustiga ef engin víxlv.

---

almennar aðferðir lærast á afl fr. gr. og afl fr. I

Skilgr.

$$\left.\begin{aligned} X_q &= \frac{1}{2}(x_1 + x_2) \\ P_q &= P_1 + P_2 \end{aligned}\right\}$$

$$\left.\begin{aligned} X_R &= x_1 - x_2 \\ P_R &= \frac{1}{2}(P_1 - P_2) \end{aligned}\right\}$$

$[x_1, P_1] = i\hbar$

$[x_2, P_2] = i\hbar$

$[X_R, P_R] = i\hbar$

$[X_q, P_q] = i\hbar$

$[X_q, P_R] = 0$

$[X_R, P_q] = 0$

$$H = H_q + H_R + m\omega^2 a^2 \frac{4\lambda}{1+4\lambda}$$

$$H_q = \frac{P_q^2}{2\mu_q} + \frac{1}{2}\mu_q \omega_q^2 x_q^2 \qquad \mu_R = \frac{m}{2}, \quad \mu_q = 2m$$

$$H_R = \frac{P_R^2}{2\mu_R} + \frac{1}{2}\mu_R \omega_R^2 \left\{ x_R - \frac{2a}{1+4\lambda} \right\}^2$$

$$\rightarrow E_{np} = \hbar\omega_q\left(n+\tfrac{1}{2}\right) + \hbar\omega_R\left(n+\tfrac{1}{2}\right) + m\omega^2 a \frac{4\lambda}{1+4\lambda}$$

$\omega_q = \omega$

$\omega_R = \omega\sqrt{1+4\lambda}$

Víxlverkunin $\longrightarrow$ margfeldni hverfur

$\updownarrow$

Klofnun orkustiga

hættir

Orkuhliðrun

tvær sýndareindir sem ekki víxlast

titringsorka	$\leftarrow$ innri hnit
CM-orka	$\leftarrow$ ytri hnit

Samfasa ástönd sveifils GV

Eiginástönd $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$

$|\varphi_n\rangle$ með orku $E_n = \hbar\omega\left(n+\tfrac{1}{2}\right)$ $n = 0, 1, \ldots$

leiða til

$$\langle p\rangle_n = \langle x\rangle_n = 0$$

sem sést best frá því að

$$\hat{p} = \frac{i}{\sqrt{2}}(a^+ - a), \qquad \hat{x} = \frac{1}{\sqrt{2}}(a^+ + a)$$

í sígildri eðlisfræði eru p og x lotubundin föll í tíma

> Er hægt að finna ástönd fyrir H sem haga sér „svipað" sígildum ástöndum sveifils?

Við munum sjá að eigin ástönd a^{+} og a eru þannig að um þau gildir

$$\Delta x \Delta p = \frac{\hbar}{2}$$

(þ.e. minnsta hugsanlega óvissa)

og

$$\langle x \rangle (t) \sim \cos \omega t$$

$$\langle p \rangle (t) \sim \sin \omega t$$

rétt „eins" og fyrir sígildan sveifil

> Ástöndin auka ekki óvissuna með tímanum og eru því kölluð samfasa

Gerum ráð fyrir að til sé ket þ.a.

$$a|\alpha\rangle = \alpha|\alpha\rangle$$

hvernig má liða $|\alpha\rangle$ í eiginvigragrunni H?

$$\langle n|a|\alpha\rangle = \alpha\langle n|\alpha\rangle$$

$$\|$$

$$\sqrt{n+1}\,\langle n+1|\alpha\rangle = \alpha\langle n|\alpha\rangle$$

$\longrightarrow$ þrepum á ~~þessu~~ (sem $\frac{\sqrt{n+1}}{\alpha}\langle n+1|\alpha\rangle = \langle n|\alpha\rangle$)

$\frac{\sqrt{n}}{\alpha}\langle n|\alpha\rangle = \langle n-1|\alpha\rangle$

gefur

$$\langle n|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}}\langle 0|\alpha\rangle$$

Liðunin er (almennt)

$$|\alpha\rangle = \sum_{n=0}^{\infty} |n\rangle\langle n|\alpha\rangle$$

$$\longrightarrow |\alpha\rangle = \langle 0|\alpha\rangle \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

$\{|n\rangle\}$ er einingaréttur grunnur

$$\rightarrow \quad \langle\alpha|\alpha\rangle = |\langle 0|\alpha\rangle|^2 \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!}$$

$$= |\langle 0|\alpha\rangle|^2 e^{|\alpha|^2}$$

því má norma $|\alpha\rangle$ (og velja fasa þess miðað við $|0\rangle$) með

$$\langle 0|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}$$

$$\rightarrow \quad \boxed{|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle}$$

líkindi þess að finna kerfið í ástandi $|n\rangle$ eru því

$$P_n(\alpha) = |\langle n|\alpha\rangle|^2 = e^{-|\alpha|^2} \frac{\alpha^{2n}}{n!}$$

er Poissondreifing með meðalgildi $|\alpha|^2$

Óvissa

$$\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle\alpha|(a^\dagger + a)|\alpha\rangle$$

$$\langle p\rangle = i\sqrt{\frac{m\hbar\omega}{2}} \langle\alpha|(a^\dagger - a)|\alpha\rangle$$

$$\rightarrow \quad \langle x\rangle = \sqrt{\frac{2\hbar}{m\omega}} \,\mathrm{Re}(\alpha)$$

$$\langle p\rangle = \sqrt{2m\hbar\omega} \,\mathrm{Im}(\alpha)$$

(6)

