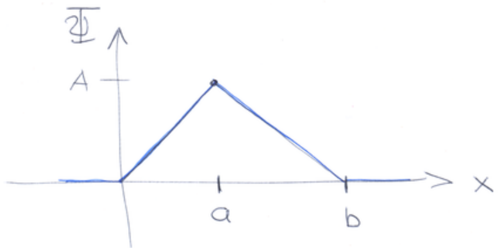
(1)

(1.4) Klukkan $t=0$ er bylgjufall eindar

$$\Phi(x,0) = \begin{cases} A\frac{x}{a} & \text{ef } 0 \le x \le a \\ A\frac{(b-x)}{(b-a)} & \text{ef } a \le x \le b \\ 0 & \text{annars} \end{cases}$$

A, a, b eru fastar (jákvæðir)

Teiknum upp til að sjá útlitið



Hér væri sniðugra að gera graf af $\frac{\Phi}{A}$ v.s. $\frac{x}{a}$ og velja gildi á b/a.

(2)

a) Staðla Φ

Líkindi ~~þess~~ að finna eindina á öllu svæðinu eru

$$\int_{-\infty}^{\infty} dx\, |\Phi(x,0)|^2 = 1$$

$$= \int_0^a dx\, |\Phi(x,0)|^2 + \int_a^b dx\, |\Phi(x,0)|$$

$$= |A|^2 \int_0^a dx \left(\frac{x}{a}\right)^2 + |A|^2 \int_a^b dx \left(\frac{b-x}{b-a}\right)^2$$

$$|A|^2 \left[a \int_0^a \frac{dx}{a} \left(\frac{x}{a}\right)^2 + \frac{a^3}{(b-a)^2} \int_a^b \frac{dx}{a} \left(\frac{b}{a} - \frac{x}{a}\right)^2 \right]$$

(3)

$$= |A|^2 a \left[\int_0^1 du\, u^2 + \frac{a^2}{(b-a)^2} \int_1^{b/a} du \left(\frac{b}{a} - u\right)^2 \right]$$

$$= |A|^2 a \left\{ \frac{1}{3} + \frac{a^2}{(b-a)^2} \frac{1}{3} \left(\left(\frac{b}{a}\right)^3 - 3\left(\frac{b}{a}\right)^2 + 3\left(\frac{b}{a}\right) - 1 \right) \right\}$$

$$= |A|^2 a \frac{1}{3} \left\{ 1 + \frac{a^2}{(b-a)^2} \left(\left(\frac{b}{a}\right) - 1 \right)^3 \right\} = \frac{a}{3} |A|^2 \left\{ 1 + \frac{(b-a)}{a} \right\}$$

$$= \frac{a}{3} |A|^2 \frac{b}{a} = \frac{b}{3} |A|^2 = 1$$

$\rightarrow A = \sqrt{\frac{3}{b}}$ er lausn

A hefur víddina $\frac{1}{\sqrt{L}}$ eins og normeringsfastinn $\underbrace{\int dx\, |\Psi|^2}_{\text{víddarlaust}} = 1$

(4)

b) sjá 1. blað.

c) Hvar er líklegast að finna eindina klukkan $t=0$?

Í hápunkti $|\Psi|^2$ í $x=a$

d) Hver eru líkindin fyrir því að finna eindina f. $x<a$

$$P(x<a) = \int_0^a dx\, |\Phi(x,0)|^2 = |A|^2 a \int_0^1 du\, u^2$$

$$= |A|^2 \frac{a}{3} = \frac{3}{b}\frac{a}{3} = \frac{a}{b}$$ hreintala, án víddar

Þegar $a \rightarrow b \longrightarrow P(x<a) \rightarrow 1$, enda er allt bylgjuf. á vinstra megin við a

(5)

þegar $b \to 2a$, ~~því~~ þá $a \to \frac{b}{2}$

$\to P(x < a) = \frac{1}{2}$ enda er bylgjufallið þá samhverft um $x = a$

e) Væntigildi $\langle x \rangle$?

$$\langle x \rangle = \int_{-\infty}^{\infty} dx \cdot x \, |\Phi(x,0)|^2$$

$$= \int_0^a dx \; x \, |\Phi(x,0)|^2 + \int_a^b dx \cdot x \, |\Phi(x,0)|^2$$

$$= |A|^2 a^2 \left\{ \int_0^1 du \, u^3 + \frac{a^2}{(b-a)^2} \int_1^{b/a} du \; u \left(u - \frac{b}{a}\right)^2 \right\}$$

(6)

$$= |A|^2 a^2 \left\{ \frac{b^2 + 2ab}{12 a^2} \right\} = \frac{3}{b} \; \frac{b^2 + 2ab}{12}$$

$$= \frac{b + 2a}{4}$$ með réttu vídd

(7)

1.14 $P_{ab}(t)$ eru líkur ~~þess að~~ fyrir eind á bilinu (a,b) á tíma t

a) Sýna að

$$d_t P_{ab} = J(a,t) - J(b,t)$$

þar sem

$$J(x,t) = \frac{i\hbar}{2m} \left\{ \Phi \, \partial_x \Phi^* - \Phi^* \partial_x \Phi \right\}$$

Við vitum að

$$P_{ab}(t) = \int_a^b dx \, |\Phi(x,t)|^2$$

$$d_t P_{ab}(t) = d_t \left\{ \int_a^b dx \, |\Phi(x,t)|^2 \right\} = \int_a^b dx \; d_t \left[|\Phi(x,t)|^2 \right]$$

(8)

x is here independent of t

$$\to d_t P_{ab}(t) = \int_a^b dx \, \partial_t |\Phi(x,t)|^2 = \int_a^b dx \left\{ (\partial_t \Phi^*) \Phi + \Phi^* (\partial_t \Phi) \right\}$$

Notum jöfnu Schrödingers

$$i\hbar \partial_t \Phi = H \Phi$$

$$-i\hbar \partial_t \Phi^* = H \Phi^*$$

$$d_t P_{ab}(t) = \int_a^b dx \left\{ \left(\frac{-1}{i\hbar} H \Phi^*\right) \Phi + \Phi^* \left(\frac{1}{i\hbar} H \Phi\right) \right\}$$

9

Ef nú $H = \frac{p^2}{2m} + V \quad \to \quad -\frac{\hbar^2}{2m}\partial_x^2 + V$

þá fæst

$$d_t P_{ab}(t) = \int_a^b dx \left\{ \frac{\hbar}{2mi}(\partial_x^2 \Psi^*)\Psi - \frac{\hbar}{2mi}\Psi^*(\partial_x^2\Psi)\right\}$$

{krossliðirnir styttast út þ. afleiðan er tekin}

$$d_t P_{ab}(t) = \int_a^b dx\, \partial_x \left\{\frac{\hbar}{2mi}\left[(\partial_x\Psi^*)\Psi - \Psi^*(\partial_x\Psi)\right]\right\}$$

$$= \int_a^b dx\,\partial_x\left\{\frac{i\hbar}{2m}\left[\Psi^*(\partial_x\Psi) - (\partial_x\Psi^*)\Psi\right]\right\}$$

$$= -\int_a^b dx\,\partial_x J(x,t) = -J(b,t) + J(a,t)$$

10

Breytingin á líkindunum innan bilsins eru aðeins vegna strauma inn eða út úr bilinu á jöðrum þess. Líkindin eru víddarlaus $\to$ straumur, $d_t P_{ab}$ hefur vídd T^{-1}

b) $$\Psi(x,t) = A\exp\left[-a\left(\frac{mx^2}{\hbar} + it\right)\right]$$

Hér er $\Psi(x,t) = \phi(x)e^{-ait}$ þ.s. $\phi(x)\in\mathbb{R}$

$\to J(x,t) = 0$

1

2.4 Óendanlegur brunnur, Reikna $\langle x\rangle, \langle x^2\rangle, \langle p\rangle, \langle p^2\rangle$ og σ_x og σ_p

Ástand $|n\rangle$

$$\Psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

$$\langle x\rangle = \int_0^a dx\,\Psi_n^*(x)\,x\,\Psi_n(x) = \frac{2}{a}\int_0^a dx\,x\sin^2\left(\frac{n\pi}{a}x\right)$$

$$= \frac{a}{4n^2\pi^2}\left\{1 - 2n\pi\sin(2n\pi) - \cos(2\pi n) + 2n^2\pi^2\right\}$$

$$= \frac{a}{4n^2\pi^2}\left\{1-1+2n^2\pi^2\right\} = \frac{a}{2}$$

Ψ_n er alltaf jafnstætt eða oddstætt svo niðurstaðan kemur ekki á óvart

2

$$\langle x^2\rangle = \int_0^a dx\,\Psi_n^*(x)\,x^2\,\Psi_n(x) = \frac{2}{a}\int_0^a dx\,x^2\sin^2\left(\frac{n\pi}{a}x\right)$$

$$= \frac{2}{a}\left\{\frac{-6a^3n\pi + 4a^3n^3\pi^3}{24n^3\pi^3}\right\} = \frac{-6a^2n\pi + 4a^2n^3\pi^3}{12n^3\pi^3}$$

$$= a^2\left\{\frac{1}{3} - \frac{1}{2\pi^2n^2}\right\}$$

$$\langle p\rangle = \int_0^a dx\,\Psi_n^*\, p\, \Psi_n = -i\hbar\int_0^a dx\,\Psi_n^*(x)\left(\frac{\partial}{\partial x}\Psi_n(x)\right)$$

$$= m\frac{d\langle x\rangle}{dt} = 0$$

notum (1.31) úr bók

3

$$\langle p^2\rangle = -\hbar^2 \int_0^a dx\, \Phi_n(x)\left\{\frac{\partial^2}{\partial x^2}\Phi_n(x)\right\}$$

$$= +\hbar^2\, \frac{n^2\pi^2}{a^2} \int_0^a dx\, |\Phi_n(x)|^2 = \frac{\hbar^2 n^2\pi^2}{a^2}$$

þ.s. við notum að $\Phi_n''(x) = -\frac{n^2\pi^2}{a^2}\Phi_n(x)$

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = a\sqrt{\left\{\frac{1}{3} - \frac{1}{2(\pi n)^2}\right\} - \frac{1}{4}}$$

$$= a\sqrt{\frac{1}{12} - \frac{1}{2(\pi n)^2}} = \frac{a}{2}\sqrt{\frac{1}{3} - \frac{2}{(\pi n)^2}}$$

4

$$\sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \frac{\hbar n\pi}{a}$$

$$\rightarrow \sigma_x\sigma_p = \frac{\hbar}{2}\left\{n\pi\sqrt{\frac{1}{3} - \frac{2}{(\pi n)^2}}\right\}$$

$\sigma_x\sigma_p \geq \frac{\hbar}{2}$ ef $n\pi\sqrt{\frac{1}{3} - \frac{2}{(\pi n)^2}} \geq 1$

$\rightarrow$ ef $\sqrt{\frac{n^2\pi^2}{3} - 2} \geq 1$ sem er alltaf rétt fyrir $n = 1, 2, \ldots$

Lægst er óvissan fyrir $n=1$

5

(2.8) Eind með massa m hefur jafnar líkur á að finnast vinstra megin í óendanlegum brunni klukkan $t=0$

a) Finna $\Phi(x,0)$

$$\Phi(x,0) = \begin{cases} A & \text{ef } 0 < x < \frac{a}{2} \\ 0 & \text{annars} \end{cases}$$

$$1 = \int_0^a dx\, |\Phi(x,0)|^2 = |A|^2 \int_0^{a/2} dx = |A|^2 \frac{a}{2}$$

$\rightarrow A = \sqrt{\frac{2}{a}}$ er möguleg lausn

6

b) Með hvaða líkum fæst $1 \cdot \frac{\pi^2\hbar^2}{2ma^2} = E_0 \cdot 1$ í orkumælingu

---

Orkurófið er eigingildi H. Eiginástönd H eru

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

Þurfum liðun $\Phi(x,0)$ í ~~þessum~~ grunni

$$\Phi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

Mælingin setur kerfið í eiginástönd H. Vogi ψ_1, c_1 er þá líkindavísirinn

$$c_n = \int_0^a dx\, \Phi(x,0)\, \psi_n^*(x) = \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\Phi(x,0)\,dx$$

(7)

$$C_n = \frac{2}{a}\int_0^{a/2} dx \, \sin\left(\frac{n\pi}{a}x\right) = 2\int_0^{1/2} du \, \sin(n\pi u)$$

$$= \frac{2}{n\pi}\left\{1-\cos\left(\frac{n\pi}{2}\right)\right\}$$

$\to C_1 = \frac{2}{\pi} \to$ líkurnar eru $|C_1|^2 = \frac{4}{\pi^2}$

$\simeq 0,4$

(1)

2.10 Hreintóna sveifill

a) finna $\psi_2(x)$

$$\psi_n(x) = \frac{1}{\sqrt{n!}}(a_+)^n \psi_0(x)$$

$$\psi_0(x) = \frac{1}{\sqrt{a\sqrt{\pi}}} e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}$$

$$a_+ = \frac{\hbar}{\sqrt{2\hbar m\omega}}\left\{-\frac{ip}{\hbar} + \frac{m\omega x}{\hbar}\right\}$$

$$= \frac{a}{\sqrt{2}}\left\{-\frac{ip}{\hbar} + \frac{x}{a^2}\right\}$$

ef $a = \sqrt{\frac{\hbar}{m\omega}}$

$$a_+ = \frac{1}{\sqrt{2}}\left\{-a\partial_x + \frac{x}{a}\right\}$$

$$\to \psi_2(x) = \frac{1}{\sqrt{2}\,2}\frac{1}{\sqrt{a\sqrt{\pi}}}\left(-a\partial_x + \frac{x}{a}\right)\left(-a\partial_x + \frac{x}{a}\right)e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}$$

$$= \cdot \quad \cdot \quad \cdot \quad \cdot \, \cdot \, e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}\left(\frac{x}{a} + \frac{x}{a}\right)$$

