(1)

Eind er lýst með bylgjufallinu

$$\psi(x) = A x^2 \exp\left(-\left(\frac{x}{a}\right)^2\right)$$

(1) Finna A

$$\int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = |A|^2 \int_{-\infty}^{\infty} dx\, x^4 \exp\left\{-2\left(\frac{x}{a}\right)^2\right\}$$

$$= |A|^2 a^5 \int_{-\infty}^{\infty} \frac{dx}{a} \left(\frac{x}{a}\right)^4 \exp\left\{-2\left(\frac{x}{a}\right)^2\right\} = |A|^2 a^5 \int_{-\infty}^{\infty} du\, u^4 e^{-2u^2}$$

$$= |A|^2 a^5 \frac{3\sqrt{\pi}}{2^{9/2}} = 1 \quad \to \quad A = \frac{2^{9/4}}{\sqrt{3\sqrt{\pi}\, a^5}}$$ er lausn

(2)

(2) Reikna $\langle x\rangle$ og $\langle x^2\rangle$

$$\langle x\rangle = \int_{-\infty}^{\infty} dx\, x\, |\psi(x)|^2 = A^2 \int_{-\infty}^{\infty} dx\, x^5 \exp\left(-2\left(\frac{x}{a}\right)^2\right) = 0$$

því fallið undir heildinu er oddstætt.

$$\langle x^2\rangle = A^2 \int_{-\infty}^{\infty} dx\, x^6 \exp\left\{-2\left(\frac{x}{a}\right)^2\right\} = A^2 a^7 \int_{-\infty}^{\infty} du\, u^6 e^{-2u^2}$$

$$= A^2 a^7 \frac{15\sqrt{\pi}}{2^{13/2}} = \frac{2^{9/2} a^7}{3\sqrt{\pi}\, a^5} \frac{15\sqrt{\pi}}{2^{13/2}} = \frac{5}{4} a^2$$

(3)

(3) Reikna $\langle p\rangle$ og $\langle p^2\rangle$

$$p\psi(x) = -i\hbar \partial_x \psi(x) = -i\hbar A\, \partial_x \left\{x^2 \exp\left(-\left(\frac{x}{a}\right)^2\right)\right\}$$

$$= -i\hbar A \left\{-\frac{2}{a^2}\left(x^3 - a^2 x\right) e^{-\left(\frac{x}{a}\right)^2}\right\}$$

$$p^2\psi(x) = -\hbar^2 \partial_x^2 \psi(x) = -\hbar^2 A \partial_x^2 \left\{x^2 e^{-\left(\frac{x}{a}\right)^2}\right\}$$

$$= -\hbar^2 A \left\{\frac{2}{a^4}\left(2x^4 - 5a^2x^2 + a^4\right) e^{-\left(\frac{x}{a}\right)^2}\right\}$$

$$\langle p\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x) p\, \psi(x) = +i\hbar |A|^2 \frac{2}{a^2} \int_{-\infty}^{\infty} dx \left\{x^5 - a^2 x^3\right\} e^{-2\left(\frac{x}{a}\right)^2} = 0$$

fallið er oddstætt á $(-\infty, \infty)$

(4)

$$\langle p^2\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x) p^2 \psi(x)$$

$$= -\hbar^2 |A|^2 \frac{2}{a^4} \int_{-\infty}^{\infty} dx \left\{2x^6 - 5a^2x^4 + a^4x^2\right\} e^{-2\left(\frac{x}{a}\right)^2}$$

$$= -\hbar^2 |A|^2 2a^3 \int_{-\infty}^{\infty} d\left(\frac{x}{a}\right) \left\{2\left(\frac{x}{a}\right)^6 - 5\left(\frac{x}{a}\right)^4 + \left(\frac{x}{a}\right)^2\right\} e^{-2\left(\frac{x}{a}\right)^2}$$

$$= -\hbar^2 |A|^2 2a^3 \int_{-\infty}^{\infty} du \left\{2u^6 - 5u^4 + u^2\right\} e^{-2u^2}$$

$$= -\hbar^2 |A|^2 2a^3 \left\{-\frac{7\sqrt{\pi}}{2^{11/2}}\right\} = +\hbar^2 2a^3 \left\{\frac{2^{9/2}}{3\sqrt{\pi}\, a^5}\right\}\left\{\frac{7\sqrt{\pi}}{2^{11/2}}\right\}$$

(1) Eind í brunni með lengd a í ástandi lýst með

$$\Psi(x,0) = A\{\psi_3(x) - i\psi_5(x)\}$$

(1) Finnið A. $\psi_n(x)$ eru stöðluð og hornrétt (raungild)

$$1 = |A|^2\int_0^a dx\,\{\psi_3(x) - i\psi_5(x)\}^*\{\psi_3(x) - i\psi_5(x)\}$$

$$= |A|^2\int_0^a dx\,\{\psi_3(x) + i\psi_5(x)\}\{\psi_3(x) - i\psi_5(x)\}$$

$$= |A|^2\int_0^a dx\,\{\underbrace{|\psi_3(x)|^2 + |\psi_5(x)|^2}_{\text{eru stöðluð}}\underbrace{- i\psi_3(x)\psi_5(x) + i\psi_5(x)\psi_3(x)}_{\text{eru hornrétt}}\} = 2|A|^2$$

$\rightarrow |A|^2 = \frac{1}{2}$ og við veljum $A = \frac{1}{\sqrt{2}}$

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left[\psi_3(x)e^{-i\omega_3 t} - i\psi_5(x)e^{-i\omega_5 t}\right]$$

þ.s. $\omega_n = \frac{E_n}{\hbar} = \frac{E_1}{\hbar}n^2 = \omega_1 n^2$

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

(2) Finna $\langle x\rangle$

$$\langle x\rangle = \int_0^a dx\,\Psi^*(x,t)\,x\,\Psi(x,t)$$

$$= \frac{1}{2}\int_0^a dx\left[\psi_3(x)e^{i\omega_3 t} + i\psi_5(x)e^{i\omega_5 t}\right] x \left[\psi_3(x)e^{-i\omega_3 t} - i\psi_5(x)e^{-i\omega_5 t}\right]$$

$$= \frac{1}{2}\int_0^a dx\left\{|\psi_3(x)|^2 x + |\psi_5(x)|^2 x + ix\psi_5(x)\psi_3(x)\left[e^{i(\omega_5-\omega_3)t} - e^{-i(\omega_5-\omega_3)t}\right]\right\}$$

$$= \frac{a}{2} + \Delta(t)$$

$$\Delta(t) = -\int_0^a dx\,\underbrace{\left[x\psi_5(x)\psi_3(x)\right]}_{\text{(tvískauts fylgjastak)}}\underbrace{\sin((\omega_5-\omega_3)t)}_{\text{óháð } x} = 0$$

$\langle x\rangle = \frac{a}{2}$ ekki háð tíma

(3)
$$|\Psi(x,t)|^2 = \frac{1}{2}\left\{|\psi_3(x)|^2 + |\psi_5(x)|^2 - 2\psi_5(x)\psi_3(x)\sin[(\omega_5-\omega_3)t]\right\}$$

$$= \frac{1}{2}\left\{|\psi_3^2(x)| + |\psi_5(x)|^2 - 2\psi_5(x)\psi_3(x)\sin[16\omega_1 t]\right\}$$

$$\langle p^2\rangle = \frac{\hbar^2}{a^2}\cdot\frac{7}{3}$$

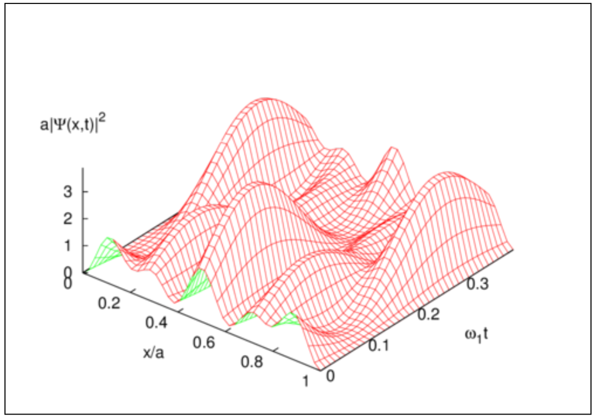
(4) Reiknum Δx og Δp

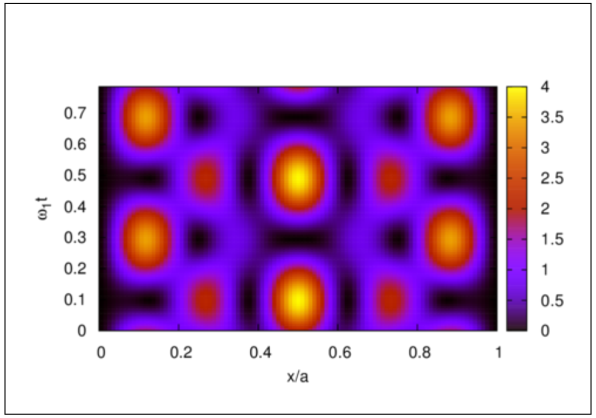
$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\langle x^2\rangle} = \sqrt{\frac{5}{4}}\,a$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\langle p^2\rangle} = \frac{\hbar}{a}\sqrt{\frac{7}{3}}$$

(5)
$$\Delta x\cdot\Delta p = \hbar\sqrt{\frac{5\cdot 7}{4\cdot 3}} = \hbar\sqrt{\frac{35}{12}} \sim \hbar\cdot 1{,}708 \gg \frac{\hbar}{2}$$

Þannig að óvissulögmálið er uppfyllt fyrir þetta ástand! →





(4)

(4) Ef orka $\Psi(x,t)$ er mæld?