Eftir sömmu leiðum

$$\langle x^2\rangle = \frac{\hbar}{2m\omega}\left\{(\alpha+\alpha^*)^2+1\right\}$$

$$\langle P^2\rangle = \frac{m\hbar\omega}{2}\left\{1-(\alpha-\alpha^*)^2\right\}$$

$$\longrightarrow \boxed{\Delta x\,\Delta P = \frac{\hbar}{2}}$$

<u>hvernig þróast ástöndin í tíma?</u>

Setjum $|\alpha_0\rangle = |\alpha\rangle$

$$\| $$

$$|\alpha(t=0)\rangle$$

þá er

$$|\alpha(t)\rangle = \sum_{n=0}^{\infty} e^{-iE_n t/\hbar}\, e^{-\frac{1}{2}|\alpha_0|^2}\frac{|n\rangle}{\sqrt{n!}}\alpha_0^n$$

$$= e^{-\frac{i\omega t}{2}}\sum_{n=0}^{\infty}\left(e^{-i\omega t}\alpha_0\right)^n \frac{e^{-\frac{1}{2}|\alpha_0|^2}|n\rangle}{\sqrt{n!}}$$

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

(7)

Því sést að $|\alpha(t)\rangle$ er eiginvegur a með eigingildi $e^{-i\omega t}\alpha_0$ þ.a.

$$|\alpha(t)\rangle = e^{-\frac{i\omega t}{2}}\,|e^{-i\omega t}\alpha_0\rangle$$

$\boxed{\text{ástandið er því áfram samfasa}}$!!

Ef þetta er notað í $\langle x\rangle$ og $\langle p\rangle$ fæst

$$\boxed{\begin{aligned}\langle x\rangle(t) &= \sqrt{\frac{2\hbar}{m\omega}}\,|\alpha_0|\cos(\omega t)\\ \langle P\rangle(t) &= -\sqrt{2m\hbar\omega}\,|\alpha_0|\sin(\omega t)\end{aligned}}$$

$\longrightarrow$ <u>$|\alpha_0|$ er útslag sveiflunnar</u> og væntigildin haga sér eins og $x(t)$ og $P(t)$ í sígildri aflsfræði

8

samfasa ástönd eru ekki hornrétt

$$|\langle\beta|\alpha\rangle|^2 = e^{-|\alpha+\beta|^2}$$

þau mynda samt grunn

$$\int |\alpha\rangle\langle\alpha|\, d\alpha = 1$$

Í raun getur þurft að velja hlut mengi samfasa ástanda til þess að fá grunn sem er ekki „over complete"

V. Bargmann Rep. Math. Phys. 2 221 (1971)

Notkun
⋮

R. J. Glauber Phys. Rev. 130 2529 (63)
Phys. Rev. 131 2766 (63)

1

Hverfiþungi

$\mathbb{L}$: brautarhverfiþungi einnar agnar — klassísk hliðstæða

S : spuni — engin kl. hliðst.

$\mathbb{J}$: heildar hverfiþ. kerfis

---

nota klassíska skilgr.

$$\vec{L} = \vec{R} \times \vec{P}$$

$$\rightarrow L_x = yP_z - zP_y$$

y og P_z , z og P_y víxlast
$\rightarrow$ ekki þarf að gera L_x samhverfann

→ skammta virkinn

$$\hat L_x \equiv \hat y \hat p_z - \hat z \hat p_y$$

$$\hat L_y \equiv \hat z \hat p_x - \hat x \hat p_z$$

athuga

$$[\hat L_x, \hat L_y] = [\hat y \hat p_z - \hat z \hat p_y \,,\, \hat z \hat p_x - \hat x \hat p_z]$$

$$= [\hat y \hat p_z, \hat z \hat p_x] + [\hat z \hat p_y, \hat x \hat p_z]$$

$$= \hat y [\hat p_z, \hat z] \hat p_x + \hat x [\hat z, \hat p_z] \hat p_y$$

$$= -i\hbar \hat y \hat p_x + i\hbar \hat x \hat p_y$$

$$= i\hbar L_z$$

$$\left.\begin{aligned} [L_x, L_y] &= i\hbar L_z \\ [L_y, L_z] &= i\hbar L_x \\ [L_z, L_x] &= i\hbar L_y \end{aligned}\right\} \quad [L_i, L_j] = \epsilon_{ijk} L_k \, i\hbar$$

$$\epsilon_{iik} = 0$$

$$\epsilon_{ijk} = -\epsilon_{jik}$$

$$\epsilon_{123} = 1$$

$$\epsilon_{ijk} = \epsilon_{kij} = \epsilon_{jki}$$

<u>hverfiþungi er hvaða</u> 3 mælistærðir sem uppfylla

$$[\hat J_i, \hat J_j] = i\hbar \epsilon_{ijk} \hat J_k$$

p.s. í raun verða „víxlin" til vegna eiginleika snúnings í 3D

$$\hat J^2 \equiv \hat J_x^2 + \hat J_y^2 + \hat J_z^2$$

$$\to \quad [\hat J^2, \hat J] = 0$$

$[\hat J^2, \hat J_i]$ $i = x, y, z$

Ef ögn er í miðjumætti

$$\longrightarrow \quad \underbrace{[\hat H, \hat J]}_{[\hat H, \hat J_i] = 0} = 0$$

$\hat J$ er Hermite virki → $\hat J^2$ er einnig

En þar sem L_i víxlast ekki er ekki hægt ~~að~~ mæla þau öll samtímis fullkomið mengi víxlandi mælistærða er því

$$\boxed{\hat{H},\ \hat{J}^2,\ \hat{J}_z}$$

stigreina

Allir eiginbitar hverfiþunga koma frá $[J_i, J_j] \simeq \epsilon_{ijk} J_k$

$$\left.\begin{array}{l} J_+ \equiv J_x + i J_y \\ J_- \equiv J_x - i J_y \end{array}\right\} \to J_+^{+} = J_-$$

ekki Hermit virkjar, svipar til a, a^+ í H.O.