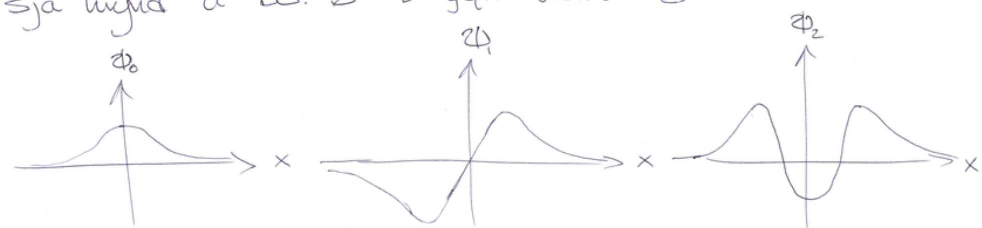
(2)

$$\psi_2(x) = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{a\sqrt{\pi}}}\left(-a\partial_x + \frac{x}{a}\right)\frac{x}{a}e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}$$

$$= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{a\sqrt{\pi}}}\left[\left(\frac{x}{a}\right)^2 - 1 + \left(\frac{x}{a}\right)^2\right]e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}$$

$$= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{a\sqrt{\pi}}}\left\{2\left(\frac{x}{a}\right)^2 - 1\right\}e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}$$

b) sjá myndir á bls. 8 í fyrirlestri 5



(3)

c)

$$\int_{-\infty}^{\infty} dx \, \psi_0(x)\psi_1(x) = 0$$

← odd stakt fall

$$\int_{-\infty}^{\infty} dx \, \psi_2(x)\psi_3(x) = 0$$

$$\int_{-\infty}^{\infty} dx \, \psi_0(x)\psi_2(x) = \frac{1}{\sqrt{2}}\frac{1}{a\sqrt{\pi}}\int_{-\infty}^{\infty} dx \left\{2\left(\frac{x}{a}\right)^2 - 1\right\}e^{-\left(\frac{x}{a}\right)^2}$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} du \left\{2u^2 - 1\right\}e^{-u^2} = 0$$

samkvæmt Maxima

(2.11) Rekna $\langle x\rangle, \langle p\rangle, \langle x^2\rangle$ og $\langle p^2\rangle$

fyrir ψ_0 og ψ_1 ~~med~~ heildum

$$\psi_0(x) = \frac{1}{\sqrt{a\sqrt{\pi}}} e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}, \quad \psi_1(x) = \frac{\sqrt{2}}{\sqrt{a\sqrt{\pi}}}\left(\frac{x}{a}\right) e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}$$

$n=0$

$\psi_0(x)$ er samhverft um $x=0$ $\rightarrow$ $\langle x\rangle$ og $\langle p\rangle$ hverfa

$$\langle x^2\rangle = \int dx\, \psi_0(x) x^2 \psi_0(x) = \frac{1}{a\sqrt{\pi}}\int dx\; x^2 e^{-\left(\frac{x}{a}\right)^2}$$

$$= \frac{a^3}{a\sqrt{\pi}}\int \frac{dx}{a}\left(\frac{x}{a}\right)^2 e^{-\left(\frac{x}{a}\right)^2} = \frac{a^2}{\sqrt{\pi}}\int_{-\infty}^{\infty} du\; u^2 e^{-u^2} = \frac{a^2}{2}$$

(4)

$$\langle p^2\rangle = \int dx\, \psi_0(x)\, p^2 \psi_0(x) = \frac{1}{a\sqrt{\pi}}\int dx\, e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}\left\{-\hbar^2\partial_x^2 e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}\right\}$$

$$= -\frac{\hbar^2}{a^2\sqrt{\pi}}\int \frac{dx}{a}\, e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}\left\{a^2\partial_x^2 e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}\right\}$$

$$= -\frac{\hbar^2}{a^2}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} du\; e^{-\frac{u^2}{2}}\left\{\partial_u^2 e^{-\frac{u^2}{2}}\right\}$$

$$= -\frac{\hbar^2}{a^2}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} du\; e^{-u^2}\left\{u^2-1\right\} = -\frac{\hbar^2}{a^2}\frac{1}{\sqrt{\pi}}\left(-\frac{\sqrt{\pi}}{2}\right)$$

$$= \frac{\hbar^2}{2a^2}$$

(5)

$n=1$

$\psi_1(x)$ er antisamhverft $\rightarrow$ $|\psi_1|^2$ er samhverft

$\rightarrow$ $\langle x\rangle$ og $\langle p\rangle$ hverfa

$$\langle x^2\rangle = \frac{2}{a\sqrt{\pi}}\int dx \left(\frac{x}{a}\right)^2 x^2 e^{-\left(\frac{x}{a}\right)^2} \qquad \text{(sjå (2.62))}$$

$$= \frac{2a^2}{\sqrt{\pi}}\int_{-\infty}^{\infty} du\; u^4 e^{-u^2} = \frac{2a^2}{\sqrt{\pi}}\frac{3\sqrt{\pi}}{4} = \frac{3a^2}{2}$$

$$\langle p^2\rangle = \frac{2}{a\sqrt{\pi}}\int dx\left(\frac{x}{a}\right)e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}\left\{-\hbar^2\partial_x^2\left(\frac{x}{a}\right)e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}\right\}$$

$$= \frac{2}{a^2\sqrt{\pi}}\int\frac{dx}{a}\left(\frac{x}{a}\right)e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}\left\{-\hbar^2 a^2\partial_x^2\left(\frac{x}{a}\right)e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}\right\}$$

(6)

$$\langle p^2\rangle = -\frac{2\hbar^2}{a^2\sqrt{\pi}}\int_{-\infty}^{\infty} du\; u e^{-u^2/2}\left\{\partial_u^2\, u e^{-u^2/2}\right\}$$

$$= -\frac{2\hbar^2}{a^2\sqrt{\pi}}\int_{-\infty}^{\infty} du\; u^2 e^{-u^2}\left\{u^2-3\right\}$$

$$= \left(-\frac{2\hbar^2}{a^2\sqrt{\pi}}\right)\left(-\frac{3\sqrt{\pi}}{4}\right) = \frac{3\hbar^2}{2a^2}$$

b) $n=0$ $\quad \sigma_x = \frac{a}{\sqrt{2}}, \quad \sigma_p = \frac{\hbar}{\sqrt{2}\,a}$

$$\rightarrow \sigma_x\sigma_p = \frac{\hbar}{2}$$

(7)

8

$n=1$

$$\sigma_x = \sqrt{\tfrac{3}{2}}\, a, \qquad \sigma_p = \sqrt{\tfrac{3}{2}}\, \frac{\hbar}{a}$$

$$\to \sigma_x \sigma_p = \tfrac{3}{2}\hbar$$

c)

$$\langle T\rangle = \frac{\langle p^2\rangle}{2m}$$

$$\langle V\rangle = \tfrac{1}{2} m\omega^2 \langle x^2\rangle$$

$n=0$

$$\left.\begin{aligned} \langle T\rangle &= \frac{\hbar^2}{4ma^2} \\ \langle V\rangle &= \tfrac{1}{4} m\omega^2 a^2 \end{aligned}\right\} \quad \langle T\rangle + \langle V\rangle = \tfrac{1}{4}\left\{\frac{\hbar^2}{ma^2} + m\omega^2 a^2\right\} = \tfrac{1}{4}\left\{\hbar\omega + \hbar\omega\right\} = \underline{\underline{\frac{\hbar\omega}{2}}}$$

9

$n=1$

$$\left.\begin{aligned} \langle T\rangle &= \frac{3\hbar^2}{4ma^2} \\ \langle V\rangle &= \tfrac{3}{4} m\omega^2 a^2 \end{aligned}\right\} \to \langle T\rangle + \langle V\rangle = \underline{\underline{\frac{3\hbar\omega}{2}}}$$

Í samræmi við 2 lægstu eigingildi hreintóna sveifils

1

Fjórði skammtur

Finna dreifiástönd mættisins $V(x) = \alpha\delta(x+a)$ sem staðsett er fyrir framan óendanlegan háan vegg í $x = 0$

Hugsum okkur innbylgju með bylgjuvigur k

Tvö svæði þar sem við þurfum að finna $\psi(x)$, þar er ekkert mætti → notum frjálsa lausn (fyrir frjálsa eind)

I $\quad \psi_I(x) = e^{ikx} + Be^{-ikx}$

II $\quad \psi_{II}(x) = Ce^{ikx} + De^{-ikx}$

Jaðar-skilyrði

$\psi(0) = 0$

Innbylgja

$\psi_{II}(-a) = \psi_I(-a)$

Brot í afleiðu

$\psi'(-a^+) - \psi'(-a^-) = \frac{2m\alpha}{\hbar^2}\psi(a)$

2

$\psi(0) = 0 \to D = -C$

Samfella í $x=-a$:

$$e^{-ika} + Be^{ika} = Ce^{-ika} + De^{ika} = C\{e^{-ika} - e^{ika}\} = -C2i\sin(ka) \qquad \text{(A)}$$

Brot í afleiðu:

$$Cike^{-ika} + Cike^{ika} - ike^{-ika} + ike^{ika}B = \frac{2m\alpha}{\hbar^2}\{e^{-ika} + Be^{ika}\}$$

$$C\,2\cos(ka) + e^{ika}B - \beta Be^{ika} = e^{-ika}(1+\beta), \quad \beta = \frac{2m\alpha}{\hbar^2 ik}$$

$$\boxed{2C\cos(ka) + B(1-\beta)e^{ika} = (1+\beta)e^{-ika}} \qquad \text{(B)}$$

3

Umrituum (A)

$$\boxed{\begin{aligned} &Be^{ika} + C\,2i\sin(ka) = -e^{-ika} && (A) \\ &B(1-\beta)e^{ika} + 2C\cos(ka) = (1+\beta)e^{-ika} && (B) \end{aligned}}$$

og (B)

Tvær línulegar jøfnur fyri ókendu stødirnar B og C

(A) gevur

$$C = -\frac{e^{-ika} + Be^{ika}}{2i\sin(ka)} \qquad (**)$$

notum í (B)

$$i\frac{\left(e^{-ika} + Be^{ika}\right)}{\sin(ka)}\cos(ka) + B(1-\beta)e^{ika} = (1+\beta)e^{-ika}$$

4

Soa

$$B\left\{ie^{ika}\cot(ka) + (1-\beta)e^{ika}\right\} = e^{-ika}\left\{-i\cot(ka) + (1+\beta)\right\}$$

$$\to B = \frac{e^{-2ika}\left\{-i\cot(ka) + (1+\beta)\right\}}{\left\{i\cot(ka) + (1-\beta)\right\}}$$

$$\to |B|^2 = B\cdot B^* = \frac{|1+\beta|^2 + \cot^2(ka)}{|1-\beta|^2 + \cot^2(ka)}$$

$$= \frac{(1+\gamma^2) + \cot^2(ka)}{(1+\gamma^2) + \cot^2(ka)} = 1$$

ef $i\gamma = \beta$

$|1+\beta|^2 = |1+i\gamma|^2 = 1+\gamma^2$

$|1-\beta|^2 = |1-i\gamma|^2 = 1+\gamma^2$

5

Allar eindir sum streyma móti molinum fara einhvørntíman frá tí aftur, en hér er mangt falið! Stoðum.

Bylgjufallið á (II) er

$$\psi_{II}(x) = 2iC\sin(kx)$$

C fæst við tí at seta B í jøfnu (**)

$$\boxed{C = ie^{-ika}\,\frac{\left[1 + \frac{\{(1+i\gamma) - i\cot(ka)\}}{\{(1-i\gamma) + i\cot(ka)\}}\right]}{2\sin(ka)}}$$

$$\gamma = -\frac{2m\alpha}{\hbar^2 k}$$

6

Frjálseind

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2ma^2}(ka)^2 = E_1\cdot(ka)^2$$

$$\gamma = -\frac{2m\alpha}{\hbar^2 k} = -\frac{\alpha}{a}\,\frac{2ma^2}{\hbar^2(ka)} = -\left(\frac{\alpha}{aE_1}\right)\frac{1}{ka}$$

víddarleysar stødir

$$(ka)^2 = \frac{E}{E_1} \to ka = \sqrt{\left(\frac{E}{E_1}\right)}$$

$$\to \frac{\alpha}{aE_1} = -(ka)\gamma$$

Notum sum stika í grøfum

Við höfum að $|B|^2 = 1$ sem táknar að allar eindir koma einhverntíman til baka

$\lim_{\gamma \to 0} |C|^2 = 1$ því þegar $\gamma \to 0$ eða $\alpha \to 0$ er enginn δ-toppur og þá flæða öll líkindin alveg að veggnum

$|C|^2$ hefur sérstöðupunkta, eins og gröfin sýna og jafnan fyrir C bendir til. Það eru hermur, þá festist eindin einhvern tíma milli δ-topps og veggs