$\Psi(x,t)$ er ekki eiginástand H, en það er sett saman úr tveimur eigin ástöndum með sama vogi

því fæst E_3 með líkum $\frac{1}{2}$

og E_5 —||—

Eftir mælingu er eindin annaðhvort í ástandi 3 eða 5

(5)

$$\langle H \rangle = \int_0^a dx\, \Psi^*(x,t)\, H\, \Psi(x,t)$$

$$= \frac{1}{2}\int_0^a dx \left[\psi_3(x) e^{i\omega_3 t} + i\psi_5(x) e^{i\omega_5 t}\right]\left\{E_3 \psi_3(x) e^{-i\omega_3 t} - i E_5 \psi_5(x) e^{-i\omega_5 t}\right\}$$

(5)

$$= \frac{1}{2}\int_0^a dx \left\{E_3 |\psi_3(x)|^2 + E_5 |\psi_5(x)|^2\right\} = \frac{E_3 + E_5}{2}$$

eins og við mátti búast af líkunum á undan.

② Eind í óendanlegum brunni lýst með

$$\Psi(x) = A\cdot x\cdot(a-x)\cdot\left(x-\frac{a}{2}\right)$$

① Normun

$$1 = \int_0^a dx\; |A|^2\, x^2(a-x)^2\cdot\left(x-\frac{a}{2}\right)^2 = |A|^2\cdot\frac{a^7}{840}$$

Veljum því $A = \sqrt{\frac{840}{a^7}}$

Hér er ágætt að athuga hvernig bylgjufallið hefur þá rétta vídd

② Hvað gefur orkumæling?

Hvernig er hægt að liða Ψ í grunnföllum (eiginföllum) Hamiltonvirkjans, orkuvirkjans?

$$\Psi(x) = \sum_{n=1}^{\infty} C_n \phi_n(x)$$

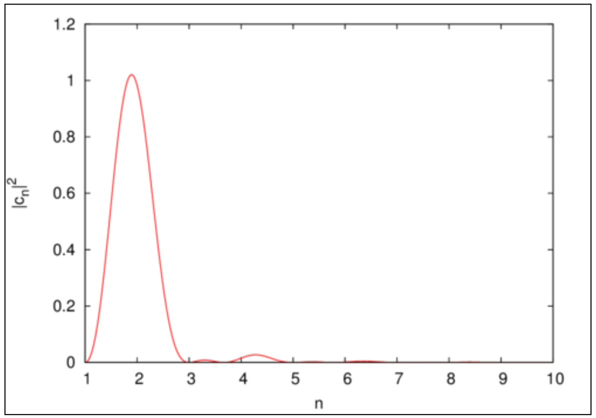
$$C_n = \int_0^a dx\; f(x)\,\phi_n^*(x) = \sqrt{\frac{1680}{a^8}}\int_0^a dx\; x(a-x)\left(x-\frac{a}{2}\right)\sin\left(n\pi\frac{x}{a}\right)$$

$$= \sqrt{1680}\int_0^1 du\; u\cdot(1-u)\cdot\left(u-\frac{1}{2}\right)\cdot\sin(n\pi u)$$

$$= \sqrt{1680}\left\{-\frac{(n^2\pi^2-12)\sin(\pi n)+6\pi n\cos(\pi n)}{2\pi^4 n^4} - \frac{3}{n^3\pi^3}\right\}$$

Mæling gefur $E_n = E_1\cdot n^2$ með líkum $|C_n|^2$

$C_1 = 0$, sjá mynd



③ Væntigildi H

$$\langle H\rangle = \int_0^a dx\; \Psi^*(x)\, H\, \Psi(x) = \sum_{n=1}^{\infty} |C_n|^2 E_n$$

$$= E_1\sum_{n=1}^{\infty} |C_n|^2 n^2 = E_1\, 1680 \sum_{n=1}^{\infty}\left\{\frac{3[(-1)^n+1]}{\pi^3 n^3}\right\}^2 n^2$$

$$= E_1\; 1680\cdot\frac{9}{\pi^6}\sum_{n=1}^{\infty}\left\{\frac{(-1)^n+1}{n^3}\right\}^2 n^2 \approx E_1\cdot 4+\delta$$

$$\approx E_2+\delta$$

(1)

① Væntigildi p^4 og x^4 fyrir n-ástand H.O.

Byrjum á p^4

$$a_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left\{\mp ip + mx\right\}$$

$$\to \quad a_+ - a_- = \frac{1}{\sqrt{2\hbar m\omega}}\left\{-ip - ip\right\} = -\sqrt{\frac{2}{\hbar m\omega}}\, ip$$

$$= -\frac{ip}{\hbar}\sqrt{\frac{2\hbar}{m\omega}} = -\frac{i}{\hbar}\sqrt{2}\, a\, p$$

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

$$\to \quad p = \frac{i\hbar}{a}\frac{1}{\sqrt{2}}(a_+ - a_-)$$

(2)

$$p^4 = \frac{\hbar^4}{a^4}\frac{1}{4}(a_+ - a_-)^4$$

$$\langle p^4\rangle = \int dx\, \psi_n^*(x)\, p^4\, \psi_n(x)$$

Munum að ψ_n mynda hornréttan grunn

$$\to \quad \int dx\, \psi_n^*(x)\psi_m(x) = \delta_{n,m}$$

Einu liðirnir sem ekki hverfa í $\langle p^4\rangle$ eru liðir með jafnan fjölda hækkunar og lækkunarvirkja

$$\langle p^4\rangle = \frac{\hbar^4}{a^4 4}\int dx\, \psi^*(x)\{a_+a_+a_-a_- + a_-a_-a_+a_+ + a_+a_-a_+a_- + a_-a_+a_-a_- + a_+a_-a_-a_+ + a_-a_+a_+a_-\}\psi_n(x)$$

(3)

notum $a_-\psi_n = \sqrt{n}\,\psi_{n-1}$ og $a_+\psi_n = \sqrt{n+1}\,\psi_{n+1}$

$$\langle p^4\rangle = \frac{\hbar^4}{4a^4}\int dx\, \psi_n^*(x)\{n(n-1) + (n+1)(n+2) + n^2 + (n+1)^2 + n(n+1) + (n+1)n\}\psi_n(x)$$

$$= \frac{\hbar^4}{4a^4}\left\{6n^2 + 6n + 3\right\} = \frac{\hbar^4}{a^4}\left\{\frac{3}{2}n^2 + \frac{3}{2}n + \frac{3}{4}\right\}$$

Gætum notað sömu aðferð fyrir x^4, en ég reyni aðra aðferð

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

(4)

Vitum

$$\left.\begin{aligned} H_0 &= 1 \\ H_1 &= 2x \\ H_2 &= 4x^2 - 2 \\ H_3 &= 8x^3 - 12x \\ H_4 &= 16x^4 - 48x^2 + 12 \end{aligned}\right\} \to \quad x^4 = \left\{\frac{1}{16}H_4(x) + \frac{3}{4}H_2(x) + \frac{3}{4}H_0(x)\right\}$$

því er

$$\langle x^4\rangle = \int_{-\infty}^{\infty} dx\, \psi_n^*(x)\, x^4\, \psi_n(x)$$

$$= \frac{a^4}{2^n n!\sqrt{\pi}}\int_{-\infty}^{\infty} du\, H_n(u)H_n(u)e^{-u^2}\left\{\frac{1}{16}H_4(u) + \frac{3}{4}H_2(u) + \frac{3}{4}H_0(u)\right\}$$

⑤

Notum GR- 7.375.2

$$\int_{-\infty}^{\infty} e^{-x^2} H_k(x) H_m(x) H_n(x) dx = \frac{2^{\frac{m+n+k}{2}} \sqrt{\pi}\, k!\, m!\, n!}{(s-k)!\,(s-m)!\,(s-n)!}$$

$2s = m+n+k$ (k+m+n er jöfn tala)

$m=n$, k er 0, 2, 4 hjá okkur

$$\langle x^4 \rangle = \frac{a^4}{2^n n! \sqrt{\pi}} \frac{2^n \sqrt{\pi}\, n!\, n!}{1} \left\{ \frac{2^2 \cdot 4!}{16 \cdot (n-2)!\,(2)!\,(2)!} + \frac{2 \cdot 2! \cdot 3}{4 \cdot (n-1)!\,(1)!\,(1)!} + \frac{3}{4\,(n)!\,0!\,0!} \right\}$$

⑥

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

$$= a^4 \left\{ \frac{3}{2} n^2 + \frac{3}{2} n + \frac{3}{4} \right\}$$

svipað $\langle p^4 \rangle$? . . . . . .