þá fæst

$$[J_z, J_+] = \hbar J_+$$

$$[J_z, J_-] = -\hbar J_-$$

$$[J_+, J_-] = 2\hbar J_z$$

$$[J^2, J_+] = [J^2, J_-] = [J^2, J_z] = 0$$

$\leftarrow$

$$\left.\begin{array}{l} J_+ J_- = J^2 - J_z^2 + \hbar J_z \\ J_- J_+ = J^2 - J_z^2 - \hbar J_z \end{array}\right\} J^2 = \tfrac{1}{2}(J_+J_- + J_-J_+) + J_z^2$$

Eigingildi $\hat{J}^2$ og J_z

$\langle\psi|J^2|\psi\rangle = \langle\psi|J_x^2|\psi\rangle + \cdots$
$= \| J_x|\psi\rangle\|^2 + \cdots$

Öll eigingildi $\hat{J}^2$ eru ≥ 0

Eigingildin eru á forminu $\lambda\hbar^2$

veljum

$$\lambda = j(j+1)$$
$$\text{með } j \geq 0$$

er hægt því $j(j+1) = \lambda$ hefur aðeins eina (enga aðra) lausn með $j \geq 0$

fyrir J_z eru eigingildin valin sem

$m\hbar$

Eiginvektorar $\hat{J}^2$ og $\hat{J}_z$ eru því merktir með j og m, sem nægja ekki til að tilgreina ástand (J^2 og J_z eru ekki fullkomið mengi víxlandi mælistærða)

$$\rightarrow \quad J^2|k,j,m\rangle = j(j+1)\hbar^2|k,j,m\rangle$$

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

(i) fyrir m má sanna

$$-j \leq m \leq j$$

---

athuga

$$\| J_+|k,j,m\rangle\|^2 = \langle k,j,m|J_-J_+|k,j,m\rangle \geq 0$$

$$\| J_-|k,j,m\rangle\|^2 = \langle k,j,m|J_+J_-|k,j,m\rangle \geq 0$$

og

$$\langle k,j,m|J_-J_+|k,j,m\rangle = j(j+1)\hbar^2 - m^2\hbar^2 - m\hbar^2 \geq 0$$

$$\langle k,j,m|J_+J_-|k,j,m\rangle = j(j+1)\hbar^2 - m^2\hbar^2 + m\hbar^2 \geq 0$$

$$\longrightarrow$$

$$j(j+1) - m(m+1) = (j-m)(j+m+1) \geq 0$$

$$j(j+1) - m(m-1) = (j-m+1)(j+m) \geq 0$$

$$-(j+1) \leq m \leq j$$

$$-j \leq m \leq j+1$$

$$\longrightarrow \quad -j \leq m \leq j$$

(ii) vanrækja mætti

Ef $m=-j \Leftrightarrow J_-|k,j,-j\rangle = 0$

$m > -j$ $\quad J_-|k,j,m\rangle$ er eiginvektor J^2 og J_z með eigingildi $j(j+1)\hbar^2$ og $(m-1)\hbar$

---

höfum séð

$$\| J_-|k,j,m\rangle\|^2 = j(j+1)\hbar^2 - m^2\hbar^2 + m\hbar^2 \geq 0$$

$$= 0 \quad \text{ef} \quad m=-j$$

$$\longrightarrow \quad J_-|k,j,m\rangle = 0$$

og öfugt

ef $m > -j$

$$\| J_- |k,j,m\rangle \|^2 \neq 0 \quad \to J_- |k,j,m\rangle \neq 0.$$

$$[J^2, J_\pm] = 0$$

sama $J_-|kjm\rangle$ er eiginv. J^2 og J_z með $j(j+1)\hbar^2$ og $(m-1)\hbar$

$$\hookrightarrow [J^2, J_-]|k,j,m\rangle = 0$$

$$\to J^2 J_- |kjm\rangle = J_- J^2 |kjm\rangle$$
$$= j(j+1)\hbar^2 J_- |kjm\rangle$$

$\to J_-|kjm\rangle$ er eiginvektor J^2 með $j(j+1)\hbar^2$

$$[J_z, J_-] = -\hbar J_-$$

$$\hookrightarrow J_z J_- |kjm\rangle = J_- J_z |kjm\rangle - \hbar J_- |kjm\rangle$$
$$= m\hbar J_- |kjm\rangle - \hbar J_- |kjm\rangle$$
$$= (m-1)\hbar J_- |kjm\rangle$$

$\to J_-|kjm\rangle$ er eiginv. J_z með $(m-1)\hbar$

Samsvarar fyrir J_+

(iii) ef $m = j$ $\quad J_+|kjj\rangle = 0$

ef $m < j$ $\quad J_+|kjm\rangle \neq 0$ eiginvektor J^2 og J_z með eigingildi $j(j+1)$ og $(m+1)\hbar$

Nú má nota þetta til að sýna að einu möguleikar á gildum fyrir j eru $0, 1/2, 1, 3/2, 2, 5/2, 3 \ldots$ og $m = -j, -j+1, \ldots, j-1, j$

<u>En þessi gildi þurfa ekki að koma öll fyrir í sama kerfinu.</u>

$$\langle k_2 jm | J_\mp J_\pm | k_1 jm \rangle$$

$$= \langle k_2 jm | (J^2 - J_z^2 \mp \hbar J_z) | k_1 jm \rangle$$

$$= \{ j(j+1) - m(m \pm 1) \} \hbar^2 \langle k_2 jm | k_1 jm \rangle$$

$|k, j, m\rangle$ – grunnur (staðal grunnur)