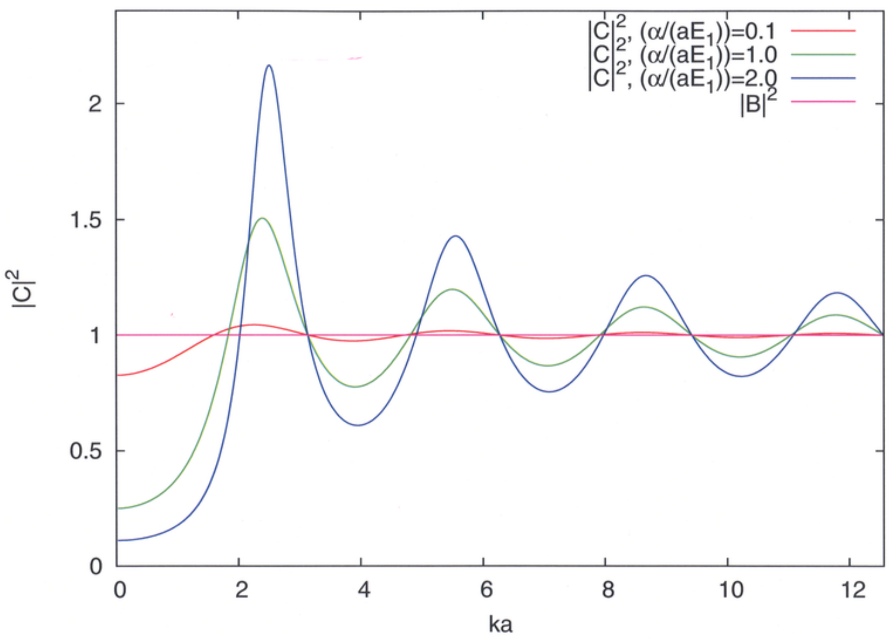
↑ eindin eyðir löngum tíma þar -> meiri líkindin á því að finna hana þar,

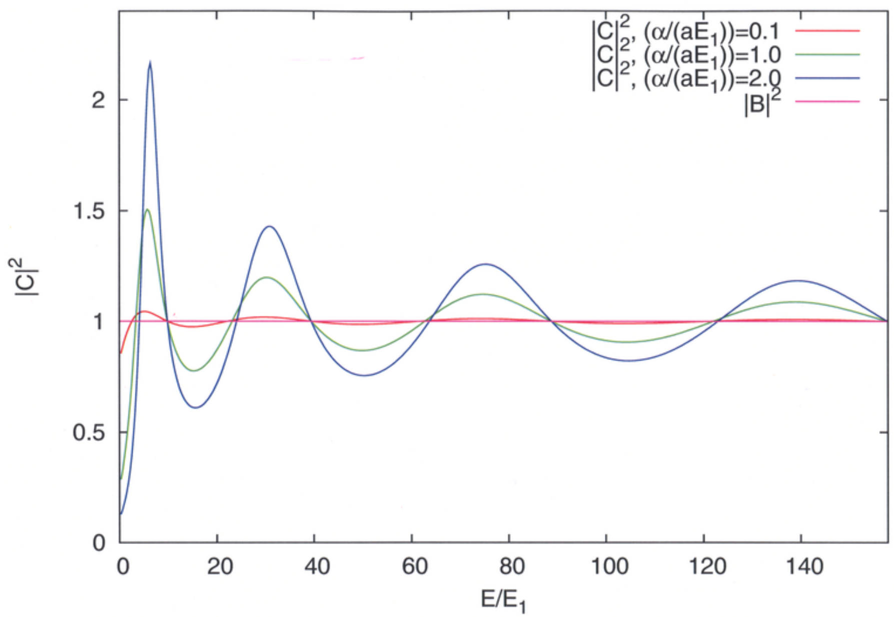
háð bylgjuvigri ka

Hár toppur $\alpha \to \infty$ lítil líkindi að eind finnist milli topps og veggs, nema fyrir hermuástand

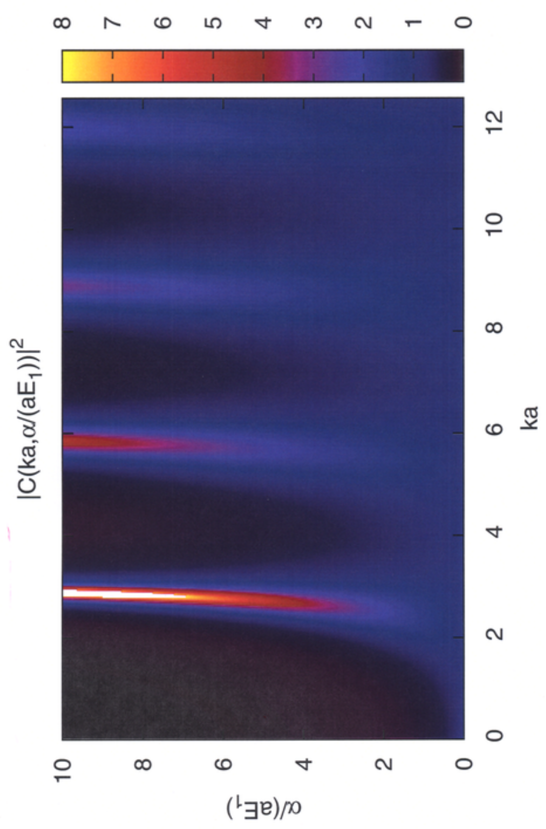
Í hermu passar bylgjulengd eindar milli topps og veggs (hálf eða heilt margfeldi hálfrar)

Hermuástönd færast til í orku þegar α vex og nálgast ráfið fyrir óendanlegan brunn þegar $\alpha \to \infty$





(11)



(12)


```
#!/usr/bin/gnuplot -persist
#
#
#       G N U P L O T
#       Version 4.6 patchlevel 0    last modified 2012-03-04
#       Build System: Linux x86_64
#
#       Copyright (C) 1986-1993, 1998, 2004, 2007-2012
#       Thomas Williams, Colin Kelley and many others
#
#       gnuplot home:     http://www.gnuplot.info
#       faq, bugs, etc:   type "help FAQ"
#       immediate help:   type "help"  (plot window: hit 'h')
#
#       Type `load "all.dem"` to display a large number of examples.
#       They are located at /usr/share/doc/packages/gnuplot/demo/*
#
 set terminal postscript landscape enhanced defaultplex \
   leveldefault color colortext \
   solid dashlength 1.0 linewidth 1.0 butt noclip \
   nobackground \
   palfuncparam 2000,0.003 \
   "Helvetica" 18  fontscale 1.0
 set output 'C2-ka.ps'

set xlabel "ka"
set xlabel  offset character 0, 0, 0 font "" textcolor lt -1 norotate
set x2label ""
set x2label  offset character 0, 0, 0 font "" textcolor lt -1 norotate
set xrange [ * : * ] noreverse nowriteback
set x2range [ * : * ] noreverse nowriteback
set ylabel "|C|^2"
set ylabel  offset character 0, 0, 0 font "" textcolor lt -1 rotate by -270
set y2label ""
set y2label  offset character 0, 0, 0 font "" textcolor lt -1 rotate by -270
set yrange [ * : * ] noreverse nowriteback
set y2range [ * : * ] noreverse nowriteback
set zlabel ""
set zlabel  offset character 0, 0, 0 font "" textcolor lt -1 norotate
set zrange [ * : * ] noreverse nowriteback
set cblabel ""
set cblabel  offset character 0, 0, 0 font "" textcolor lt -1 rotate by -270
set cbrange [ * : * ] noreverse nowriteback
set zero 1e-08
set locale "en_US.UTF-8"
set key right top
# ---------------------- Föll -------------------------------
I={0.0,1.0}  # þvereining i
# x=ka
# y=gamma
icot(x) = I/tan(x)
gp(x)  = (1.0+I*x)
gm(x)  = (1.0-I*x)
C(x,y) = (I*exp(-I*x)/(2*sin(x)))*(1+(gp(y)-icot(x))/(gm(y)+icot(x)))
#-----------------------------------------------------------
#
plot [0:4.0*pi][0:2.4] abs(C(x,-0.1/x))**2 w l title '|C|^2, ({/Symbol a}/(aE_1))=0.1' lw 2,\
                       abs(C(x,-1.0/x))**2 w l title '|C|^2, ({/Symbol a}/(aE_1))=1.0' lw 2,\
                       abs(C(x,-2.0/x))**2 w l title '|C|^2, ({/Symbol a}/(aE_1))=2.0' lw 2,\
                       1.0 w l title '|B|^2' lt 4 lw 2
#    EOF
```

(13)


```
#!/usr/bin/gnuplot -persist
#
#
#       G N U P L O T
#       Version 4.6 patchlevel 0    last modified 2012-03-04
#       Build System: Linux x86_64
#
#       Copyright (C) 1986-1993, 1998, 2004, 2007-2012
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#
#       gnuplot home:     http://www.gnuplot.info
#       faq, bugs, etc:   type "help FAQ"
#       immediate help:   type "help"  (plot window: hit 'h')
#
#       Type `load "all.dem"` to display a large number of examples.
#       They are located at /usr/share/doc/packages/gnuplot/demo/*
#
 set terminal postscript landscape enhanced defaultplex \
   leveldefault color colortext \
   solid dashlength 1.0 linewidth 1.0 butt noclip \
   nobackground \
   palfuncparam 2000,0.003 \
   "Helvetica" 18  fontscale 1.0
 set output 'C2-E.ps'

set xlabel "E/E_1"
set xlabel  offset character 0, 0, 0 font "" textcolor lt -1 norotate
set x2label ""
set x2label  offset character 0, 0, 0 font "" textcolor lt -1 norotate
set xrange [ * : * ] noreverse nowriteback
set x2range [ * : * ] noreverse nowriteback
set ylabel "|C|^2"
set ylabel  offset character 0, 0, 0 font "" textcolor lt -1 rotate by -270
set y2label ""
set y2label  offset character 0, 0, 0 font "" textcolor lt -1 rotate by -270
set yrange [ * : * ] noreverse nowriteback
set y2range [ * : * ] noreverse nowriteback
set zlabel ""
set zlabel  offset character 0, 0, 0 font "" textcolor lt -1 norotate
set zrange [ * : * ] noreverse nowriteback
set cblabel ""
set cblabel  offset character 0, 0, 0 font "" textcolor lt -1 rotate by -270
set cbrange [ * : * ] noreverse nowriteback
set zero 1e-08

set locale "en_US.UTF-8"
set key right top
# ---------------------- Föll -------------------------------
I={0.0,1.0}  # þvereining i
# x=ka
# y=gamma
icot(x) = I/tan(x)
gp(x)  = (1.0+I*x)
gm(x)  = (1.0-I*x)
C(x,y) = (I*exp(-I*x)/(2*sin(x)))*(1+(gp(y)-icot(x))/(gm(y)+icot(x)))
#-----------------------------------------------------------
#
plot [0:16.0*pi**2][0:2.4] abs(C(sqrt(x),-0.1/sqrt(x)))**2 w l title '|C|^2, ({/Symbol a}/(aE_1))=0.1' lw 2,\
                       abs(C(sqrt(x),-1.0/sqrt(x)))**2 w l title '|C|^2, ({/Symbol a}/(aE_1))=1.0' lw 2,\
                       abs(C(sqrt(x),-2.0/sqrt(x)))**2 w l title '|C|^2, ({/Symbol a}/(aE_1))=2.0' lw 2,\
                       1.0 w l title '|B|^2' lt 4 lw 2
#    EOF
```

(14)


```
#!/usr/bin/gnuplot -persist
#
#
#       G N U P L O T
#       Version 4.6 patchlevel 0    last modified 2012-03-04
#       Build System: Linux x86_64
#
#       Copyright (C) 1986-1993, 1998, 2004, 2007-2012
#       Thomas Williams, Colin Kelley and many others
#
#       gnuplot home:     http://www.gnuplot.info
#       faq, bugs, etc:   type "help FAQ"
#       immediate help:   type "help"  (plot window: hit 'h')
#
#       Type `load "all.dem"` to display a large number of examples.
#       They are located at /usr/share/doc/packages/gnuplot/demo/*
#
 set terminal postscript landscape enhanced defaultplex \
   leveldefault color colortext \
   solid dashlength 1.0 linewidth 1.0 butt noclip \
   nobackground \
   palfuncparam 2000,0.003 \
   "Helvetica" 18  fontscale 1.0
 set output 'C2-ka-3D.ps'

set xlabel "ka"
set xlabel  offset character 0, 0, 0 font "" textcolor lt -1 norotate
set x2label ""
set x2label  offset character 0, 0, 0 font "" textcolor lt -1 norotate
set xrange [ * : * ] noreverse nowriteback
set x2range [ * : * ] noreverse nowriteback
set ylabel "{/Symbol a}/(aE_1)"
set ylabel  offset character 0, 0, 0 font "" textcolor lt -1 rotate by -270
set y2label ""
set y2label  offset character 0, 0, 0 font "" textcolor lt -1 rotate by -270
set yrange [ * : * ] noreverse nowriteback
set y2range [ * : * ] noreverse nowriteback
set zlabel ""
set zlabel  offset character 0, 0, 0 font "" textcolor lt -1 norotate
set zrange [ * : * ] noreverse nowriteback
set cblabel ""
set cblabel  offset character 0, 0, 0 font "" textcolor lt -1 rotate by -270
set cbrange [ * : * ] noreverse nowriteback
set zero 1e-08
set lmargin  -1
set bmargin  -1
set rmargin  -1
set tmargin  -1
set locale "en_US.UTF-8"
set pm3d explicit at s
set pm3d scansautomatic
set pm3d interpolate 1,1 flush begin noftriangles nohidden3d corners2color mean
set palette positive nops_allcF maxcolors 0 gamma 1.5 color model RGB
set palette rgbformulae 7, 5, 15
set colorbox default
set colorbox vertical origin screen 0.9, 0.2, 0 size screen 0.05, 0.6, 0 front bdefault
set style boxplot candles range  1.50 outliers pt 7 separation 1 labels auto unsorted
set loadpath
set fontpath
set psdir
set fit noerrorvariables
# ---------------------- Föll -------------------------------
I={0.0,1.0}  # þvereining i
# x=ka
# y=gamma
icot(x) = I/tan(x)
gp(x)  = (1.0+I*x)
```

File: /home2/vidar/Instruado/IaSF/Dæmi-2012/Gröf/C2-ka-3D.gnu

```
gm(x)  = (1.0-I*x)
C(x,y) = (I*exp(-I*x)/(2*sin(x)))*(1+(gp(y)-icot(x))/(gm(y)+icot(x)))
#------------------------------------------------------------------
#
unset key
set title '|C(ka,{/Symbol a}/(aE_1))|^2'
set pm3d map
set samples 400
set isosamples 400
splot [0:4.0*pi][0:10][0:8.0] abs(C(x,-y/x))**2 w pm3d
#    EOF
```