② $[A,B] = AB - BA$

því er líka $[A,B] = -[B,A]$

$[A,BC] = ABC - BCA$

$$\left.\begin{aligned} B[A,C] &= BAC - BCA \\ [A,B]C &= ABC - BAC \end{aligned}\right\} \rightarrow \begin{aligned} &B[A,C] + [A,B]C \\ &= [A,BC] \end{aligned}$$

⑦

② frh

$[x,H]$, $H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

$$\rightarrow [x,H] = \frac{1}{2m}[x,p^2] \qquad \{\text{því } [x,x]=0\}$$

$$= \frac{1}{2m}\left\{p[x,p] + [x,p]p\right\} = \frac{i\hbar \cdot 2p}{2m}$$

$$= \frac{i\hbar p}{m} \qquad ([x,p] = i\hbar)$$

$$[p,H] = \frac{1}{2} m\omega^2 [p,x^2] = \frac{1}{2} m\omega^2 \left\{x[p,x] + [p,x]x\right\}$$

$$= \frac{1}{2} m\omega^2 \left\{-x \cdot 2i\hbar\right\} = -m\omega^2 i\hbar x$$

⑧

③

$$[a_-,H] = [a_-, \hbar\omega(a_+a_- + \tfrac{1}{2})] = \hbar\omega [a_-, a_+a_-]$$

$$= \hbar\omega \left\{ a_+[a_-,a_-] + [a_-,a_+]a_- \right\}$$

$$= \hbar\omega [a_-,a_+]a_- = \hbar\omega a_-$$

$$[a_+,H] = \hbar\omega [a_+, a_+a_-]$$

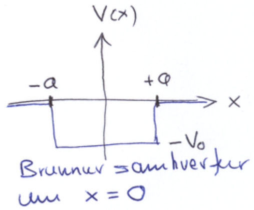
$$= \hbar\omega\, a_+ [a_+,a_-] = -\hbar\omega a_+$$

(1)

Skoða oddstæða lausn í endanlega brunninum.
Finna óbeinu jöfnuna fyrir orku ástandsins.

Grunnástandið er jafnstætt, það er fundið í bók, jafna (2.151)

$$\psi(x) = \begin{cases} F e^{-\kappa x} & x > a \\ D\cos(lx) & 0 < x < a \\ \psi(-x) & x < 0 \end{cases}$$



óbeina jafnan vegna samfellu ψ og ψ' verða þá (2.154)

$$\kappa = l\tan(la)$$

$$l = \frac{\sqrt{2m(E+V_0)}}{\hbar}, \quad \kappa = \frac{\sqrt{-2mE}}{\hbar}$$ ← því hér er leitað af bundnum ástöndum

(2)

Fyrir oddstæðu lausnina gerum við það fyrir

$$\psi(x) = \begin{cases} F e^{-\kappa x} & x > a \\ D\sin(lx) & 0 < x < a \\ -\psi(-x) & \end{cases}$$ ← til þess að lýsa andsamhverfunni

$\psi(x)$ er samfellt í $x = a$

$$\rightarrow F e^{-\kappa a} = D\sin(la)$$

$\psi'(x)$ er samfellt í $x = a$

$$\rightarrow -F\kappa e^{-\kappa a} = Dl\cos(la)$$

$$\rightarrow -\kappa = l\frac{\cos(la)}{\sin(la)} = l\cot(la)$$

(Við höfum skilgreint ψ þ.a. þá verður samfeldnin sjálfkrafa uppfyllt í $x=-a$)

(3)

eða $-\kappa a = la\cot(la)$ t.a. gefa jöfnuna víddarlausa

Í bók er notuð táknunin $z = la$ og $z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$

$$\rightarrow \kappa^2 a^2 = -\frac{2mE}{\hbar^2}a^2 = -l^2a^2 + z_0^2 = -z^2 + z_0^2$$

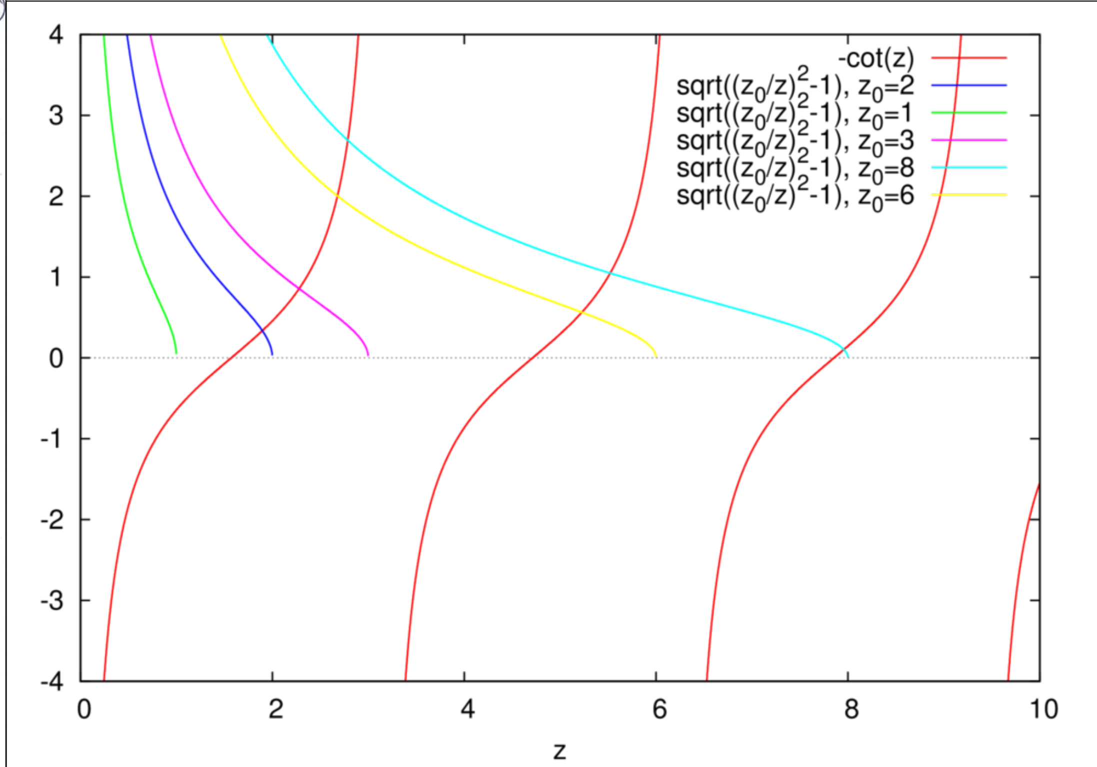
eða $\kappa^2 a^2 = z_0^2 - z^2$

og því verður óbeina jafnan

$$\sqrt{z_0^2 - z^2} = -z\cot(z)$$

eða

$$-\cot(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$



(5)

Markgildi

Víður + djúpur

$z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$ verður stór tala

Graf sýnir að núllstöður færast að $\pi, 2\pi, 3\pi \ldots$

$z_n \approx (n\pi)^2$ eða $(la)_n^2 = \frac{2m(E_n+V_0)a^2}{\hbar^2} \approx (n\pi)^2$

$$\rightarrow E_n + V_0 = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = \frac{\hbar^2 (n \cdot 2)^2 \pi^2}{2m(2a)^2}$$

sem er orkan í óendanlegum brunni

Hér þarf að fara varlega með „n", ef miðað er við 2a fæst einmitt önnur hver lausn fyrir óendanlega brunninn með lengd 2a

(6)

Grunnur þröngur brunnur

$z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$ er lítil tala

Grafið sýnir að engin lausn fæst fyrir $z_0 < \frac{\pi}{2}$ þá er engin bundin oddstöðu lausn til

$z_0 < \frac{\pi}{2}$ jafngildir

$$\frac{a}{\hbar}\sqrt{2mV_0} < \frac{\pi}{2} \rightarrow \frac{a^2}{\hbar^2}2mV_0 < \frac{\pi^2}{4}$$

$$\rightarrow V_0 < \frac{\pi^2\hbar^2}{8ma^2}$$

(7)

lausn fyrir $z_0 = 2$

það er lausn á

$$\sqrt{\left(\frac{4}{z}\right)^2 - 1} + \cot(z) = 0$$

fyrir lægsta oddstöðu fallið.