<u>fylkisstök $\bar{J}$</u>

höfum

$$J_z |kjm\rangle = m\hbar |kjm\rangle$$

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

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

$\longrightarrow$

$$\langle kjm | J_z | k'j'm' \rangle = m\hbar \delta_{kk'} \delta_{jj'} \delta_{mm'}$$

$$\langle kjm | J_\pm | k'j'm' \rangle = \hbar \sqrt{j(j+1) - m'(m' \pm 1)}\, \delta_{kk'} \delta_{jj'} \delta_{m, m' \pm 1}$$

$j = 1/2 \rightarrow$

$$\left\{ \begin{array}{l} (J_z)^{1/2} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (J_+)^{1/2} = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ (J_-)^{1/2} = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad (J_x)^{1/2} = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ (J_y)^{1/2} = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad (J^2)^{1/2} = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{array} \right.$$

$j = 1$

$$(J)_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$(J_+) = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \qquad (J_-) = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

$$(J_x) = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad (J_y) = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$(J^2) = 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

---

fylkin uppfylla einnig víxlin

$$[J_i, J_j] = i\hbar \epsilon_{ijk} J_k$$

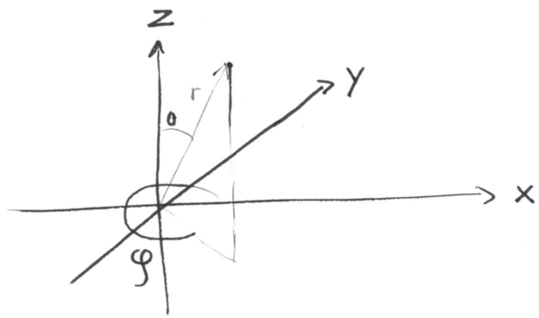
spunalaus ögn

Brautarhverfiþungi í $\{|r\rangle\}$ framsetningu

$$\bar{L} = \bar{R} \times \bar{P} \qquad \langle \bar{r} | \bar{R} | \psi \rangle = \bar{r}\,\psi(\bar{r})$$
$$\langle \bar{r} | \bar{P} | \psi \rangle = -i\hbar \bar{\nabla} \psi(\bar{r})$$

$$\longrightarrow \begin{cases} L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ L_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{cases}$$

skipta um hnit $\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases}$ Kúluhnit



$$\begin{cases} L_x = i\hbar\left(\sin\varphi \frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right) \\ L_y = i\hbar\left(-\cos\varphi \frac{\partial}{\partial\theta} + \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right) \\ L_z = -i\hbar\frac{\partial}{\partial\varphi} \end{cases}$$

$$\begin{cases} \bar{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) \\ L_+ = \hbar e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) \\ L_- = \hbar e^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) \end{cases}$$

höfðum séð

$$\hat{L}^2 |klm\rangle = \hbar^2 l(l+1) |klm\rangle$$

$$L_z |klm\rangle = \hbar m |klm\rangle$$

$$\langle \bar{r}| \cdot \longrightarrow \boxed{\begin{aligned} \bar{L}^2\psi &= \hbar^2 l(l+1)\psi \\ L_z\psi &= \hbar m\psi \end{aligned}}$$

↗ leysa þessar diffurjöfnur

Lausnin verður

$$\psi_{lm}(r,\theta,\varphi) = f(r)\, Y_{lm}(\theta,\varphi)$$

$f(r)$: frjálst fall hér $\longrightarrow L^2$ og L_z mynda ekki FSVM

Veljum normun $\displaystyle\int_0^\infty r^2 dr\, |f(r)|^2 = 1$

$$\int d\Omega\, |Y_{lm}|^2 = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta\, |Y_{lm}(\theta,\varphi)|^2 = 1$$

Í ljós mun koma að visst val á L og m er aðeins ein lausn Y_{lm}

Eiginleitar lausna

$$-i\hbar\partial_\varphi Y_{lm} = m\hbar Y_{lm}$$

$$\longrightarrow Y_{lm}(\theta,\varphi) = F_{lm}(\theta)\, e^{im\varphi}$$

Samfelldni

$$\longrightarrow \quad Y_{lm}(\theta,0) = Y_{lm}(\theta,2\pi)$$

$$\longrightarrow \quad e^{2\pi i m} = 1 \quad \longrightarrow \quad m \in \mathbb{Z} \quad \longrightarrow$$ frá fyrri síðum $l \in \mathbb{N} \cup 0$

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

$$\longrightarrow \quad -\left\{ \frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} - \frac{m^2}{\sin^2\theta} \right\} F_{lm}(\theta) = l(l+1) F_{lm}(\theta)$$

$$\longrightarrow \quad Y_{lm}(\theta,\varphi) = \sqrt{\left(\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right)} \, P_l^m(\cos\theta) \, e^{im\varphi}$$

{hin óháða lausnin $Q_l^m(\cos\theta)$ hefur sérstöðupunkta við $x = \pm 1$}

þar sem

$$P_l^m(x) = \frac{(-1)^m}{2^l \, l!} (1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (x^2-1)^l$$

eru Legendre fleirliðar skilgreindar á bilinu $[-1,1]$

t.d.

$$P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x)$$

Lausnir einungis til fyrir

$$l \geq 0$$

$$-l \leq m \leq l$$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,1} = -\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{i\varphi}$$