5

1

2.51 Skoðum mættið

$$V(x) = -\frac{\hbar^2 a^2}{m}\,\mathrm{Sech}^2(ax)$$

$[ax]$

$[a] = L^{-1}$

Vidda a

$$= -2E_0\,\mathrm{Sech}^2(ax)$$

þar sem E_0 er einhver náttúrulegur orkustuðull mættisins

$$E_0 = \frac{\hbar^2 a^2}{2m}$$

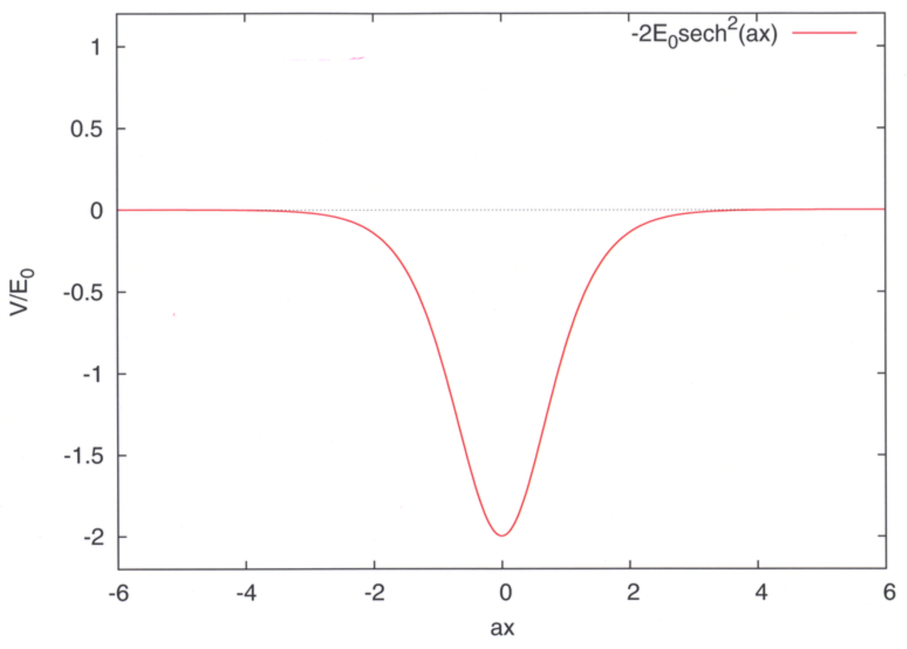
því er eðlilegt að teikna upp V/E_0 v.s. ax

a) sjá næstu síðu

b) Sýna að $\phi_0(x) = A\,\mathrm{sech}(ax)$

sé bylgjufall grunnástandsins, finna A og orku grunnástandsins

2



3

Ég nota wxmaxima til þess að finna

$$d_x \phi_0(x) = -Aa\,\mathrm{sech}(ax)\tanh(ax)$$

$$d_x^2 \phi_0(x) = Aa^2\left\{\mathrm{sech}(ax)\tanh^2(ax) - \mathrm{sech}^3(ax)\right\}$$

Schrödinger jafnan fyrir grunnástandið er

$$\left\{-\frac{\hbar^2}{2m}d_x^2 - \frac{\hbar^2 a^2}{m}\mathrm{Sech}^2(ax)\right\}\phi_0(x) = \varepsilon_0\phi_0(x)$$

Reynum

$$\left\{-\frac{\hbar^2}{2m}d_x^2 - \frac{\hbar^2 a^2}{m}\mathrm{sech}^2(ax)\right\}\phi_0(x) = +\frac{\hbar^2 a^2}{m}A\left\{\frac{\mathrm{sech}^3(ax) - \mathrm{sech}(ax)\tanh^2(ax)}{2} - \mathrm{sech}^3(ax)\right\}$$

4

$$= -\frac{\hbar^2 a^2}{2m}\left\{\mathrm{sech}^3(ax) + \mathrm{sech}(ax)\tanh^2(ax)\right\}A$$

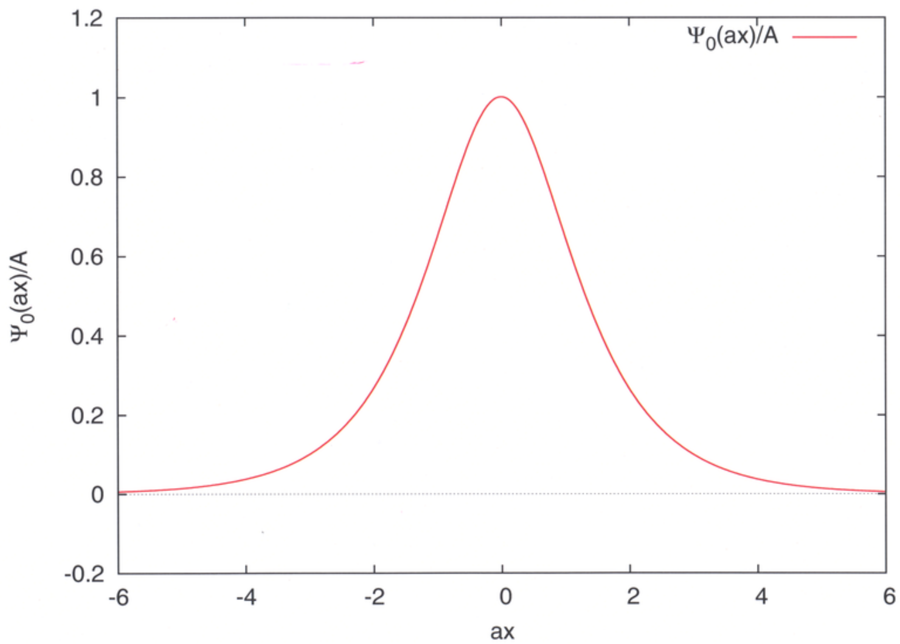
$$= -\frac{\hbar^2 a^2}{2m}\left\{\frac{1}{\cosh^3(ax)} + \frac{\sinh^2(ax)}{\cosh^3(ax)}\right\}A = -\frac{\hbar^2 a^2}{2m}\left\{\frac{1+\sinh^2(ax)}{\cosh^3(ax)}\right\}A$$

$$= -\frac{\hbar^2 a^2}{2m}\frac{A}{\cosh(ax)} = -\frac{\hbar^2 a^2}{2m}A\,\mathrm{sech}(ax) = -\frac{\hbar^2 a^2}{2m}\psi_0(x)$$

$$\rightarrow \mathcal{E}_0 = -\frac{\hbar^2 a^2}{2m} = -E_0$$

Eins og séð á næstu mynd má búast við að $\psi_0(x)$ sé bylgjufall grunnástandsins, engin núllstöð, samhverft.

5



6

Staðla $\psi_0 = A\,\mathrm{sech}(ax) = A\frac{1}{\cosh(ax)}$

$$1 = |A|^2\int_{-\infty}^{\infty}dx\,\mathrm{sech}^2(ax) = \frac{a}{2}$$

samkvæmt wxmaxima

$\rightarrow A = \sqrt{\frac{a}{2}}$ er mögulegt val fyrir A.

7

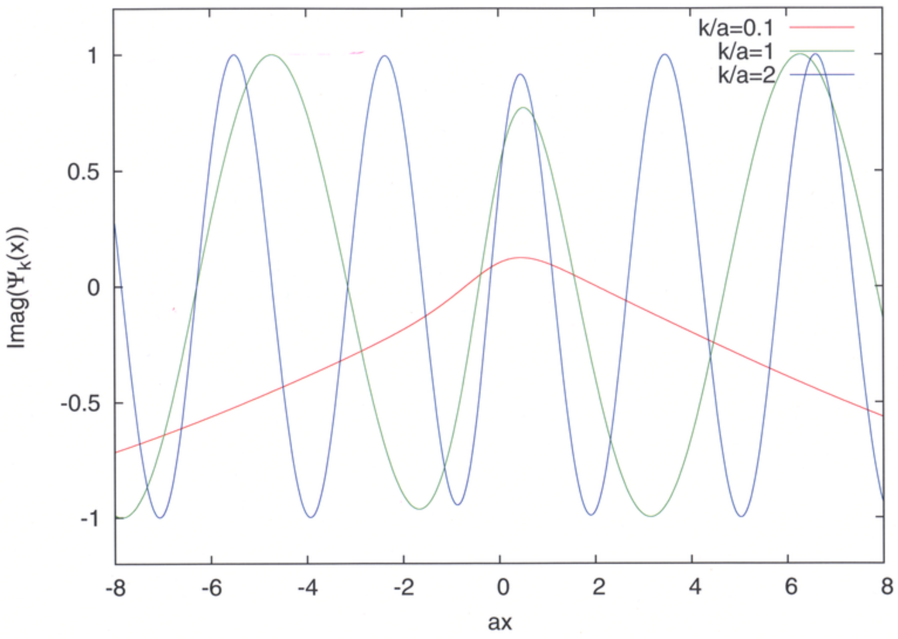
c) Sýna að

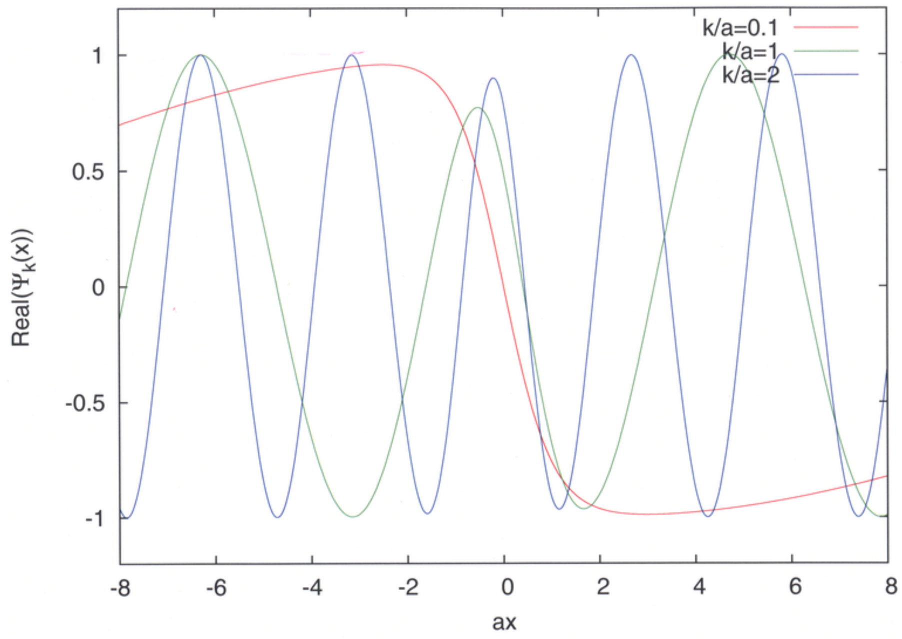
$$\psi_k(x) = A\left\{\frac{ik - a\tanh(ax)}{ik + a}\right\}e^{ikx}$$

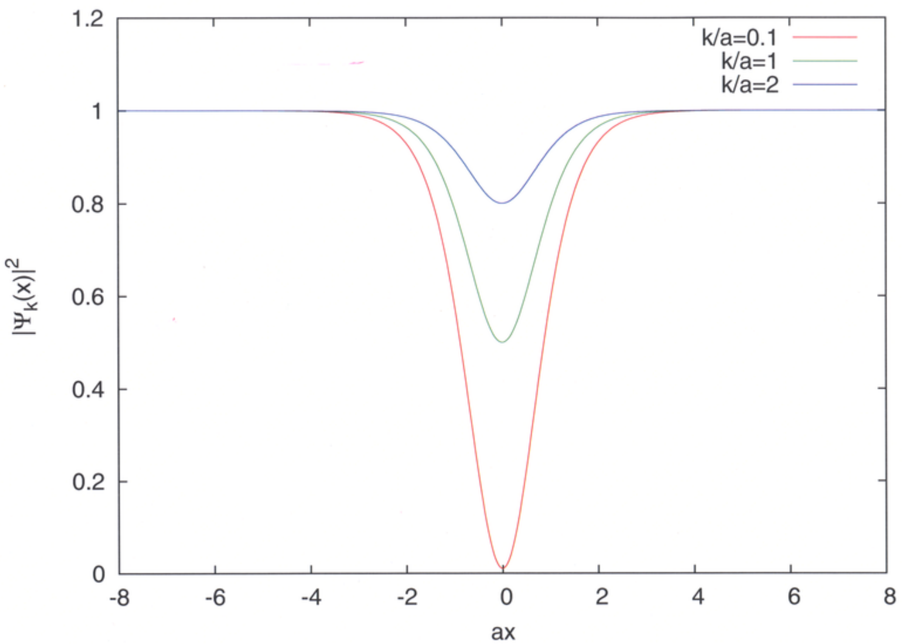
með $k = \frac{\sqrt{2mE}}{\hbar}$ sé lausn á jöfnu Schrödingers fyrir hvaða E sem er.

$$\psi_k(x) = A\left\{\frac{i\left(\frac{k}{a}\right) - \tanh(ax)}{i\left(\frac{k}{a}\right) + 1}\right\}e^{i\left(\frac{k}{a}\right)(ax)}$$

Skoðum graf fyrst







Reynum

$$H\psi_k(x) = A\left\{-\frac{\hbar^2}{2m}d_x^2 - \frac{\hbar^2 a^2}{m}\mathrm{sech}^2(ax)\right\}\left\{\frac{ik - a\tanh(ax)}{ik+a}\right\}e^{ikx}$$

$$d_x^2\psi_k(x) = A\left[-\frac{k^2e^{ikx}(ik-a\tanh(ax))}{ik+a} + \frac{2a^3e^{ikx}\mathrm{sech}^2(ax)\tanh(ax)}{ik+a} - \frac{2ia^2ke^{ikx}\mathrm{sech}^2(ax)}{ik+a}\right]$$

$$H\psi_k(x) = -\frac{A\hbar^2}{2m}\left[k^2e^{ikx}\left\{\frac{ik-a\tanh(ax)}{ik+a}\right\} + \frac{2a^3e^{ikx}\mathrm{sech}^2(ax)\tanh(ax)}{\cancel{ik+a}} - \frac{2ia^2ke^{ikx}\mathrm{sech}^2(ax)}{ik+a} + 2a^2\cancel{\mathrm{sech}^2(ax)}\left\{\frac{ik-a\tanh(ax)}{\cancel{ik+a}}\right\}e^{ikx}\right]$$

(10)

$$H\psi_k(x) = -\frac{\hbar^2 k^2}{2m} A e^{ikx} \left\{ \frac{ik - a\tanh(ax)}{ik+a} \right\} = \underbrace{-\frac{\hbar^2 k^2}{2m}}_{\text{orka frjálsrar eindar}} \psi_k(x)$$

$$\left.\begin{aligned} \lim_{x\to\infty} \tanh(x) &= +1 \\ \lim_{x\to-\infty} \tanh(x) &= -1 \end{aligned}\right\}$$

Aðfellu form innbylgju er

$$\psi_k(x) \xrightarrow[x\to-\infty]{} A e^{ikx}$$

Aðfellu form útbylgju er

$$\psi_k(x) \xrightarrow[x\to\infty]{} A\left\{\frac{ik-a}{ik+a}\right\} e^{ikx} \to \underbrace{|\psi_k(x)|^2 \xrightarrow[x\to\pm\infty]{} A}$$

engin endurkast bylgja!