Grafið á blaðsíðu 4 gefur til kynna að lausnin sé á bilinu $1{,}5 < z < 2$

Maxima gefur $z_{rót} = 1.8955$

$$(z_{rót})^2 = (la)^2 = \frac{2m(E+V_0)a^2}{\hbar^2}$$

$$\rightarrow (E+V_0) = \frac{\hbar^2 (z_{rót})^2}{2ma^2} = \frac{\hbar^2 4 (z_{rót})^2}{2m(2a)^2}$$

(8)

$$(E+V_0) = E_1 \cdot \frac{4}{\pi^2}(z_{rót})^2, \quad E_1 = \frac{\hbar^2\pi^2}{2m(2a)^2}$$

Eins fæst frá $z_0 = 2 = \frac{a}{\hbar}\sqrt{2mV_0}$

að $V_0 = \frac{\hbar^2 4}{2ma^2} = \frac{\hbar^2 16}{2m(2a)^2} = E_1 \cdot \frac{16}{\pi^2}$

$$\rightarrow E = E_1\left\{\frac{4}{\pi^2}(z_{rót})^2 - \frac{16}{\pi^2}\right\}$$

$$= \frac{E_1 4}{\pi^2}\left\{(z_{rót})^2 - 4\right\} =$$

$$= -\frac{E_1 4}{\pi^2} \cdot 0{,}407 \approx -0{,}165 \cdot E_1$$

2.30 (9)

Stoða ψ í jöfnu (2.151) og ákvarða D og F

$$\psi(x) = \begin{cases} Fe^{-Kx} & x > a \\ D\cos(lx) & 0 < x < a \\ \psi(-x) & x < 0 \end{cases}$$

Lausnin er jafnstæð

$$\rightarrow 1 = 2\int_0^\infty dx\, |\psi(x)|^2$$

$$= 2\left\{ \int_0^a dx\, |\psi(x)|^2 + \int_a^\infty dx\, |\psi(x)|^2 \right\}$$

(10)

$$= 2\left\{ |D|^2 \int_0^a dx\, \cos^2(lx) + |F|^2 \int_a^\infty dx\, e^{-2Kx} \right\}$$

$$= 2\left\{ |D|^2 \left[\frac{\sin(2al) + 2al}{4l} \right] + |F|^2 \frac{e^{-2Ka}}{2K} \right\}$$

F og D eru tengd vegna samfellu ψ

$$\psi(a^+) = \psi(a^-) \rightarrow Fe^{-Ka} = D\cos(la)$$

$$\rightarrow F = De^{Ka}\cos(la)$$

því er stöðlunin

$$1 = 2|D|^2 \left\{ \frac{\sin(2al) + 2al}{4l} + \frac{\cos^2(la)}{2K} \right\}$$

(11)

K og l þarf líka að tengja saman

$$(2.154) \rightarrow K = l\tan(la)$$

$$\rightarrow 1 = 2|D|^2 \left\{ \frac{a}{2} + \frac{\sin(2al)}{4l} + \frac{\cos^2(la)}{2l\tan(la)} \right\}$$

$$= 2|D|^2 \left\{ \frac{a}{2} + \frac{\sin(la)\cos(la)}{2l} + \frac{\cos^3(la)}{2l\sin(la)} \right\}$$

$$= |D|^2 \left\{ a + \frac{\sin(la)\cos(la)}{l} + \frac{\cos^3(la)}{l \cdot \sin(la)} \right\}$$

$$= |D|^2 \left\{ a + \frac{\cos(la)}{l\sin(la)} \left[\sin^2(la) + \cos^2(la) \right] \right\}$$

(12)

$$1 = |D|^2 \left\{ a + \frac{\cos(la)}{l\sin(la)} \right\} = |D|^2 \left\{ a + \frac{1}{l\tan(la)} \right\}$$

$$= |D|^2 \left\{ a + \frac{1}{K} \right\} \rightarrow D = \frac{1}{\sqrt{a + \frac{1}{K}}}$$

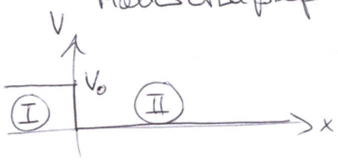
er lausn

og áður fékkst $F = De^{Ka}\cos(la)$

$$\rightarrow F = \frac{e^{Ka}\cos(la)}{\sqrt{a + \frac{1}{K}}}$$

er lausn fyrir F

① Mættisalturþrep



I

$$\left\{-\frac{\hbar^2}{2m}\partial_x^2 + V_0\right\}\psi = E\psi$$

lausn $\psi(x) = e^{ikx} + Be^{-ikx}$

og því

$$\frac{\hbar^2 k^2}{2m} + V_0 = E$$

$$k^2 = \frac{2m}{\hbar^2}(E-V_0)$$ jákvæð tala $E > V_0$

$\to k \in \mathbb{R}$ og lausn

$$\psi(x) = e^{ikx} + Be^{-ikx}, \quad k = \sqrt{\frac{2m}{\hbar^2}(E-V_0)}$$

II

$$-\frac{\hbar^2}{2m}\partial_x^2\psi = E\psi$$

Lausn $\psi(x) = Ce^{iqx}$ bara bylgja til hægri

með $\frac{\hbar^2 q^2}{2m} = E > 0 \to q = \sqrt{\frac{2mE}{\hbar^2}}$

Lausn samfeld í $x=0$

$$\psi^{I}(0) = \psi^{II}(0)$$

$$1 + B = C \quad (1)$$

②

Afleiða samfeld

$$ik - ikB = iqC$$

$$\to k(1-B) = qC \quad (2)$$

umritum

$$B - C = -1$$

$$kB + qC = k$$

$$\begin{pmatrix} 1 & -1 \\ k & q \end{pmatrix}\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} -1 \\ k \end{pmatrix}$$

Með lausn

$$B = -\frac{q-k}{q+k}$$

$$C = \frac{2k}{q+k}$$

Athugum líkinda straumþéttleika

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

$$= \frac{i\hbar}{2m}|A|^2\{-ik-ik\} = \frac{\hbar k}{m}|A|^2$$

ef bylgjufallið væri

$$\Psi_k(x,t) = A\exp\{i(kx - \omega_k t)\}$$

③

líkindastraumur innbylgju er þá

$$J_{inn} = \frac{\hbar k}{m}$$

líkindastraumur endurkasts

$$J_R = -\frac{\hbar k}{m}|B|^2$$

og frambylgju

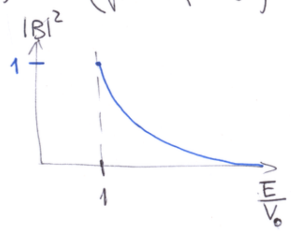
$$J_T = \frac{\hbar q}{m}|C|^2$$

a) líkindi endurkasts eru

$$\left|\frac{J_R}{J_{inn}}\right|^2 = |B|^2 = R$$

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

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

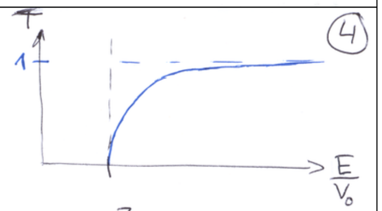


b) líkindi framförslu eru

$$\left|\frac{J_T}{J_{inn}}\right| = \frac{q}{k}|C|^2 = \frac{4qk}{(q+k)^2} = T$$

④

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



c)

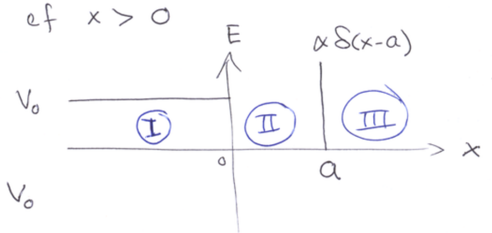
$$R + T = \frac{(q-k)^2}{(q+k)^2} + \frac{4qk}{(q+k)^2} = \frac{(q+k)^2}{(q+k)^2} = 1$$

þannig að inn streyma jafnmikið og út

(1)

① Mætti

$$V(x) = \begin{cases} V_0 & \text{ef } x < 0 \\ \alpha\delta(x-a) & \text{ef } x > 0 \end{cases} \qquad V_0 > 0,\ a > 0$$



Gerum ráð fyrir að $\alpha > 0$

leitum dreifilausna með $E > V_0$

Eind kemur inn frá vinstri

I

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

$$k^2 = \frac{2m}{\hbar^2}(E - V_0)$$

III

$$\psi_{III}(x) = Fe^{iqx}$$

$$q^2 = \frac{2m}{\hbar^2}E$$

Á þessu svæði getur engin bylgja komið frá hægri

II

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

$$q^2 = \frac{2m}{\hbar^2}E$$

(2)