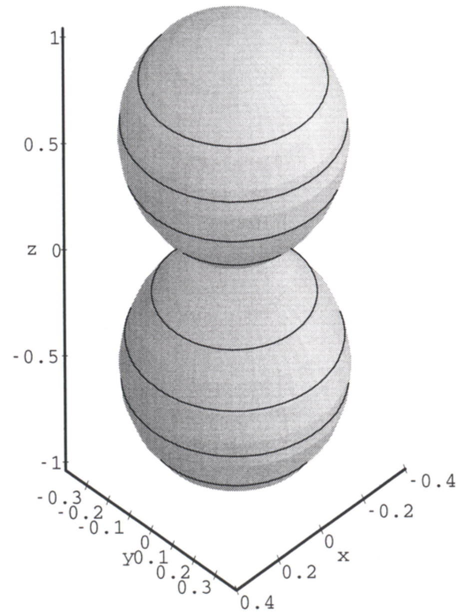
$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$\vdots$$

$$\int d\Omega \, Y^*_{lm} Y_{l'm'} = \delta_{l,l'} \delta_{m,m'}$$ } hornétt og normuð

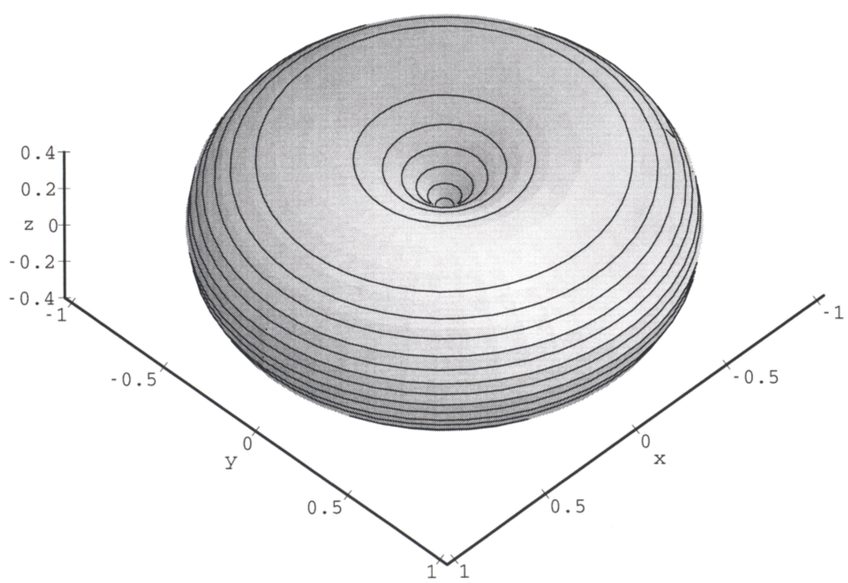
$$Y_{l,-m} = (-1)^m Y^*_{l,m}$$

Y10



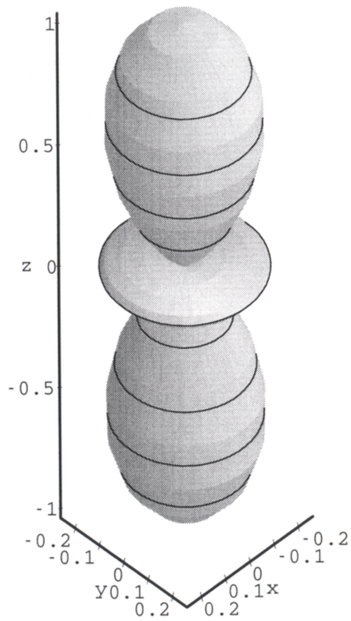
1
0.5
z 0
-0.5
-1
-0.3
-0.2
-0.1
0
y0.1
0.2
0.3
0.4
0.2
0
x
-0.2
-0.4