(11)

Nú er hægt að spyrja eru til önnur svona mætti? Einfaldari spurning er: Er til mætti $V(x,\alpha)$ við stika α þ.a. eigingildi jöfnu Schrödingers breytist ekki þegar α er hnikað til. Hægt er að sýna að mætti sem uppfylla ólínulegu jöfnuna {Korteweg-deVries}

$$\partial_\alpha V + V[\partial_x V] + \partial_x^3 V = 0$$

skila þannig mættum. → Lausnir á óháðu eiginverkefni fyrir línulegu jöfnu Schrödinger leiða til lausna á ólínulegum jöfnum ..... eintera lausnir .....

(12)

2.45 Engar margfaldar lausnir í einvídd fyrir bundin ástönd

Gefum okkur að til séu tvær lausnir ψ_1 og ψ_2 með sömu orku E

$$\left\{-\frac{\hbar^2}{2m}d_x^2 + V(x)\right\}\psi_1 = E\psi_1 \qquad \text{margfalda með } \psi_2$$

$$\left\{-\frac{\hbar^2}{2m}d_x^2 + V(x)\right\}\psi_2 = E\psi_2 \qquad \text{-||-} \quad \psi_1$$

draga frá

$$\to \quad -\psi_2 \frac{\hbar^2}{2m}\psi_1'' + \psi_1 \frac{\hbar^2}{2m}\psi_2'' = E\{\psi_2\psi_1 - \psi_1\psi_2\} = 0$$

$$\to \quad \psi_1\psi_2'' - \psi_2\psi_1'' = 0$$

(13)

Athugum

$$d_x\{\psi_1 d_x\psi_2 - \psi_2 d_x\psi_1\} = \{\psi_1 d_x^2\psi_2 - \psi_2 d_x^2\psi_1\} + \{\psi_1'\psi_2' - \psi_2'\psi_1'\}$$

$$= \{\psi_1\psi_2'' - \psi_2\psi_1''\} = 0 \quad \leftarrow \text{eins og sást áðer}$$

$$\to \{\psi_1\psi_2' - \psi_2\psi_1'\} = C \leftarrow \text{fasti}$$

Bundin ástönd $\to$ $\left.\begin{aligned}\psi_1(x)\\ \psi_2(x)\end{aligned}\right. \xrightarrow[x\to\pm\infty]{} 0$ $\Bigg\}$ $\to$ $C=0$

→ $\{\psi_1\psi_2' - \psi_2\psi_1'\} = 0$ fyrir öll x

→ $\psi_1\psi_2' = \psi_2\psi_1'$ → $\dfrac{\psi_2'}{\psi_2} = \dfrac{\psi_1'}{\psi_1}$

→ $\ln\psi_1 = \ln\psi_2 + C_1$

→ $\boxed{\psi_1 = C_1\psi_2}$

sama bylgjufallið

3.10 Eind í óendanlegum brunni, er grunnástandið eigin ástand skriðþungavirkjan p?

Hamiltonvirkinn er

$$H = \frac{p^2}{2m} + V(x) \quad \text{með} \quad V(x) = \begin{cases} 0 & \text{ef } 0 \le x \le a \\ \infty & \text{annars} \end{cases}$$

Grunnástandið er

$$\psi_1(x) = \sqrt{\frac{2}{a}}\,\sin\left(\pi\frac{x}{a}\right)$$

$p = -i\hbar\partial_x$ → $p\psi_1(x) = \sqrt{\frac{2}{a}}\,\frac{\pi}{a}\cos\left(\pi\frac{x}{a}\right)$

$\neq$ fasti $\cdot\, \psi_1(x)$

Grunnástandið er því ekki eiginástand p !

Hví ekki ?

$$[p, H] = [p, V] \neq 0$$

→ því geta p og H ekki haft sameiginleg eiginástönd !

Veggirnir í $x = 0, a$ valda speglunum → alltaf verða til staðar bylgjur sem stefna í sitt hvora áttina

Hamiltonvirki tvístiga kerfis er

$$H = E\{|1\rangle\langle 1| + 2|2\rangle\langle 2| + i|1\rangle\langle 2| - i|2\rangle\langle 1|\}$$

Ástöndin $\{|n\rangle\}$ mynda fullkominn staðlaðan grunn

Við getum fundið Hamilton fylkið í þessum grunni með því að athuga fylkjastökin $\langle n|H|m\rangle$

→ $H = E\begin{pmatrix} 1 & i \\ -i & 2 \end{pmatrix}$

Stökin utan hornalínu rekka orkugildin 1E og 2E í sundur

Eigingildin eru
(maxima)

$$E_\pm = \left(\frac{3}{2} \pm \frac{\sqrt{5}}{2}\right)E \simeq \begin{cases} 2{,}618 \cdot E \\ 0{,}382 \cdot E \end{cases}$$

Eiginvigrarnir eru

$$|\pm\rangle = \left\{|1\rangle \mp i\left(\frac{\sqrt{5}\pm 1}{2}\right)|2\rangle\right\}\frac{1}{\sqrt{1+\left(\frac{\sqrt{5}\pm1}{2}\right)^2}}$$

$$= \left\{|1\rangle \mp i\alpha_\pm |2\rangle\right\}\frac{1}{\sqrt{1+\alpha_\pm^2}} \quad , \quad \alpha_\pm = \frac{\sqrt{5}\pm 1}{2}$$

Hvernig lítur H út í nýja grunninum?

$|\pm\rangle$ eru eiginvigrar H

$$\left.\begin{array}{l} \to \langle +|H|+\rangle = E_+ \\ \quad \langle -|H|-\rangle = E_- \\ \text{og } \langle \pm|H|\mp\rangle = 0 \end{array}\right\} \quad H = \begin{pmatrix} E_- & 0 \\ 0 & E_+ \end{pmatrix}$$

í nýja grunninum ef $|+\rangle \to 2$, $|-\rangle \to 1$

Í eiginástandagrunninum er H á hornalínuformi.

Hver eru væntigildi H fyrir ástöndin $|1\rangle$ og $|2\rangle$

$$\langle 1|H|1\rangle = 1E \quad , \quad \langle 2|H|2\rangle = 2E$$

eins og lesa má beint úr útsetningu H í upphaflega grunninum $\{|n\rangle\}$

4.20 Eind í mætti $V(\bar r)$, sýna fram á að

$$d_t\langle \bar L\rangle = \langle \bar N\rangle$$

þ.s. $\bar N = \bar r \times \bar F = \bar r \times (-\bar\nabla V)$

Breyting á væntigildi hverfiþunga er vegna væntigildis vægis á kerfið

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

Höfum áður séð almenna jöfnu fyrir væntigildi

$$d_t\langle Q\rangle = \frac{i}{\hbar}\langle [H,Q]\rangle + \langle \partial_t Q\rangle$$

$\bar L = \bar r \times \bar p$ → í okkar Schrödingermynd $\partial_t L = 0$

$$\to d_t\langle \bar L\rangle = \frac{i}{\hbar}\langle [H,\bar L]\rangle$$

Við þurfum því að reikna víxlin $[H,\bar L] = \left[\frac{p^2}{2m},\bar L\right] + [V,\bar L]$

Skoðum

$$[p^2, L_z] = [p_x^2+p_y^2+p_z^2, L_z] = [p_x^2, L_z] + [p_y^2, L_z] + [p_z^2, L_z]$$

$$= p_x[p_x,L_z] + [p_x,L_z]p_x + p_y[p_y,L_z] + [p_y,L_z]p_y$$

$$+ p_z[p_z,L_z] + [p_z,L_z]p_z$$

þ.s. við notum $[AC,B] = A[C,B] + [A,B]C$

$$L_z = xp_y - yp_x$$

$$\to [p_x, L_z] = [p_x, x]p_y = -i\hbar p_y$$

$$[p_y, L_z] = -[p_y, y]p_x = i\hbar p_x$$

$$[p_z, L_z] = 0$$

$$\to [p_x^2, L_z] = -i\hbar p_x p_y - i\hbar p_y p_x$$

eins fæst

$$[p_y^2, L_z] = i\hbar p_x p_y + i\hbar p_y p_x$$

$$[p_x^2 + p_y^2, L_z] = 0$$

og því í heild $[p^2, L_z] = 0$

Samskonar fæst fyrir hina þætti $\bar{L}$ og því

$$[p^2, \bar{L}] = 0$$

(hverfiþungi frjálsrar eindar er hreyfingarfasti)

Eftir stendur

$$[V(\bar{r}), \bar{L}] = [V(\bar{r}), \bar{r}\times\bar{p}]$$

$$-i\hbar[V(\bar{r}), \bar{r}\times\bar{\nabla}]$$

ef við notum útsetninguna í staðarrúminu með $\bar{p} = -i\hbar\bar{\nabla}$

Könnum

$$[V(\bar{r}), \bar{r}\times\bar{\nabla}]f(\bar{r}) = V(\bar{r})\{\bar{r}\times\bar{\nabla}f(\bar{r})\} - \bar{r}\times\bar{\nabla}\{V(\bar{r})f(\bar{r})\}$$

$$= \{-f(\bar{r})\}\bar{r}\times\bar{\nabla}V(\bar{r})$$

eða

$$-i\hbar[V(\bar{r}), \bar{r}\times\bar{\nabla}] = i\hbar\, \bar{r}\times\{\bar{\nabla}V(\bar{r})\}$$

en

$$d_t\langle\bar{L}\rangle = \frac{i}{\hbar}\langle[H, \bar{L}]\rangle = -\langle\bar{r}\times\{\bar{\nabla}V(\bar{r})\}\rangle$$

$$= \langle\bar{r}\times\{-\bar{\nabla}V(\bar{r})\}\rangle = \langle\bar{N}\rangle$$

ef $\bar{N} = \bar{r}\times\bar{F} = \bar{r}\times\{-\bar{\nabla}V\}$

Einsleitur 3D hreintóna sveifill með orkuróf

$$E_{nlm} = E_0\cdot\left(n + \frac{3}{2}\right)$$

er í ástandi

$$|\alpha\rangle = \{2|100\rangle + |211\rangle - |210\rangle + i|21{-1}\rangle\}$$

Gerum ráð fyrir því að $|nlm\rangle$ séu stöðluð, en við þurfum að staðla $|\alpha\rangle$

$$\langle\alpha|\alpha\rangle = \{4 + 1 + 1 + 1\} = 7$$

-> staðlað er

$$|\alpha\rangle = \frac{1}{\sqrt{7}}\{2|100\rangle + |211\rangle - |210\rangle + i|21{-1}\rangle\}$$

(7)

a) Væntigildi H (notum $H|nlm\rangle = E_{nlm}|nlm\rangle = E_n|nlm\rangle$)

$$\langle\alpha|H|\alpha\rangle = \frac{1}{7}\left\{4\cdot\frac{5}{2}E_0 + 1\cdot\frac{7}{2}E_0 + 1\cdot\frac{7}{2}E_0 + \frac{7}{2}E_0\right\}$$

$$= \frac{E_0}{7}\left\{\frac{20}{2} + \frac{21}{2}\right\} = E_0\cdot\frac{41}{14}$$

b) væntigildi L^2 (notum $L^2|nlm\rangle = \hbar^2 l(l+1)|nlm\rangle$)

$$\langle\alpha|L^2|\alpha\rangle = \frac{\hbar^2}{7}\left\{0 + 1\cdot2 + 1\cdot2 + 1\cdot2\right\}$$

$$= \hbar^2\frac{6}{7}$$

(8)

c) væntigildi L_z (notum $L_z|nlm\rangle = \hbar m|nlm\rangle$)

$$\langle\alpha|L_z|\alpha\rangle = \frac{\hbar}{7}\left\{0 + 1 - 0 - 1\right\} = 0$$

(1)

4.30

Almenn stefna í kúluhnitum

$$\hat r = \sin\theta\cos\phi\cdot\hat i + \sin\theta\sin\phi\,\hat j + \cos\theta\,\hat k$$