Lausn er samfeld í $x = 0$

$$\psi_I(0) = \psi_{II}(0)$$

$$\rightarrow \quad 1 + B = C + D$$

Lausn er samfeld í $x = a$

$$\psi_{II}(a) = \psi_{III}(a)$$

$$Ce^{iqa} + De^{-iqa} = Fe^{iqa}$$

Afleiða lausnar er samfeld í $x=0$

$$\psi_I'(0) = \psi_{II}'(0)$$

$$ik - ikB = iqC - iqD$$

Afleiða lausnar er ósamfeld í $x = a$

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

eða

$$iqFe^{iqa} - \{iqCe^{iqa} - iqDe^{-iqa}\} = \frac{2m\alpha}{\hbar^2}Fe^{iqa}$$

(3)

Söfnum saman jöfnum

$$B - C - D = -1$$

$$-ikB - iqC + iqD = -ik$$

$$C + e^{-2iqa}D - F = 0$$

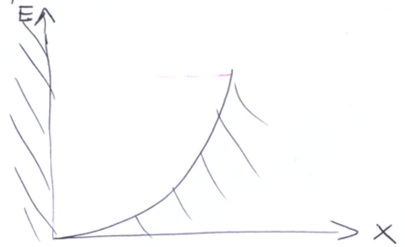
$$-iqC + iqe^{-2iqa}D + \left\{iq - \frac{2m\alpha}{\hbar^2}\right\}F = 0$$

eða

$$\begin{pmatrix} 1 & -1 & -1 & 0 \\ -ik & -iq & iq & 0 \\ 0 & 1 & e^{-2iqa} & -1 \\ 0 & -iq & iqe^{-2iqa} & \left[iq - \frac{2m\alpha}{\hbar^2}\right] \end{pmatrix} \begin{pmatrix} B \\ C \\ D \\ F \end{pmatrix} = \begin{pmatrix} -1 \\ -ik \\ 0 \\ 0 \end{pmatrix}$$

(5)

② Hálfur hreintóna sveifill



Jafna Schrödingers er sú sama, en gildir aðeins fyrir bilið $x > 0$ núna

Vegna veggsins í $x = 0$ verður að gilda $\psi(0) = 0$

→ hér eru aðeins oddstæðu lausnir hreintóna sveifils mögulegar og engar aðrar

$$E_n = \hbar\omega(n + \tfrac{1}{2}) \qquad n = 1, 3, 5, 7, \ldots$$

④

setjum $s = e^{-2iqa}$ og $r = \left\{ iq - \frac{2m\alpha}{\hbar^2} \right\}$

$$\begin{pmatrix} 1 & -1 & -1 & 0 \\ -ik & -iq & iq & 0 \\ 0 & 1 & s & -1 \\ 0 & -iq & iqs & r \end{pmatrix} \begin{pmatrix} B \\ C \\ D \\ F \end{pmatrix} = \begin{pmatrix} -1 \\ -ik \\ 0 \\ 0 \end{pmatrix}$$

lausn fundin í maxima er ef við skilgreinum

$$\Omega = q\left\{-ir(s+1) + k(s+1)\right\} + ikr(1-s) + q^2(s-1)$$

$$= q(s+1)(k-ir) + (s-1)(q^2 - ikr)$$

⑤

$$B = -\frac{q(s+1)(-k-ir) - ikr(1-s) + q^2(s-1)}{\Omega}$$

$$= \frac{q(s+1)(k+ir) - (s-1)(q^2+ikr)}{\Omega}$$

$$C = \frac{2ks(q-ir)}{\Omega}$$

$$D = \frac{2k(ir+q)}{\Omega}$$

$$F = \frac{4kqs}{\Omega}$$

⑥

Ef $\alpha = 0$, engin δ-toppar $\longrightarrow$ $r = iq$

$$\longrightarrow \Omega = q(s+1)(k+q) + (s-1)(q^2+kq)$$

$$= (s+1)(q^2+kq) + (s-1)(q^2+kq)$$

$$= 2s(q^2+kq)$$

og

$$B = \frac{q(s+1)(k-q) - (s-1)(q^2-kq)}{\Omega}$$

$$= \frac{2sq(k-q)}{2sq(q+k)} = -\frac{q-k}{q+k}$$

eins og í dæminu í síðustu viku ↑
þar sem $\alpha = 0$

⑦

Enn ef $\alpha = 0$

$$F = \frac{4kqs}{\Omega} = \frac{4kqs}{2s(q^2+kq)} = \frac{2k}{q+k}$$

eins og í dæminu í síðustu viku

Undirbúum grafík:

Miðum allt við orkuna $E_1 = \frac{\hbar^2}{2ma^2}$ ← væri orka lægsta ástands í óendanlegum brunni

$$ka = \sqrt{\frac{2ma^2}{\hbar^2}(E - V_0)} = \sqrt{\frac{E}{E_1} - \frac{V_0}{E_1}} \qquad E > V_0$$

$$qa = \sqrt{\frac{E}{E_1}} \qquad ra = \left\{ i\,qa - \left(\frac{\alpha}{a}\right)\frac{1}{E_1} \right\}$$