Y11

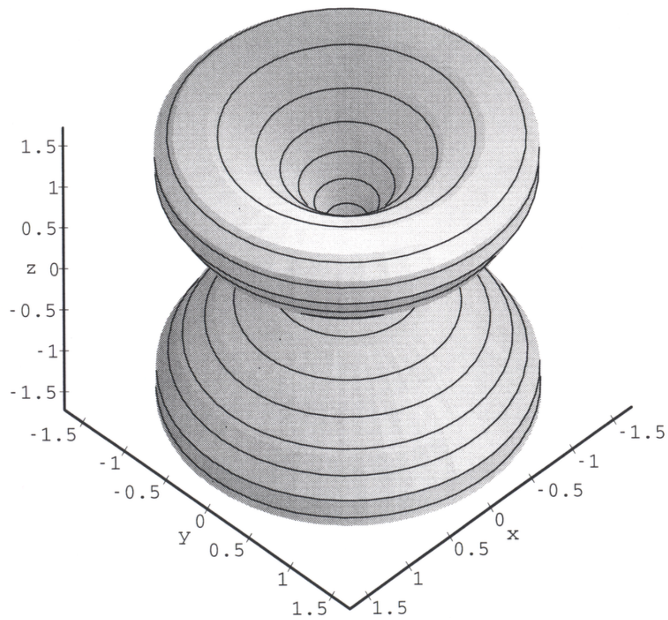


0.4
0.2
z 0
-0.2
-0.4
-1
-0.5
y
0
0.5
1
1
0.5
x
0
-0.5
-1

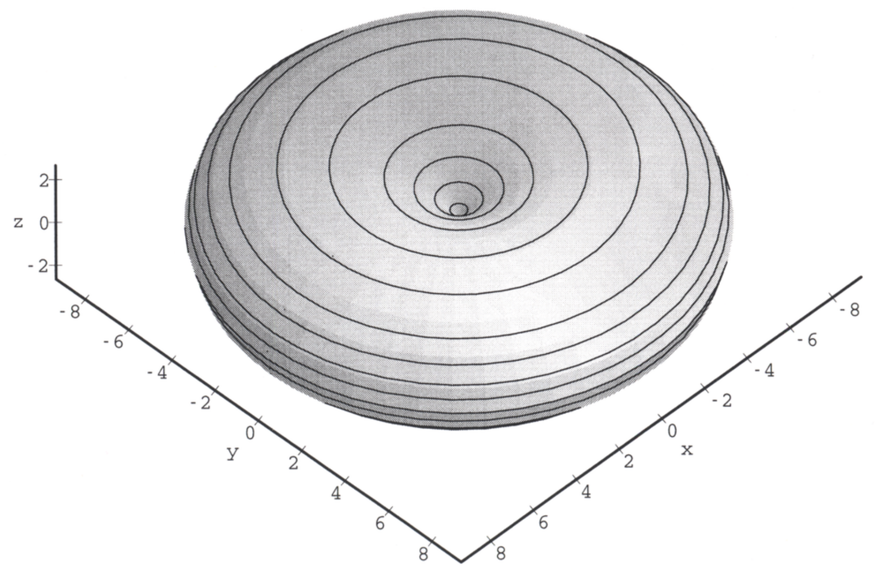
Y20


1
0.5
z 0
-0.5
-1
-0.2
-0.1
0
y 0.1
0.2
-0.2
-0.1
0
0.1 x
0.2

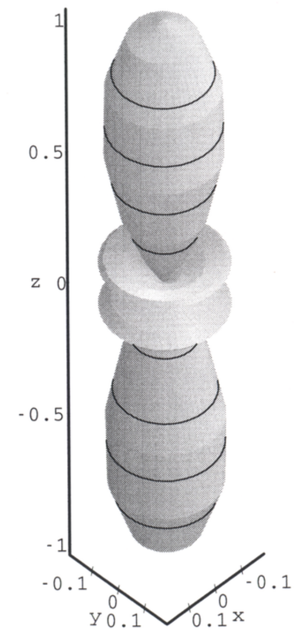
Y21


1.5
1
0.5
z 0
-0.5
-1
-1.5
-1.5
-1
-0.5
y 0
0.5
1
1.5
-1.5
-1
-0.5
0 x
0.5
1
1.5

Y22



Y30



hægt að liða föll

$$f(\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} C_{lm} Y_{lm}(\theta,\varphi)$$

$$C_{lm} = \int d\Omega\, Y^*_{lm}(\theta,\varphi) f(\theta,\varphi)$$

fullkomleiki

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\theta,\varphi) Y^*_{lm}(\theta',\varphi')$$

$$= \delta(\cos\theta - \cos\theta')\delta(\varphi-\varphi')$$

$$= \frac{1}{\sin\theta}\delta(\theta-\theta')\delta(\varphi-\varphi')$$

summuregla

$$\frac{2l+1}{4\pi} P_l(\cos\alpha) = \sum_{m=-l}^{+l} Y^*_{lm}(\theta',\varphi') Y_{lm}(\theta,\varphi)$$

$$\cos\alpha = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi-\varphi')$$

$\rightarrow$

$$\sum_{m=-l}^{l} |Y_{lm}(\theta,\varphi)|^2 = \frac{2l+1}{4\pi}$$

þægileg jafna

$$\frac{1}{|\bar{x}-\bar{x}'|} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{1}{2l+1}\left(\frac{r_<^l}{r_>^{l+1}}\right) Y^*_{lm}(\theta',\varphi') Y_{lm}(\theta,\varphi)$$

$$r_< = \min(r,r')$$

$$r_> = \max(r,r')$$

---

líkindin fyrir því að mæla samtímis $l(l+1)\hbar^2$ og $m\hbar$ fyrir L^2 og L_z

ástandi lýst með $\Psi(r,\theta,\varphi)$

liða

$$\Psi(r,\theta,\varphi) = \sum_l \sum_m a_{lm}(r) Y_{lm}(\theta,\varphi)$$

$$a_{lm}(r) = \int d\Omega\, Y^*_{lm}(\theta,\varphi)\Psi(r,\theta,\varphi)$$

$$\longrightarrow \begin{cases} \rho_{L^2,L_z}(l,m) = \int_0^\infty r^2 dr\, |a_{lm}(r)|^2 \\ \rho_{L^2}(l) = \sum_{m=-l}^{+l} \int_0^\infty r^2 dr\, |a_{lm}(r)|^2 \\ \rho_{L_z}(m) = \sum_{l \geq |m|} \int_0^\infty r^2 dr\, |a_{lm}(r)|^2 \end{cases}$$

Miðlæg mætti $\rightarrow$ Vetnisatóm

Miðlægt mætti $\longrightarrow$ $d_t \bar{L} = 0$

í $\{r\}$ framsetn. er jafna Schrödingers

$$\left\{ -\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right\} \varphi(\bar{r}) = E \varphi(\bar{r}) \qquad (1)$$

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \left(\frac{\partial^2}{\partial \theta} + \frac{1}{\tan\theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right)$$

$$= \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{L^2}{r^2}$$

því er Sch.

$$\left\{ -\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{2\mu r^2} \bar{L}^2 + V(r) \right\} \varphi(\bar{r}) = E \varphi(\bar{r})$$

og

$$H = -\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{2\mu r^2} \bar{L}^2 + V(r)$$