Finnum S_r, fylkið fyrir spuna þáttinn í þessa stefnu

$$\bar S\cdot\hat r = S_r = S_x\hat r_x + S_y\hat r_y + S_z\hat r_z$$

$$= \frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}\sin\theta\cos\phi + \frac{\hbar}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix}\sin\theta\sin\phi$$

$$+ \frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\cos\theta$$

$$= \frac{\hbar}{2}\begin{pmatrix}\cos\theta & \sin\theta(\cos\phi - i\sin\phi)\\ \sin\theta(\cos\phi + i\sin\phi) & -\cos\theta\end{pmatrix}$$

(2)

$$\to S_r = \frac{\hbar}{2}\begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta\end{pmatrix}$$

Reynum til gamans $\hat r = \hat z$ þegar $\theta = 0$, þá fæst

$$S_z = \frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

og samsvarar með samreyna fyrir x og y - þættina

Finnum eigingildi og vigra

Skoðum hvað maxima gefur

Eigingildi $-1\cdot\frac{\hbar}{2}$ og $+1\cdot\frac{\hbar}{2}$

með eiginvigra

$$\begin{pmatrix} 1 \\ -\left(\frac{1+\cos\theta}{\sin\theta}\right)e^{+i\phi} \end{pmatrix} \quad \text{og} \quad \begin{pmatrix} 1 \\ \left(\frac{1-\cos\theta}{\sin\theta}\right)e^{+i\phi} \end{pmatrix}$$

Notum $1+\cos\theta = 2\cos^2\frac{\theta}{2}$ og $\sin\theta = 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}$

$$1-\cos\theta = 2\sin^2\frac{\theta}{2}$$

þá eru vigrarnir

$$\begin{pmatrix} 1 \\ -\cot\frac{\theta}{2}\cdot e^{i\phi} \end{pmatrix} \quad \text{og} \quad \begin{pmatrix} 1 \\ \tan\frac{\theta}{2}\cdot e^{+i\phi} \end{pmatrix}$$

Normum, þá þurfum við

$$1+\tan^2\frac{\theta}{2} = \sec^2\frac{\theta}{2} = \frac{1}{\cos^2\frac{\theta}{2}}$$

$$1+\cot^2\frac{\theta}{2} = \csc^2\frac{\theta}{2} = \frac{1}{\sin^2\frac{\theta}{2}}$$

Og þá verða normuðu eiginvigrarnir

$$\underbrace{\begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}\cdot e^{+i\phi} \end{pmatrix}}_{\text{samsvarandi } -\frac{\hbar}{2}} \quad \text{og} \quad \underbrace{\begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}\cdot e^{+i\phi} \end{pmatrix}}_{\text{samsvarandi } +\frac{\hbar}{2}}$$

Vigrarnir eru greinilega hornréttir, og þar sem normunin er frjáls m.t.t. fasa skrifum við

$$\begin{pmatrix} \sin\frac{\theta}{2}\cdot e^{-i\phi} \\ -\cos\frac{\theta}{2} \end{pmatrix} \quad \text{og} \quad \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}\cdot e^{+i\phi} \end{pmatrix}$$

og sjáum fyrir $\hat{r} = \hat{z}$ þegar $\theta = 0$

$$\begin{pmatrix} 0 \\ -1 \end{pmatrix} \quad \text{og} \quad \begin{pmatrix} +1 \\ 0 \end{pmatrix}$$

eins og við þekkjum

4.33 Rafeind föst í segulsviði

$$\bar{B} = B_0\cos(\omega t)\hat{k}$$

a) finna H fyrir kerfið. Samkvæmt jöfnu (4.160)

$$H = -\gamma\,\bar{B}\cdot\bar{S} = -\gamma\, B_0\cos(\omega t)S_z$$

$$= -\gamma B_0\cos(\omega t)\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= -\frac{\gamma B_0\hbar}{2}\cos(\omega t)\begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}$$

tímaháða spuna ástandinu (kerfisins) er lýst með

$$\chi(t) = \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} \quad \text{og} \quad \boxed{i\hbar\partial_t\chi(t) = H(t)\chi(t)}$$

er hreyfijafna χ

7

b) Klukkan $t=0$ er upphafsástandið

$$\chi(0) = \chi_+^{(x)}$$ ← spuna uppástandið fyrir x-ásinn

Samkvæmt (4.151) er

$$\chi_+^{(x)} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

Jöfnurnar fyrir $\alpha(t)$ og $\beta(t)$ eru ekki tengdar og því er lausnaraðferðin einföld

finnum $\chi(t)$ fyrir $t>0$

Hreyfijöfnuna má skrifa

$$i\hbar \begin{pmatrix} \dot\alpha(t) \\ \dot\beta(t) \end{pmatrix} = -\frac{\gamma B_0 \hbar}{2} \cos(\omega t) \begin{pmatrix} \alpha(t) \\ -\beta(t) \end{pmatrix}$$

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Skoðum fyrri jöfnuna

$$\dot\alpha(t) = i\,\frac{\gamma B_0}{2} \cos(\omega t)\cdot \alpha(t)$$ 1. stigs jafna

$$\rightarrow \alpha(t) = C\cdot \exp\left\{ i\,\frac{\gamma B_0}{2\omega} \sin(\omega t)\right\}$$ ← reyna með innsetningu

upphafsskilyrði $\alpha(0) = C = \frac{1}{\sqrt{2}}$

Jafnan fyrir $\beta(t)$ er nánast eins, nema hvað er annað

$$\rightarrow \beta(t) = \frac{1}{\sqrt{2}} \exp\left\{ -i\,\frac{\gamma B_0}{2\omega} \sin(\omega t)\right\}$$

og því

$$\chi(t) = \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \exp\left\{ i\,\frac{\gamma B_0}{2\omega} \sin(\omega t)\right\} \\ \exp\left\{ -i\,\frac{\gamma B_0}{2\omega} \sin(\omega t)\right\} \end{pmatrix}$$

9

c) Hver eru líkindin að mæla S_x og fá gildi $-\frac{\hbar}{2}$?

þ.e. hve stór $\chi_-^{(x)}$ þátturinn í $\chi(t)$?

Notum innfeldið

$$\left\{\chi_-^{(x)}\right\}^* \chi(t) = \frac{1}{\sqrt{2}} (1,-1)\cdot \frac{1}{\sqrt{2}} \begin{pmatrix} \exp\left\{ i\,\frac{\gamma B_0}{2\omega} \sin(\omega t)\right\} \\ \exp\left\{ -i\,\frac{\gamma B_0}{2\omega} \sin(\omega t)\right\} \end{pmatrix}$$

$$= \frac{1}{2}\left\{ \exp\{i\ldots\} - \exp\{-i\ldots\}\right\}$$

$$= i \sin\left\{ \frac{\gamma B_0}{2\omega} \sin(\omega t)\right\}$$

líkindin

$$P_-^{(x)}(t) = \left| \left\{\chi_-^{(x)}\right\}^* \chi(t)\right|^2 = \sin^2\left\{ \frac{\gamma B_0}{2\omega} \sin(\omega t)\right\}$$

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d) Hvert er lágmarkssviðið til þess að snúa S_x alveg?

Algersnúningur verður þegar $P_-^{(x)}(t) = 1$

því við byrjuðum með spuna upp $\chi(0) = \chi_+^{(x)}$

→ hvenær verður $\sin^2\left\{ \frac{\gamma B_0}{2\omega} \sin(\omega t)\right\} = 1$

eða $\frac{\gamma B_0}{2\omega} \sin(\omega t) = \frac{\pi}{2}$

$\sin(\omega t)$ tekur gildi á $[-1,1]$

$$\rightarrow \frac{\gamma B_0}{2\omega} = \frac{\pi}{2} \rightarrow B_0 = \frac{\pi\omega}{\gamma}$$

annars tekst ekki að snúa spunanum!

1D-hreintóna sveifill

$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right), \quad n = 0, 1, 2, \ldots$$

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}\, a}} H_n\left(\frac{x}{a}\right) e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}$$

$$a = \sqrt{\frac{\hbar}{m\omega}}$$ náttúrulegur lengdarskali fleygbogamættisins

Kerfið er truflað með $H' = \alpha\delta(x)$

Skoðum 1. stigs áhrifin á orkurófið.

Einföld orkustig

$$\to E_n' = E_n + \langle n|V|n\rangle$$ er nýja orkurófið fyrir truflaða kerfið

$$\langle n|V|n\rangle = \alpha\int_{-\infty}^{\infty} dx\, \psi_n^*(x)\delta(x)\psi_n(x) = \alpha|\psi_n(0)|^2$$

$$= \alpha \frac{1}{2^n n! \sqrt{\pi}\, a}\left\{H_n(0)\right\}^2$$

$$H_n(0) = \begin{cases} 0 & \text{fyrir oddatölu } n \\ \dfrac{(-1)^{n/2}\, n!}{(\frac{1}{2}n)!} & \text{fyrir jöfnu } n \end{cases}$$

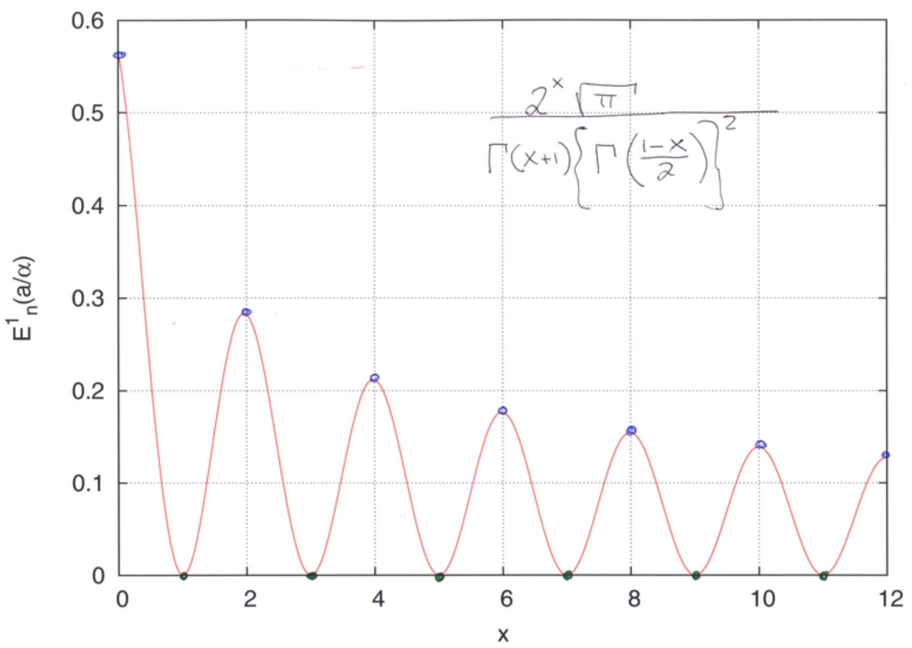
eða $$H_n(0) = \frac{2^n\sqrt{\pi}}{\Gamma\left(\frac{1-n}{2}\right)}$$

$$\langle n|V|n\rangle = \left(\frac{\alpha}{a}\right)\frac{2^n\sqrt{\pi}}{n!\left\{\Gamma\left(\frac{1-n}{2}\right)\right\}^2}$$ stærð með vídd orku

$\Gamma(-n) \to \pm\infty$ and $\Gamma(0) \to \pm\infty$ fyrir $n \geq 0$

$\to$ ástönd með oddatölu n hreyfast ekki
andsamhverf ástönd með núllstöð í 0

Ástönd með jöfnu n hliðrast upp



Tvær bósendir víxlverkast veikt með snertivíxlverkun (5)

$$V(x_1,x_2) = \alpha\,\delta(x_1-x_2) \qquad \alpha>0 \text{ fráhrinding}$$

a) Finna orku grunn- og örvaðs ástands fyrir óvíxlverkandi bósendir

Einnar-eindar ástöndin eru

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!\,\sqrt{\pi}\,a}}\, H_n\left(\frac{x}{a}\right) e^{-\frac{1}{2}\left(\frac{x}{a}\right)^2}$$

$$a = \sqrt{\frac{\hbar}{m\omega}}\;, \qquad E_n = \hbar\omega\left(n+\frac{1}{2}\right)$$

Grunnástandið er samhverft $\rightarrow$

$$\psi_g(x_1,x_2) = \psi_0(x_1)\psi_0(x_2) = \psi_g(x_2,x_1)$$

(6)

Orkan er

$$E_g = 2\cdot E_0 = \hbar\omega \quad \text{, engin víxlverkun}$$

fyrsta örvaða ástandið

samhverft fyrir bósendir

$$\psi_e(x_1,x_2) = \frac{1}{\sqrt{2}}\left\{\psi_0(x_1)\psi_1(x_2) + \psi_1(x_1)\psi_0(x_2)\right\}$$

$$E_e = E_0 + E_1 = \frac{\hbar\omega}{2} + \frac{3\hbar\omega}{2} = 2\hbar\omega$$

b) 1. stigs truflun fyrir E_g og E_e

$$E_g' = \langle g|V|g\rangle = \int_{-\infty}^{\infty} dx_1 dx_2\, \psi_g^*(x_1,x_2)V(x_1,x_2)\psi_g(x_1,x_2)$$

(7)

$$= \alpha\int_{-\infty}^{\infty} dx_1 dx_2\, \delta(x_1-x_2)\,|\psi_g(x_1,x_2)|^2 = \alpha\int_{-\infty}^{\infty} dx_1\, |\psi_g(x_1,x_1)|^2$$

$$= \frac{\alpha}{\pi a^2}\int_{-\infty}^{\infty} dx\, e^{-2\left(\frac{x}{a}\right)^2} = \left(\frac{\alpha}{a}\right)\frac{1}{\pi}\int_{-\infty}^{\infty} du\, e^{-2u^2}$$

$$= \left(\frac{\alpha}{a}\right)\frac{1}{\sqrt{2\pi}}$$

$$E_e' = \langle e|V|e\rangle = \int_{-\infty}^{\infty} dx_1 dx_2\, \psi_e^*(x_1,x_1)V(x_1,x_2)\psi_e(x_1,x_2)$$

$$= \alpha\int_{-\infty}^{\infty} dx_1\, |\psi_e(x_1,x_1)|^2 = \alpha\,\frac{4}{2}\int_{-\infty}^{\infty} dx\, \left\{\psi_0(x)\psi_1(x)\right\}^2$$