↑ víddarlausar stærðir

Styrkur δ-mattis í orku er $\frac{\alpha}{a}$, meðan hann líka við E_1

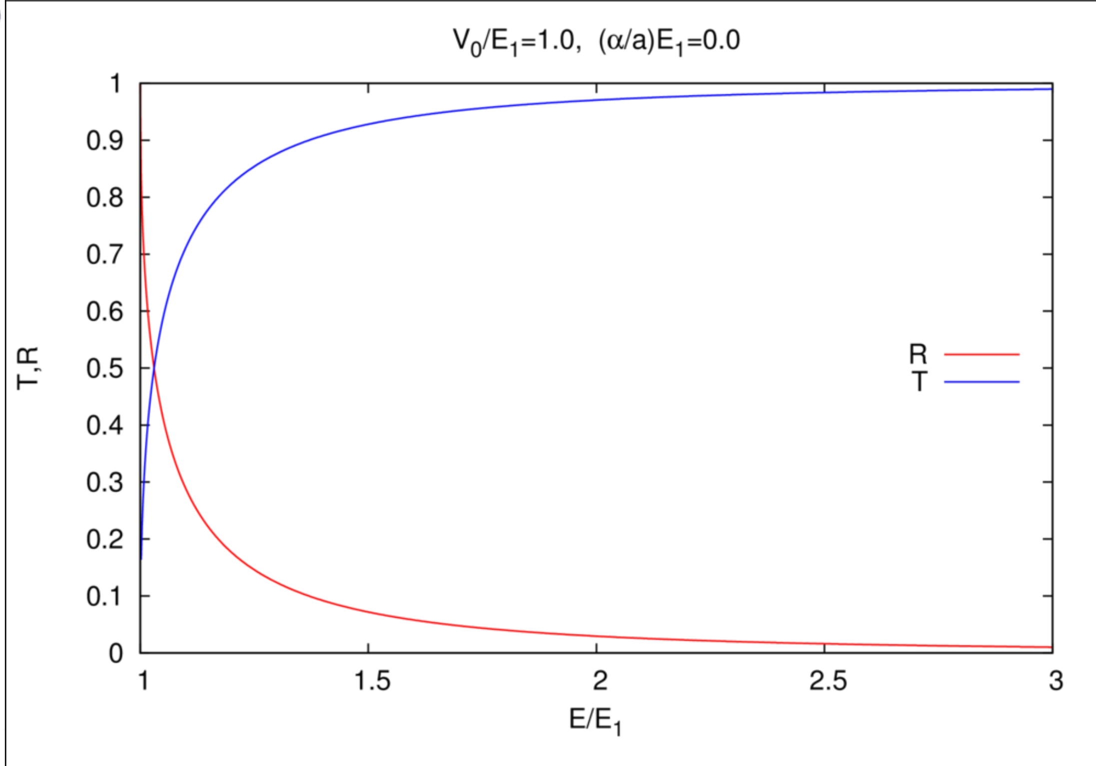
$$S = \exp\{-2iqa\}$$

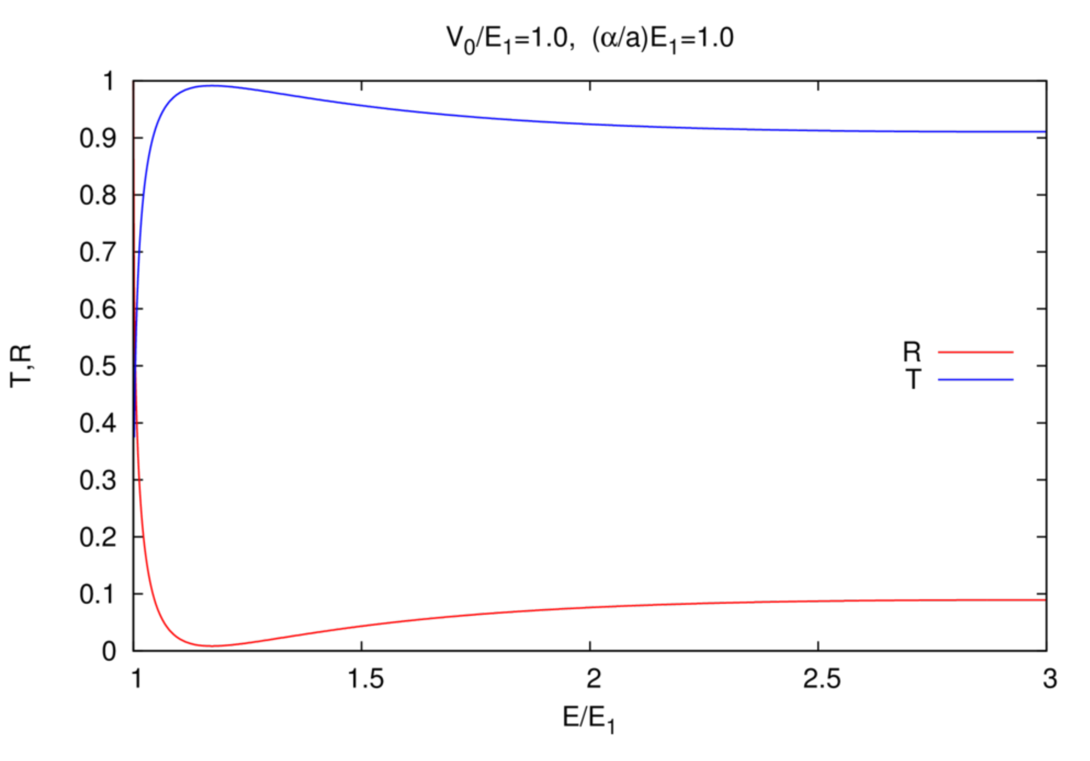
Munurin ír dominera í síðstu viku við

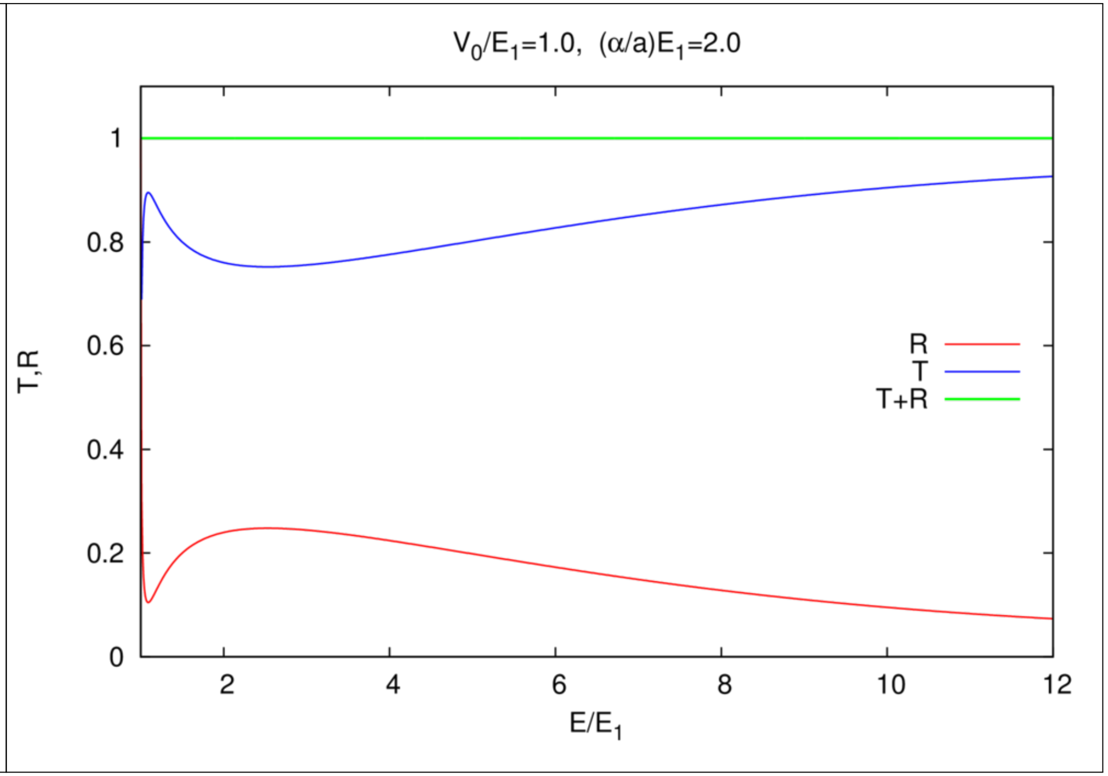
$$R = |B|^2$$

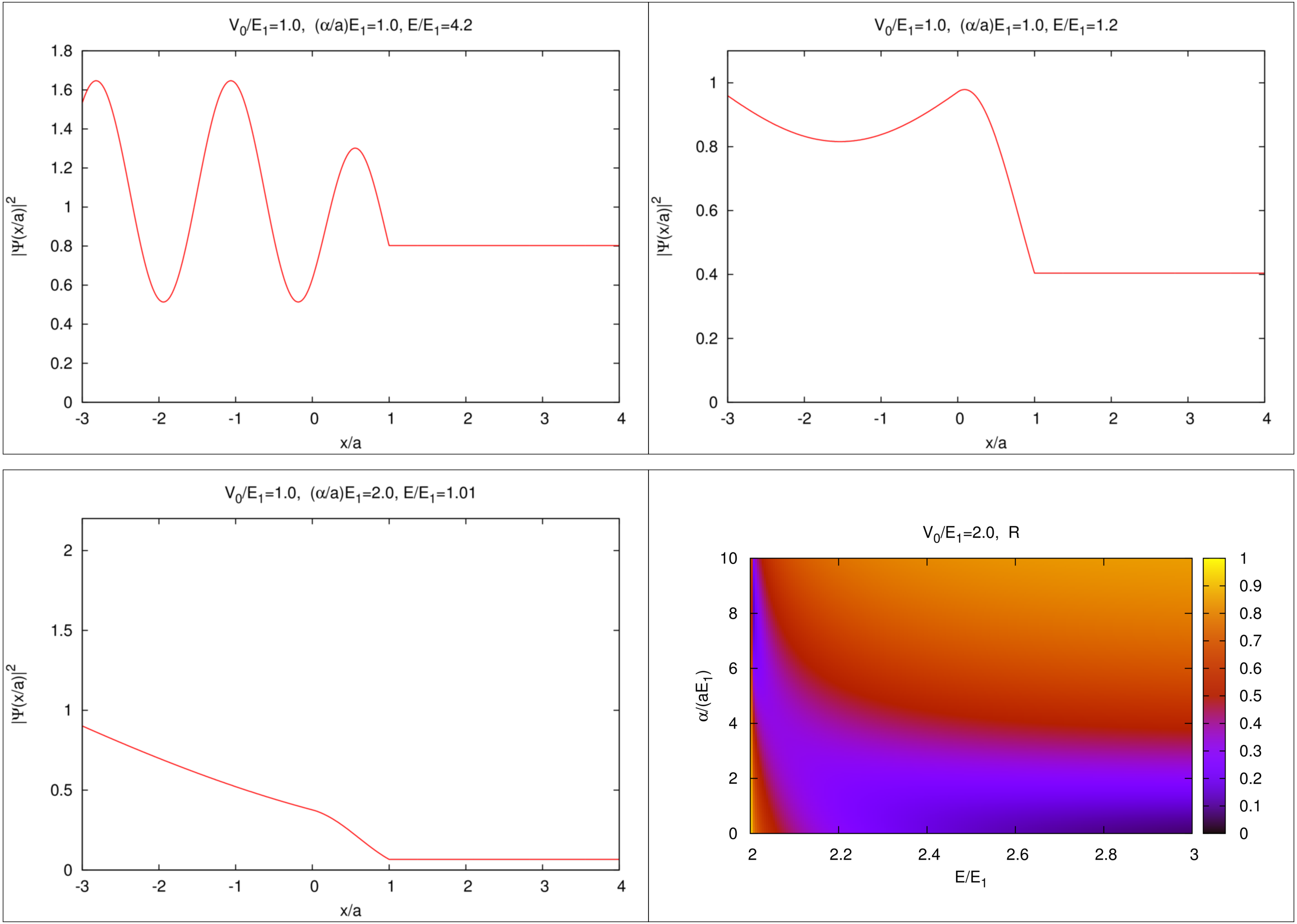
$$T = \frac{qa}{ka}|F|^2$$

(8)