2

Aðskilnaður breytistærða

$[H, \vec{L}] = 0 \quad [H, L^2] = 0 \quad [H, L_z] = 0$

því þarf að leysa jöfnu hneppið

$$\left.\begin{aligned} H\varphi(\vec{r}) &= E\varphi(\vec{r}) \\ L^2\varphi(\vec{r}) &= l(l+1)\hbar^2\varphi(\vec{r}) \\ L_z\varphi(\vec{r}) &= m\hbar\varphi(\vec{r}) \end{aligned}\right\} \to \varphi(\vec{r}) = R(r)Y_{lm}(\theta,\varphi)$$

$\to$ r-jafnan

$$\left\{-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right\}R(r) = ER(r) \qquad (2)$$

Varúð: lausn á (2) með $\varphi(\vec{r}) = R(r)Y_{lm}(\theta,\varphi)$ er ekki endilega lausn á (1) þar sem (2) er ekki skilgreind fyrir $r=0$

því þarf að velja lausnir

3

m: kemur ekki fyrir í (2)

$$R(r) \to R_{kl}(r) = \frac{1}{r}u_{kl}(r)$$

$\to$

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right\}u_{kl}(r) = E_{kl}u_{kl}(r) \qquad (3)$$

samsvarar Schrödinger jöfnunni fyrir einvíðri ögn í mættinu

fráhrinding

$$\frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)$$

að vísu en $r \geq 0$ hér

Lausnirnar um $r \sim 0$

gera ráð fyrir að $V(0)$ sé til

eða $\lim_{r\to 0} V(r) \approx \frac{1}{r^\epsilon} \qquad \epsilon \leq 1$

athugum $\quad R_{k,l}(r) \underset{r\to 0}{\sim} Cr^s$

þá fæst frá (2)

$$\left\{+\frac{\hbar^2}{2\mu r^2}\Big(-s(s+1)+l(l+1)\Big)+V(r)-E\right\}\overset{Cr^s}{\,}' = 0$$

því þarf að gilda þegar $r \to 0$

$$-s(s+1)+l(l+1)=0$$

$$\to \begin{cases} s = l \\ s = -(l+1) \end{cases}$$

aðeins $s=l$ er lausn á (1)

$$\to u_{kl}(r) \underset{r\to 0}{\sim} C r^{l+1}$$

og með (3) verður því að krefjast

$u_{kl}(0) = 0$

hægt að bera saman við einvíðu jöfnuna með $V(x<0)=\infty$

$\to u_{kl}(0) = 0$

Ath

Ef til vill þarf að leyfa (fyrir sam felda hluta rófsins)

$$\int_0^\infty r^2 dr\, R^*_{k'l}(r) R_{kl}(r) = \int_0^\infty dr\, u^*_{k'l}(r) u_{kl}(r) = \delta(k'-k)$$

þar sem $k \in \mathbb{R}$

En heildin verða að vera samleitin við lægri mörkin (svo $u(0)=0$)

og þá eru endanlegar líkur á að finna ögn í endanlegu rúmmáli

---

Kúlusamhverfa (þ.e. L_z kemur ekki fyrir í H)

$\to$ orkuástönd með mis. m_z eru margföld í orku $(2l+1)$ en hornrétt þ.s. þau eru eiginástönd L_z

$\to$ „essential" margfeldni

mismunandi k

Ef mism. l ástönd eru margföld

$\rightarrow$ „accidental" margfeldni

slysni / slembi $\}$ margfeldni

Rétt eins og í sígildri aflfræði

tvær agnir í mætti $V(\vec{r}_1 - \vec{r}_2)$

$\rightarrow$ hægt er að aðgreina innbyrðis hreyfingar og massamiðjuhreyfingu

Innbyrðishreyfingum er hægt að lýsa sem hreyfingum einnar agnar með $\mu = \dfrac{m_1 m_2}{m_1 + m_2}$

í miðjumættinu $V(r)$

Vetnisatóm $\mu = \dfrac{m_e m_p}{m_e + m_p} \simeq m_e\left(1 - \dfrac{m_e}{m_p}\right)$

$\uparrow$

$1/1800$

Vetnisatómið

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{e^2}{r}\right\} u_{k,l}(r) = E_{kl}\, u_{kl}(r)$$

veljum $\quad K = \sqrt{-\dfrac{2mE}{\hbar^2}}$ $\quad$ viljum finna bundin ástönd

og

$$x = 2kr, \qquad u(r) = y(x)$$

$$\nu = \frac{me^2}{k\hbar^2}$$

$$\rightarrow \quad y'' - \left\{\frac{l(l+1)}{x^2} - \frac{\nu}{x} + \frac{1}{4}\right\} y = 0$$

Hér kemur E aðeins fyrir í ν

Skoðum aðfellulausnir

$x \to \infty$

$$\to \quad y'' - \frac{1}{4} y \simeq 0$$

$$\to \quad y \sim e^{\pm x/2} \qquad \Leftarrow \text{velja mínus}$$

$x \to 0$

$$\to \quad y'' - \frac{l(l+1)}{x^2} y \simeq 0$$

$$\to \quad \begin{cases} y \simeq x^{l+1} & \Leftarrow \text{velja vegna } y(0) = 0 \\ y \simeq x^{-l} \end{cases}$$

Því reynum lausn

$$y(x) = e^{-x/2} x^{l+1} v(x)$$

$$\Phi(a,c,x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 dt\, t^{a-1} (1-t)^{c-a-1} e^{tz}$$

t.d. $e^z = \Phi(a,a,z)$

$$\lim_{\substack{z \to \infty \\ z \in \mathbb{R}}} \Phi(a,c,z) = \frac{\Gamma(c)}{\Gamma(a)} e^z z^{a-c}$$

$$\Phi(a,c,z) = 1 + \frac{a}{c}\frac{z}{1!} + \frac{a(a+1)}{c(c+1)}\frac{z^2}{2!} + \ldots$$