(8)

$$= 2\alpha\cdot\frac{1}{\sqrt{\pi}\,a}\,\frac{1}{2\sqrt{\pi}\,a}\int_{-\infty}^{\infty} dx\, \left(2\frac{x}{a}\right)^2 e^{-2\left(\frac{x}{a}\right)^2}$$

$$= \left(\frac{\alpha}{a}\right)\frac{4}{\pi}\int_{-\infty}^{\infty} du\, u^2 e^{-2u^2} = \left(\frac{\alpha}{a}\right)\frac{1}{\sqrt{2\pi}}$$

$$= \left(\frac{\alpha}{a}\right)\frac{1}{\sqrt{2\pi}} = E_g'$$

$\rightarrow$ örvaða ástandið $|e\rangle$ hækkar jafnmikið og grunnástandið $|g\rangle$ vegna snerti fráhrindingarinnar

(6.1) (1)

Óendanlegur brunnur með einni eind

$$\psi_n^0(x) = \sqrt{\frac{2}{a}}\,\sin\left(n\pi\frac{x}{a}\right)$$

$$E_n^0 = E_1 \cdot n^2 \,, \quad E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

Kerfið er truflað með $H' = \alpha\delta(x-\frac{a}{2})$

a) Fyrsta stigs truflun á orku-rófinu

$$E_n = E_n^0 + \langle n|V|n\rangle$$

$$\langle n|V|n\rangle = 2\frac{\alpha}{a}\int_0^a dx\,\sin^2\left(n\pi\frac{x}{a}\right)\delta\left(x-\frac{a}{2}\right)$$

(2)

$$\langle n|V|n\rangle = 2\frac{\alpha}{a}\sin^2\left(\frac{n\pi}{2}\right) = \begin{cases} 0 & \text{ef } n = 2,4,6,\ldots \\ \frac{2\alpha}{a} & \text{ef } n = 1,3,5,\ldots \end{cases}$$

ástöndin með jöfn n eru með núllstöð í $x = \frac{a}{2}$, miðjum brunni, eru andsamhverf um þennan punkt.

b) Finna lægstu liðina í leiðréttingunni á grunnástandinu

$$|\psi_1^1\rangle = \sum_{m=2}^{\infty} \frac{\langle\psi_m|H'|\psi_1^0\rangle}{E_1^0 - E_m^0}|\psi_m^0\rangle$$

Lið m=1 er sleppt, þurfum enn að sjá hvaða m er í raun summað yfir

(3)

þurfum að reikna

$$\langle\psi_m|H'|\psi_1^0\rangle = 2\frac{\alpha}{a}\int_0^a dx\,\sin\left(\pi\frac{x}{a}\right)\delta\left(x-\frac{a}{2}\right)\sin\left(m\pi\frac{x}{a}\right)$$

$$= 2\frac{\alpha}{a}\sin\left(\frac{\pi}{2}\right)\sin\left(m\frac{\pi}{2}\right) = \begin{cases} 2\frac{\alpha}{a}\sin\left(\frac{m\pi}{2}\right) & \text{ef } m = 1,3,5,7 \\ 0 & \text{ef } m = 2,4,6,\ldots \end{cases}$$

Ennfremur er

$$E_1^0 - E_m^0 = E_1 - E_1 m^2 = E_1(1-m^2)$$

$$\rightarrow |\psi_1^1\rangle = \sum_{m=3,5,7\ldots}^{\infty} \left\{\frac{2\left(\frac{\alpha}{a}\right)}{E_1}\right\} \frac{\sin\left(\frac{m\pi}{2}\right)}{1-m^2}$$

(4)

Fyrstu 3 liðirnir eru

$$|\psi_1^1\rangle \simeq \frac{2\left(\frac{\alpha}{a}\right)}{E_1}\left\{\frac{-|\psi_3^0\rangle}{1-9} + \frac{|\psi_5^0\rangle}{1-25} + \frac{-|\psi_7^0\rangle}{1-49}\right\}$$

$$= \frac{2\left(\frac{\alpha}{a}\right)}{E_1}\left\{\frac{|\psi_3^0\rangle}{8} - \frac{|\psi_5^0\rangle}{24} + \frac{|\psi_7^0\rangle}{48}\right\}$$

$$\langle x|\psi_1^1\rangle \approx \frac{2\left(\frac{\alpha}{a}\right)}{E_1}\sqrt{\frac{2}{a}}\left\{\frac{\sin\left(\frac{3\pi x}{a}\right)}{8} - \frac{\sin\left(\frac{5\pi x}{a}\right)}{24} + \frac{\sin\left(\frac{7\pi x}{a}\right)}{48}\right\}$$

Truflunin er spegilsamhverf um punktinn $x = \frac{a}{2}$ —> aðeins bylgjuföll sem eru með sömu samhverfu eru liðuð saman í truflaða bylgjufallið

(6.6) Tvö „góð" ótrufluð ástönd eru

$|\Phi_a^0\rangle$ og $|\Phi_b^0\rangle$ eru margföld

$$|\Phi_\pm^0\rangle = \alpha_\pm |\Phi_a^0\rangle + \beta_\pm |\Phi_b^0\rangle \qquad \Big| \; \langle\Phi_a^0|\Phi_c^0\rangle = \delta_{ac} \text{ með } c = a,b$$

þar sem $\alpha_\pm$ og $\beta_\pm$ eru ákvörðuð með jöfnu (6.22)

a) Sýna að $\langle\Phi_+^0|\Phi_-^0\rangle = 0$

ákvörðunarjöfnurnar eru því

$$\left.\begin{aligned} \alpha_\pm W_{aa} + \beta_\pm W_{ab} &= \alpha_\pm E'_\pm \\ \alpha_\pm W_{ba} + \beta_\pm W_{bb} &= \beta_\pm E'_\pm \end{aligned}\right\} (*)$$

$$\begin{aligned} \langle\Phi_+^0|\Phi_-^0\rangle &= \left\{\alpha_+^* \langle\Phi_a^0| + \beta_+^* \langle\Phi_b^0|\right\} \cdot \left\{\alpha_- |\Phi_a^0\rangle + \beta_- |\Phi_b^0\rangle\right\} \\ &= \alpha_+^*\alpha_- + \beta_+^*\beta_- \end{aligned}$$

Notum (*) t.þ.a. umrita $\beta_\pm$ í $\alpha_\pm$

$$\beta_\pm W_{ab} = \alpha_\pm E'_\pm - \alpha_\pm W_{aa} \;\rightarrow\; \beta_\pm = \frac{\alpha_\pm (E'_\pm - W_{aa})}{W_{ab}}$$

$$\rightarrow \beta_+^*\beta_- = \frac{\alpha_+^*\alpha_-}{W_{ab}^* W_{ab}} (E'_+ - W_{aa}^*)(E'_- - W_{aa}), \qquad W_{aa}^* = W_{aa}$$

því fæst

$$\langle\Phi_+^0|\Phi_-^0\rangle = \frac{\alpha_+^*\alpha_-}{|W_{ab}|^2}\left[|W_{ab}|^2 + (E'_+ - W_{aa})(E'_- - W_{aa})\right] \quad (**)$$

$$= \frac{\alpha_+^*\alpha_-}{|W_{ab}|^2}\left[E'_+E'_- - W_{aa}(E'_+ + E'_-) + |W_{ab}|^2 + W_{aa}^2\right]$$

en samkvæmt (6.27)

$$E'_+ + E'_- = \frac{W_{aa} + W_{bb}}{2} \cdot 2$$

og $$E'_+E'_- = \frac{1}{4}\left\{(W_{aa}+W_{bb})^2 - (W_{aa}-W_{bb})^2 - 4|W_{ab}|^2\right\}$$

$$\begin{aligned} \rightarrow \langle\Phi_+^0|\Phi_-^0\rangle = \frac{\alpha_+^*\alpha_-}{|W_{ab}|^2}\Big[&\tfrac{1}{4}(W_{aa}+W_{bb})^2 - \tfrac{1}{4}(W_{aa}-W_{bb})^2 - \cancel{|W_{ab}|^2} \\ &- W_{aa}^2 - W_{aa}W_{bb} + \cancel{|W_{ab}|^2} + W_{aa}^2 \Big] \end{aligned}$$

$$= \frac{\alpha_+^*\alpha_-}{|W_{ab}|^2}\left[\cancel{W_{aa}W_{bb}} - \cancel{W_{aa}^2} - \cancel{W_{aa}W_{bb}} + \cancel{W_{aa}^2}\right]$$

$$= 0$$

b) Sýna að $\langle\Phi_+^0|H'|\Phi_-^0\rangle = 0$

$$\langle\Phi_+^0|H'|\Phi_-^0\rangle = \left\{\alpha_+^*\langle\Phi_a^0| + \beta_+^*\langle\Phi_b^0|\right\} H' \left\{\alpha_-|\Phi_a^0\rangle + \beta_-|\Phi_b^0\rangle\right\}$$

$$\begin{aligned} &= \alpha_+^*\alpha_- \langle\Phi_a^0|H'|\Phi_a^0\rangle + \alpha_+^*\beta_- \langle\Phi_a^0|H'|\Phi_b^0\rangle \\ &\quad + \beta_+^*\alpha_- \langle\Phi_b^0|H'|\Phi_a^0\rangle + \beta_+^*\beta_- \langle\Phi_b^0|H'|\Phi_b^0\rangle \end{aligned}$$

$$= \alpha_+^*\alpha_- W_{aa} + \alpha_+^*\beta_- W_{ab} + \beta_+^*\alpha_- W_{ba} + \beta_+^*\beta_- W_{bb}$$

$$= \alpha_+^*\alpha_- \left[W_{aa} + (E'_- - W_{aa}) + \frac{(E'_+ - W_{aa})W_{ba}}{W_{ab}^*} + \frac{(E'_+ - W_{aa})}{W_{ab}^*}\frac{(E'_- - W_{aa})W_{bb}}{W_{ab}}\right.$$

$$= \alpha_+^*\alpha_-\left[W_{aa} + (E_-^1 - W_{aa}) + (E_+^1 - W_{aa}) + \frac{(E_+^1-W_{aa})(E_-^1-W_{aa})}{|W_{ab}|^2} W_{bb}\right]$$

frá (**) sést að $(E_+^1-W_{aa})(E_-^1-W_{aa}) = -|W_{ab}|^2$

$$\to \langle\psi_+^0|H'|\psi_-^0\rangle = \alpha_+^*\alpha_-\left[W_{aa} + (E_-^1-W_{aa}) + (E_+^1-W_{aa}) - W_{bb}\right]$$

$$= \alpha_+^*\alpha_-\left[E_-^1 + E_+^1 - W_{aa} - W_{bb}\right] = 0$$

samkvæmt (6.27)

c) Sýna að

$$\langle\psi_\pm^0|H'|\psi_\pm^0\rangle = E_\pm^1$$

$$\langle\psi_\pm^0|H'|\psi_\pm^0\rangle = \left\{\alpha_\pm^*\langle\psi_a^0| + \beta_\pm^*\langle\psi_b^0|\right\} H' \left\{\alpha_\pm|\psi_a^0\rangle + \beta_\pm|\psi_b^0\rangle\right\}$$

$$= |\alpha_\pm|^2 W_{aa} + \alpha_\pm^*\beta_\pm W_{ab} + \beta_\pm^*\alpha_\pm W_{ba} + |\beta_\pm|^2 W_{bb}$$

$$= |\alpha_\pm|^2\left\{W_{aa} + \frac{(E_\pm^1 - W_{aa})}{W_{ab}} W_{ab}\right\} + |\beta_\pm|^2\left\{W_{bb} + \frac{(E_\pm^1 - W_{bb})}{W_{ba}} W_{ba}\right\}$$

$$= |\alpha_\pm|^2\left\{E_\pm^1\right\} + |\beta_\pm|^2\left\{E_\pm^1\right\} = \underline{E_\pm^1}$$

$$= \left\{|\alpha_\pm|^2 + |\beta_\pm|^2\right\}E_\pm^1 = 1\cdot E_\pm^1$$

68 „Teningslagaður" óendanlegur brunnur er truflaður með

$$H' = a^3V_0\,\delta\!\left(x-\tfrac{a}{4}\right)\delta\!\left(y-\tfrac{a}{2}\right)\delta\!\left(z-\tfrac{3a}{4}\right)$$

finnum fyrsta stigs nálgun á orku grunnástandsins og lægsta örvaða ástandinu

$$E^0_{n_xn_yn_z} = E_1\cdot\left\{n_x^2+n_y^2+n_z^2\right\}, \quad E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