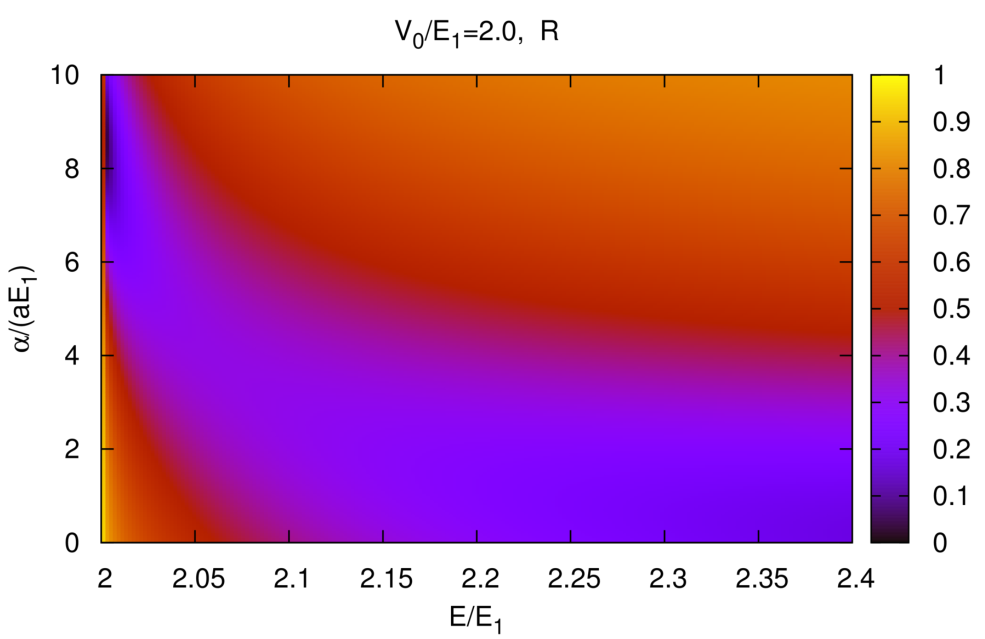


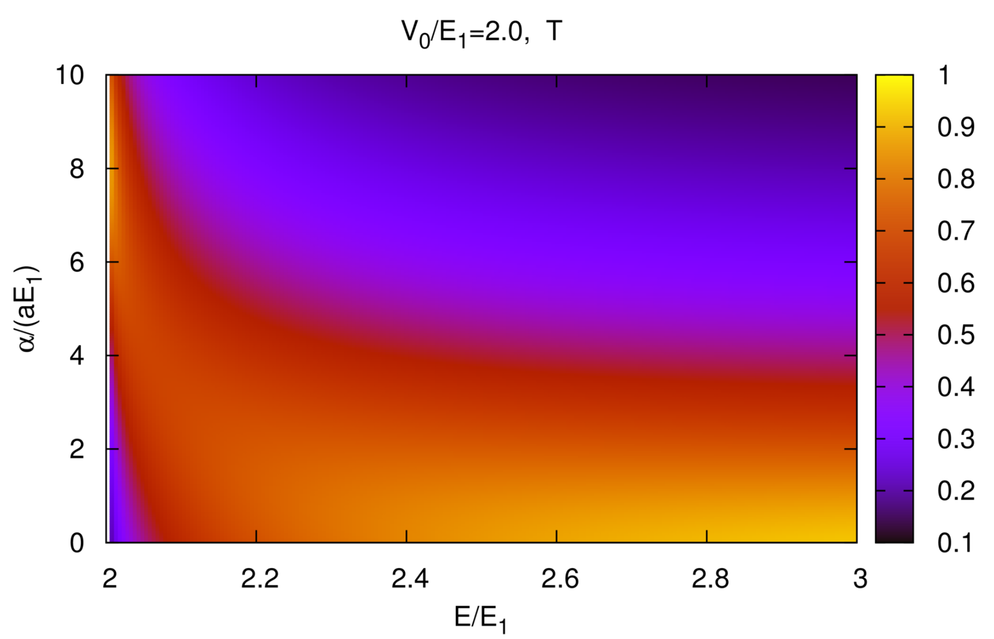


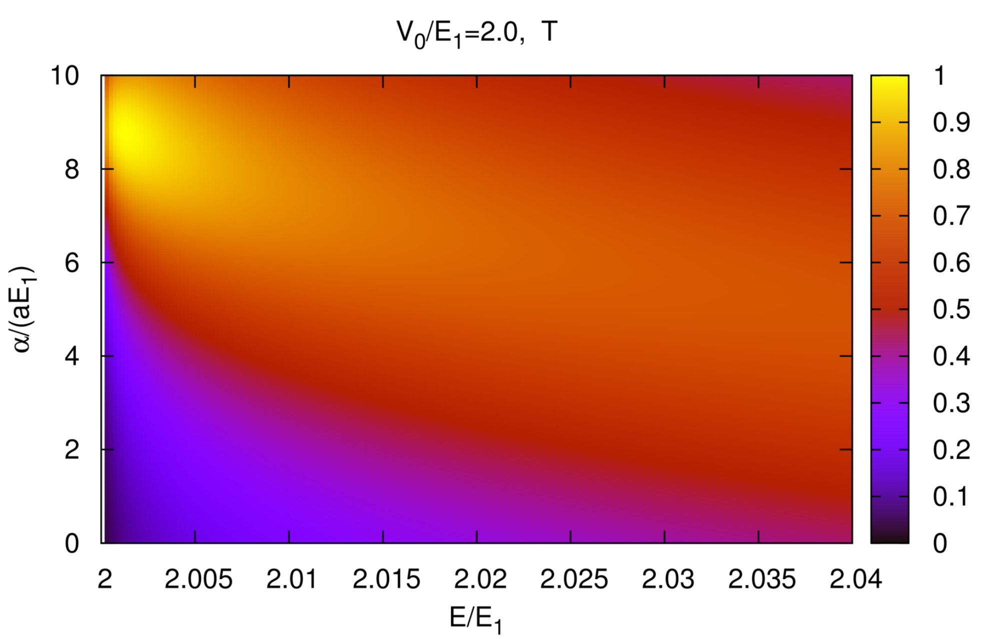




V_0/E_1=1.0, $(\alpha/a)E_1$=1.0, E/E_1=4.2
$|\Psi(x/a)|^2$
x/a
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
-3
-2
-1
0
1
2
3
4
V_0/E_1=1.0, $(\alpha/a)E_1$=1.0, E/E_1=1.2
$|\Psi(x/a)|^2$
x/a
0
0.2
0.4
0.6
0.8
1
-3
-2
-1
0
1
2
3
4
V_0/E_1=1.0, $(\alpha/a)E_1$=2.0, E/E_1=1.01
$|\Psi(x/a)|^2$
x/a
0
0.5
1
1.5
2
-3
-2
-1
0
1
2
3
4
V_0/E_1=2.0, R
$\alpha/(aE_1)$
E/E_1
0
2
4
6
8
10
2
2.2
2.4
2.6
2.8
3
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1







(1) Hreintóna sveifill

Gerum ráð fyrir ~~að~~ til sé eiginástand a_-

$$a_-|\alpha\rangle = \alpha|\alpha\rangle$$

a_- er ekki hermískur virki, því getur $\alpha \in \mathbb{C}$

a) Reiknum $\langle x\rangle$, $\langle x^2\rangle$, $\langle p\rangle$ og $\langle p^2\rangle$ fyrir $|\alpha\rangle$

Rifjum upp

$$a_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left\{\mp ip + m\omega x\right\}$$

munum líka eftir náttúrulega lengdarskalanum

$$a = \sqrt{\frac{\hbar}{m\omega}} \quad \Rightarrow \quad x = \frac{a}{\sqrt{2}}(a_+ + a_-)$$

$$p = \frac{i\hbar}{\sqrt{2}\,a}(a_+ - a_-)$$

(2)

því fæst

$$\langle x \rangle = \langle \alpha | x | \alpha \rangle = \frac{a}{\sqrt{2}} \langle \alpha | \{ a_+ + a_- \} | \alpha \rangle$$

adota virkinn

$$= \frac{a}{\sqrt{2}} \{ \langle a_- \alpha | \alpha \rangle + \langle \alpha | a_- | \alpha \rangle \} = \frac{a}{\sqrt{2}} [\alpha^* + \alpha]$$

raunhluti

$$= \sqrt{2}\, a \cdot \mathrm{Re}(\alpha)$$

$$\langle p \rangle = \langle \alpha | p | \alpha \rangle = \frac{i\hbar}{\sqrt{2}\, a} \langle \alpha | \{ a_+ - a_- \} | \alpha \rangle$$

$$= \frac{i\hbar}{\sqrt{2}\, a} \{ \alpha^* - \alpha \} = -\frac{i\hbar}{\sqrt{2}\, a} \{ \alpha - \alpha^* \}$$

$$= -\frac{i\hbar \cdot 2}{\sqrt{2}\, a} i\, \mathrm{Im}(\alpha) = \sqrt{2} \frac{\hbar}{a} \mathrm{Im}(\alpha)$$