(9)

Innsetning í jöfnu gefur

$$\boxed{x v'' + (2l+2-x) v' + (\nu - l - 1) v = 0}$$

þessi jafna hefur lausnir

$\Phi(\nu-l-1, 2l+2, x)$

og $x^{-(2l+1)} \Phi(\nu-3l-3, -2l, x)$

Confluent Hypergeometric föll

síðari lausnin er ekki skilgreind fyrir $l = 0, 1, 2, \ldots$ → kemur ekki til greina

$\Phi(\nu-l-1, 2l+2, x)$

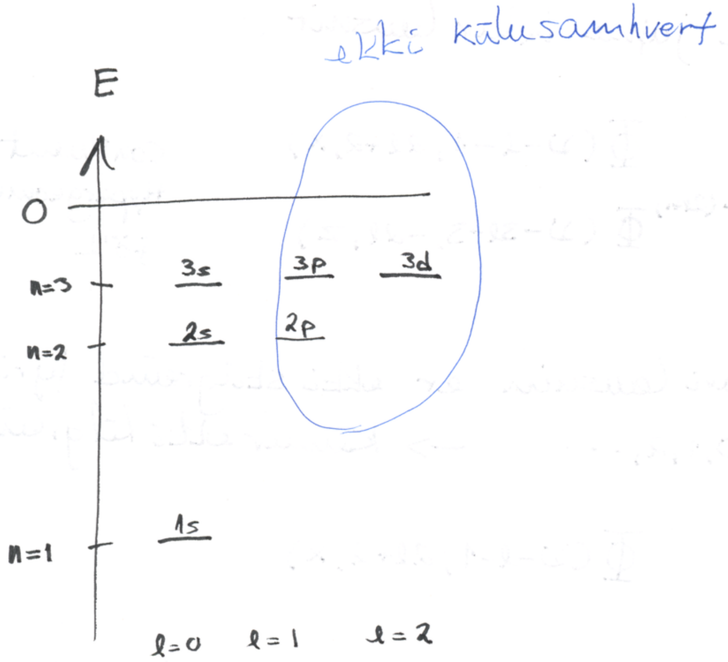
Ef $\nu - l - 1 \notin \mathbb{N} \cup \{0\}$ þá vex lausnin eins og e^x fyrir $x \to \infty$

→ lausnin væri ekki normanleg

En ef $\nu - l - 1 = 0, 1, 2, \ldots$

þá er Φ margliða

Laguerre margliða



í raun fæst $\nu - l - 1 = \overbrace{0, 1, 2 \ldots}^{k-1}$

$$\rightarrow E_{kl} = -\frac{1}{2}\alpha^2 \mu c^2 \frac{1}{(k+l)^2}$$

Velja $n = k + l$

Lausnin verður því

$$u_{n\ell}(r) \propto e^{-x/2} x^{\ell+1} L^{2\ell+1}_{n-\ell-1}(x)$$

þar sem $n = 1, 2, 3, \ldots$

$\ell = 0, 1, 2, \ldots (n-1)$

með

$$E_n = -\frac{1}{2}\alpha^2 \mu c^2 \frac{1}{n^2}$$

þ.s. $\alpha = \frac{e^2}{\hbar c} = \frac{q^2}{4\pi\epsilon_0 \hbar c} \simeq \frac{1}{137}$

cgs MKS

→ slysni margfeldni ℓ - ástanda

$$\phi_{n\ell m}(\bar{r}) = \left\{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}\right\}^{1/2} \left(\frac{2r}{na_0}\right)^\ell \exp\left\{-\frac{r}{na_0}\right\}$$

$$\cdot L^{2\ell+1}_{n-\ell-1}\left(\frac{2r}{na_0}\right) Y_{\ell m}(\theta, \varphi)$$

með

$$a_0 = \frac{\hbar^2}{me^2} = \text{Bohr geisli}$$

þessar lausnir eru ekki fullkomið mengi, það vantar lausnir fyrir $E > 0$

Einnig hefði mátt leysa jöfnuna fyrir Φ strax á hnitakerfinu í tvinntöluplaninu

$$L^b_{a-b}(x) = \frac{a!}{2\pi i} \oint e^{-xz} \frac{(z+1)^a}{z^{a-b+1}} dz$$

og nota leyfarreikning til að finna L

1

Spuni

$$\overline{M} = \frac{\mu_B}{\hbar} \overline{L} \quad : \text{ segulvogi}$$

$$\mu_B = \frac{q\hbar}{2m_e} \quad : \text{ Bohr magneton}$$

---

stöðuorka í föstu segulsviði

$$U = -\overline{M} \cdot \overline{B}$$

veljum $\overline{B} = B\hat{z}$

$$\longrightarrow \; U = -\frac{\mu_B}{\hbar} B L_z$$

---

svo möguleiki er að sjá hvert l-ástand klofið upp í $\underline{2l+1}$ ástönd í segulsviði

Zeemanhrifin

2

í atómum með Z = oddatala sáust ástönd sem klofnuðu í jafnan fjölda ástanda í segulsviði

afbrigðilegu Zeemanhrifin

$l = 0$ ástönd sáust klofin í tvennt

$$\longrightarrow \; j = 1/2$$

Einhver annar hverfiþungi heldur en brautar leggst við $\overline{L}$ því sýnt hefur verið að $l \in \mathbb{N} \cup \{0\}$

{ munum síðar sjá að heildarbrautarhverfiþungi gefur ávallt $l \in \mathbb{N} \cup \{0\}$ }