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

Grunnástandið er einfalt $|111\rangle = |g\rangle$

$$E^1_{111} = E^0_{111} + \langle g|V|g\rangle$$

$$\langle g|V|g\rangle = a^3\left(\frac{2}{a}\right)^3V_0\int_0^a dx\,dy\,dz\,\sin^2\left(\pi\frac{x}{a}\right)\sin^2\left(\pi\frac{y}{a}\right)\sin^2\left(\pi\frac{z}{a}\right)\cdot\delta\!\left(x-\tfrac{a}{4}\right)\delta\!\left(y-\tfrac{a}{2}\right)\delta\!\left(z-\tfrac{3a}{4}\right)$$

$$= 8V_0\sin^2\left(\frac{\pi}{4}\right)\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{3\pi}{4}\right)$$

$$= \frac{8V_0}{4} = 2V_0$$

fyrsta örvaða ástandið er 3-falt, hlutrúm spannað af $\{|112\rangle, |121\rangle, |211\rangle\}$ því þarf að reikna fylkja stökin fyrir öll þessi ástönd

köllum
$|112\rangle = |a\rangle$
$|121\rangle = |b\rangle$
$|211\rangle = |c\rangle$

byrjum á hornalínu

$$V_{aa} = \langle 112|V|112\rangle = a^3\left(\frac{2}{a}\right)^3 V_0 \int_0^a dxdydz\, \sin^2\left(\pi\frac{x}{a}\right)\sin^2\left(\pi\frac{y}{a}\right)\cdot$$

$$\sin^2\left(2\pi\frac{z}{a}\right)\delta\left(x-\frac{a}{4}\right)\delta\left(y-\frac{a}{2}\right)\delta\left(z-\frac{3a}{4}\right)$$

$$= 8V_0 \sin^2\left(\frac{\pi}{4}\right)\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{6\pi}{4}\right) = 8V_0\,\frac{1}{2} = 4V_0$$

$$V_{bb} = \langle 121|V|121\rangle = 8V_0 \sin^2\left(\frac{\pi}{4}\right)\sin^2(\pi)\sin^2\left(\frac{3\pi}{4}\right) = 0$$

$$V_{cc} = \langle 211|V|211\rangle = 8V_0 \sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{3\pi}{4}\right) = 8V_0\cdot\frac{1}{2} = 4V_0$$

Utan hornalínu

$$V_{ab} = \langle 112|V|121\rangle = 8V_0 \sin^2\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin(\pi)\sin\left(\frac{3\pi}{4}\right)\cdot\sin\left(\frac{6\pi}{4}\right) = 0$$

$$V_{ac} = \langle 112|V|211\rangle = 8V_0 \sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin^2\left(\frac{\pi}{2}\right)\sin\left(\frac{3\pi}{4}\right)\sin\left(\frac{6\pi}{4}\right) = 8V_0\cdot\left(-\frac{1}{2}\right) = -4V_0$$

$$V_{bc} = \langle 121|V|211\rangle = 8V_0 \sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin\left(\frac{\pi}{2}\right)\sin(\pi)\cdot\sin^2\left(\frac{3\pi}{4}\right) = 0$$

fylkjastökin eru raungild því þurfum við ekki að reikna fleiri

$$V = 4V_0 \begin{array}{c} \begin{matrix} a & b & c \end{matrix} \\ \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \end{array}$$

röð valin í fylki

Ein lína (~~eða~~ dálkur með 0) með 0 og hinar tvær eru háðar. Eru eins ef önnur er margfölduð með −1
→ aðeins eitt ástand hreyfist til í orku

Finnum eigingildi

þau eru

$8V_0$ einfalt

0 tvöfalt

$$\rightarrow E_e^0 = E_1\cdot 6 + \begin{cases} 8V_0 & \text{eitt} \\ 0 & \text{tvö} \end{cases}$$

og áður

$$E_g^0 = E_1\cdot 3 + 2V_0$$

Var hægt að sjá þetta fyrir?

$\delta(y-\frac{a}{2})$ → engin áhrif á lægstu örvun í y-átt

$\delta(x-\frac{a}{4})$ – – $\delta(z-\frac{3a}{4})$ → sama gildi en öfugt formerki fyrir lægstu örvun í x- og z-átt

→ aðeins eitt ástand hreyfist til í orku vegna truflanamættisins V

(6.17)

Fyrir leiðréttinguna vegna afstæðiskenningar höfum við

(7)

$$(*) \qquad E_r^1 = -\frac{(E_n^0)^2}{2mc^2}\left[\frac{4n}{l+\frac{1}{2}} - 3\right] \qquad E_n^0 = -\frac{R_y}{n^2}$$

fyrir spuna-brautar víxlverkun

$$(**) \qquad E_{so}^1 = \frac{(E_n^0)^2}{mc^2}\left\{\frac{n\left(j(j+1) - l(l+1) - \frac{3}{4}\right)}{l(l+\frac{1}{2})(l+1)}\right]$$

Sýnum að saman gefi þær

$$E_{fs}^1 = \frac{(E_n^0)^2}{mc^2}\left\{3 - \frac{4n}{j+\frac{1}{2}}\right]$$

Við höfum $j = l \pm \frac{1}{2}$ í vetnis atóminu, lokasvarið er í j, segjum því $l = j \pm \frac{1}{2}$

(8)

$l = j + \frac{1}{2}$

$$E_r^1 + E_{so}^1 = \frac{(E_n^0)^2}{mc^2}\left[-\frac{2n}{j+1} + \frac{3}{2} + \frac{n\left[j(j+1) - (j+\frac{1}{2})(j+\frac{3}{2}) - \frac{3}{4}\right]}{(j+\frac{1}{2})(j+1)(j+\frac{3}{2})}\right]$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{-\frac{2n}{j+1} + \frac{3}{2} - \frac{n(j+\frac{3}{2})}{(j+\frac{1}{2})(j+1)(j+\frac{3}{2})}\right]$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{-\frac{2n}{j+1} + \frac{3}{2} - \frac{n}{(j+\frac{1}{2})(j+1)}\right]$$

(9)

$$= \frac{(E_n^0)^2}{mc^2}\left\{\frac{3}{2} - \frac{2n(j+\frac{1}{2}) + n}{(j+1)(j+\frac{1}{2})}\right] = \frac{(E_n^0)^2}{2mc^2}\left\{3 - \frac{4n}{j+\frac{1}{2}}\right]$$

$l = j - \frac{1}{2}$

$$E_r^1 + E_{so}^1 = \frac{(E_n^0)^2}{mc^2}\left\{-\frac{2n}{j} + \frac{3}{2} + \frac{n\left[j(j+1) - (j-\frac{1}{2})(j+\frac{1}{2}) - \frac{3}{4}\right]}{(j-\frac{1}{2})j(j+\frac{1}{2})}\right]$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{\frac{3}{2} - \frac{2n}{j} + \frac{n\left[j^2 + j - j^2 + \frac{1}{4} - \frac{3}{4}\right]}{(j-\frac{1}{2})j(j+\frac{1}{2})}\right]$$

$$= \frac{(E_n^0)^2}{mc^2}\left[\frac{3}{2} - \frac{2n}{j} + \frac{n(j-\frac{1}{2})}{(j-\frac{1}{2})j(j+\frac{1}{2})}\right]$$

(10)

$$= \frac{(E_n^0)^2}{mc^2}\left[\frac{3}{2} - \frac{2n}{j} + \frac{n}{j(j+\frac{1}{2})}\right]$$

$$= \frac{(E_n^0)^2}{mc^2}\left[\frac{3}{2} + \frac{-2n(j+\frac{1}{2}) + n}{j(j+\frac{1}{2})}\right]$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{\frac{3}{2} - \frac{2n}{(j+\frac{1}{2})}\right]$$

$$= \frac{(E_n^0)^2}{2mc^2}\left\{3 - \frac{4n}{j+\frac{1}{2}}\right]$$

9.3 Tveggja stiga kerfi truflað með $H' = U\delta(t)$ (1)

Gerum ráð fyrir að $U_{aa} = U_{bb} = 0$, $U_{ab} = U_{ba}^* \equiv \alpha$

og ég bæti við $\alpha \in \mathbb{R}$

Gerum ráð fyrir að $\begin{pmatrix} C_a(-\infty) \\ C_b(-\infty) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ upphafsskilyrði

Finna á $C_a(t)$ og $C_b(t)$, kanna að $|C_a(t)|^2 + |C_b(t)|^2 = 1$

Í fyrirlestri skrifaði ég hreyfijöfnuna sem

$$\boxed{i\hbar\partial_t \begin{pmatrix} C_a \\ C_b \end{pmatrix} = \begin{pmatrix} H'_{aa} & H'_{ab}e^{-i\omega_0 t} \\ H'_{ba}e^{+i\omega_0 t} & H'_{bb} \end{pmatrix} \begin{pmatrix} C_a \\ C_b \end{pmatrix}}$$

(2)

eða $$i\hbar\partial_t \bar{C}(t) = H'(t)\bar{C}(t)$$

Með tímaheildun get ég komið upphafsskilyrðunum fyrir í jöfnunni sem breytist í heildisjöfnu

$$\boxed{\bar{C}(t) = \bar{C}(-\infty) + \frac{1}{i\hbar}\int_{-\infty}^{t} ds\, H'(s)\bar{C}(s)}$$

eða

$$\begin{pmatrix} C_a(t) \\ C_b(t) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{i\hbar}\int_{-\infty}^{t} ds \begin{pmatrix} 0 & \alpha\delta(s)e^{-i\omega_0 s} \\ \alpha\delta(s)e^{+i\omega_0 s} & 0 \end{pmatrix} \begin{pmatrix} C_a(s) \\ C_b(s) \end{pmatrix}$$

δ-fallið verður alltaf til vandræða, hvort sem við leysum heildis eða afleiðujöfnuna. Því notum við markgildi fyrir það

(3)

$$\delta_\epsilon(t) = \begin{cases} \frac{1}{2\epsilon} & \text{fyrir } -\epsilon < t < \epsilon \\ 0 & \text{annars} \end{cases}$$

Gott er að sannreyna að þessi stikun leiðir til $\delta(t)$ þ.e. $\epsilon \to 0$ fyrir $\int dx\, f(x)\delta_\epsilon(x)$

Lesum aðeins úr heildisjöfnunni

$$\begin{pmatrix} C_a(t) \\ C_b(t) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{fyrir } t < -\epsilon \qquad \{\text{eða uppað } t = 0\}$$

á bilinu $-\epsilon < t < \epsilon$ verður snögg breyting

og eftir $t > \epsilon$ eru $\begin{pmatrix} C_a(t) \\ C_b(t) \end{pmatrix}$ ekki háðir t lengur

{δ_ϵ-fallið klippir á efri mörk heildisins við $t = \epsilon$}

(4)

Við þurfum því að leysa

$$\begin{pmatrix} C_a(\epsilon) \\ C_b(\epsilon) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{\alpha}{2\epsilon i\hbar}\int_{-\epsilon}^{+\epsilon} ds \begin{pmatrix} 0 & e^{-i\omega_0 s} \\ e^{+i\omega_0 s} & 0 \end{pmatrix} \begin{pmatrix} C_a(s) \\ C_b(s) \end{pmatrix}$$

Þetta eru tvær tengdar heildisjöfnur. Ef ég reyni að leysa þær þ.a. ég nálga

$$\int_{-\epsilon}^{\epsilon} ds\, f(s)C(s) \simeq \frac{1}{2}\{f(\epsilon)C(\epsilon) + f(-\epsilon)C(-\epsilon)\}2\epsilon$$

þá fæst lausn fyrir $\begin{pmatrix} C_a \\ C_b \end{pmatrix}$ sem er aðeins lægsta nálgun í α. Ég reyndi það til gamans og sá að $|C_a|^2 + |C_b|^2 = 1$, en við verðum að gera betur hér. Uppbygging heildisjöfnunnar segir okkur að $\begin{pmatrix} C_a \\ C_b \end{pmatrix}$ er fall af α.

Notum ítrun og vonumst til þess að við bennum keunsl á raðirnar sem fást. (5)

Lægsta nálgun
$$\begin{pmatrix} C_a(\epsilon) \\ C_b(\epsilon) \end{pmatrix}^{(0)} \simeq \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \bar{C}^{0}(\epsilon)$$

Setjum $\bar{C}^{(0)}(\epsilon)$ inn í stað $\bar{C}(s)$ í heildinu og fáum
$$\begin{pmatrix} C_a(\epsilon) \\ C_b(\epsilon) \end{pmatrix}^{(1)} \simeq \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{i\alpha}{\epsilon\hbar\omega_0} \begin{pmatrix} 0 \\ \sin(\omega_0\epsilon) \end{pmatrix}$$

notum í stað $\bar{C}(s)$ í heildinu til að fá
$$\begin{pmatrix} C_a(\epsilon) \\ C_b(\epsilon) \end{pmatrix}^{(2)} \simeq \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{i\alpha}{\epsilon\hbar\omega_0} \begin{pmatrix} 0 \\ \sin(\omega_0\epsilon) \end{pmatrix} + \frac{1}{4}\left(\frac{\alpha}{\epsilon\hbar\omega_0}\right)^2 \begin{pmatrix} \sin(2\omega_0\epsilon) \\ 0 \end{pmatrix}$$

tökum markgildið $\epsilon \to 0$ og notum (6)

Hamiltoni er einfalt að finna með maxima

$$\lim_{\epsilon\omega_0 \to 0} \frac{\sin(\omega_0\epsilon)}{\omega_0\epsilon} = 1$$

$$\begin{pmatrix} C_a(0) \\ C_b(0) \end{pmatrix} \simeq \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{\alpha}{\hbar}\begin{pmatrix} 0 \\ -i \end{pmatrix} + \left(\frac{\alpha}{\hbar}\right)^2 \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} + \cdots\cdots$$

$$= \begin{pmatrix} \cos\left(\frac{\alpha}{\hbar}\right) \\ -i\sin\left(\frac{\alpha}{\hbar}\right) \end{pmatrix}$$

Uppbygging jöfnunnar leiðir til tveggja raða, önnur í jöfnum veldum og hin í odda veldum af $\left(\frac{\alpha}{\hbar}\right)$.

Augljóst er að $|C_a(0)|^2 + (C_b(0))^2 = 1$

Upphaflega var kerfið í ástandi $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ líkindi þess að finna það í $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ eru

$$\boxed{|C_b|^2 = \sin^2\left(\frac{\alpha}{\hbar}\right)}$$

fyrir $t > 0$

Þetta er nákvæm lausn án truflanareiknings
Sveiflur með sterk púls!