Munum að væntigildi p og x í eigin-falla grunni H hverfa

(3)

$$\langle x^2 \rangle = \frac{a^2}{2} \langle \alpha | [a_+ + a_-]^2 | \alpha \rangle = \frac{a^2}{2} \langle \alpha | \{ a_+ a_+ + a_+ a_- + a_- a_+ + a_- a_- \} | \alpha \rangle$$

Hér er best að nota $[a_-, a_+] = 1$

$$\rightarrow \quad a_- a_+ = a_+ a_- + 1$$

$$\rightarrow \quad \langle x^2 \rangle = \frac{a^2}{2} \langle \alpha | \{ a_+ a_+ + a_+ a_- + a_+ a_- + 1 + a_- a_- \} | \alpha \rangle$$

$$= \frac{a^2}{2} \langle \alpha | \{ (\alpha^*)^2 + 2\alpha^* \alpha + 1 + \alpha^2 \} | \alpha \rangle$$

$$= \frac{a^2}{2} \{ (\alpha^* + \alpha)^2 + 1 \} = \frac{a^2}{2} \{ (2\,\mathrm{Re}(\alpha))^2 + 1 \}$$

(4)

$$\langle p^2 \rangle = -\frac{\hbar^2}{2a^2} \langle \alpha | \{ a_+ - a_- \}^2 | \alpha \rangle$$

$$= -\frac{\hbar^2}{2a^2} \langle \alpha | \{ a_+ a_+ - a_+ a_- - a_- a_+ + a_- a_- \} | \alpha \rangle$$

$$= -\frac{\hbar^2}{2a^2} \{ (\alpha^*)^2 - 2\alpha^* \alpha - 1 + \alpha^2 \}$$

$$= \frac{\hbar^2}{2a^2} [1 - (\alpha - \alpha^*)^2] = \frac{\hbar^2}{2a^2} \{ 1 + (2\,\mathrm{Im}(\alpha))^2 \}$$

---

b) finna σ_x og σ_p fyrir $|\alpha\rangle$

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{a^2}{2} \{ 4(\mathrm{Re}(\alpha))^2 + 1 \} - 2a^2 (\mathrm{Re}(\alpha))^2}$$

$$= \frac{a}{\sqrt{2}}$$

(5)

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{\hbar^2}{2a^2} \{ 1 + 4(\mathrm{Im}(\alpha))^2 \} - 2\frac{\hbar^2}{a^2} (\mathrm{Im}(\alpha))^2}$$

$$= \frac{\hbar}{\sqrt{2}\, a}$$

$$\rightarrow \quad \sigma_x \cdot \sigma_p = \frac{\hbar}{2}$$ minnsta mögulega gildið

Vitum að eiginástönd H mynda fullkominn grunn

$$\rightarrow \quad |\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$$

finna c_n

$$\rightarrow \quad \langle m | \alpha \rangle = c_m$$

því $\langle m | n \rangle = \delta_{m,n}$

6

En við vorum búin að finna

$$|n\rangle = A_n (a_+)^n |0\rangle \quad \text{með} \quad A_n = \frac{1}{\sqrt{n!}}$$

$$\rightarrow c_m = \langle m|\alpha\rangle = \frac{1}{\sqrt{m!}} \langle (a_+)^m 0|\alpha\rangle$$

$$= \frac{1}{\sqrt{m!}} \langle 0|(a_-)^m|\alpha\rangle = \frac{1}{\sqrt{m!}} \alpha^m \langle 0|\alpha\rangle$$

$$\rightarrow \boxed{c_m = \frac{1}{\sqrt{m!}} \alpha^m \cdot c_0}$$

d) Finnum c_0

Við vitum að $\sum_{n=0}^{\infty} |c_n|^2 = 1$

7

$$\rightarrow \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} |c_0|^2 = |c_0|^2 \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!}$$

$$= |c_0|^2 \cdot e^{|\alpha|^2} = 1$$

$$\rightarrow |c_0|^2 = e^{-|\alpha|^2}$$

og því gæti verið

$$c_0 = e^{-\frac{|\alpha|^2}{2}}$$

e) Hvernig er $|\alpha\rangle$ háð tíma?

$$|n(t)\rangle = |n\rangle e^{-i\omega_n t} \quad \text{með} \quad \omega_n = \frac{E_n}{\hbar} = \omega(n+1/2)$$

8

því fæst

$$|\alpha(t)\rangle = \sum_{n=0}^{\infty} c_n e^{-i\omega(n+\frac{1}{2})t} |n\rangle$$

$$= e^{-\frac{i\omega t}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-\frac{|\alpha|^2}{2}} e^{-i\omega n t} |n\rangle$$

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

> því $a_-|\alpha(t)\rangle$
> $$= e^{-\frac{i\omega t}{2}} \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}} e^{-\frac{|\alpha|^2}{2}} \sqrt{n}|n-1\rangle$$
> $$= \alpha e^{-i\omega t} e^{-\frac{i\omega t}{2}} \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\omega t})^{n-1}}{\sqrt{(n-1)!}} e^{-\frac{|\alpha|^2}{2}} |n-1\rangle$$
> $$= \alpha e^{-i\omega t} |\alpha(t)\rangle$$
> þegar summuhlaupabreytunni er breytt $(n-1) \rightarrow m$

Ef við látum a_- verka á $|\alpha(t)\rangle$ fæst eigingildið

$$e^{-i\omega t}\alpha = \alpha(t)$$

$|\alpha\rangle$ og $|\alpha(t)\rangle$ eru því sama ástandið með

9

tímaháða eigin gildið $\alpha(t) = \alpha e^{-i\omega t}$

f) $|0\rangle$ er líka svona ástand því

$a_-|0\rangle = 0$ með eigingildi 0

Rifjum aðeins upp: $\langle x\rangle = \sqrt{2}\, a\, \mathrm{Re}(\alpha)$

$$\langle x(t)\rangle = \sqrt{2}\, a \cdot \mathrm{Re}(\alpha e^{-i\omega t})$$

Veljum α þ.a. upphafið er með α sem rauntölu

$$\rightarrow \langle x(t)\rangle = \sqrt{2}\, a\, \alpha \cos(\omega t)$$

ástandið sveiflast fram og aftur án þess að dreifast

(2)

$$H = E\{ |1\rangle\langle 1| + 2|2\rangle\langle 2| + i|1\rangle\langle 2| - i|2\rangle\langle 1| + 3|3\rangle\langle 3| + |3\rangle\langle 1| + |1\rangle\langle 3| \}$$

Þrívíða kerfi $\{|i\rangle\}$ mynda ~~stað~~laðan grunn

Útsetning H í honum gefur

$$H = E\begin{pmatrix} 1 & i & 1 \\ -i & 2 & 0 \\ 1 & 0 & 3 \end{pmatrix} = \begin{pmatrix} \langle 1|H|1\rangle & \langle 1|H|2\rangle & \langle 1|H|3\rangle \\ \langle 2|H|1\rangle & \langle 2|H|2\rangle & \langle 2|H|3\rangle \\ \langle 3|H|1\rangle & \langle 3|H|2\rangle & \langle 3|H|3\rangle \end{pmatrix}$$

Nú má finna eigingildin og vigrana nákvæmlega, en ég leyfi mér tölulega að ~~fara~~

þá fæst með vigra

$$E_1 \simeq 0.12061\cdot E \qquad E_2 \simeq 2.3473\cdot E \qquad E_3 \simeq 3.5321\cdot E$$

$$|1) = \begin{pmatrix} a \\ ib \\ -c \end{pmatrix} \qquad |2) \simeq \begin{pmatrix} c \\ -ia \\ -b \end{pmatrix} \qquad |3) = \begin{pmatrix} b \\ ic \\ a \end{pmatrix}$$

$a \simeq 0.84403$
$b \simeq 0.44910$
$c \simeq 0.29313$

Hvernig lítur H út í nýja grunninum, finna $(i|H|j)$

$|i)$ fyrir $i = 1, 2$ og 3 eru eigingildi H

$\Rightarrow$ í nýja grunninum er fylki $\breve{H}$

$$\breve{H} = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix}$$

$\{$því $(i|H|j) = (i|E_j|j) = (i|j)E_j = \delta_{ij} E_j \}$

Einnig er gaman að raða eiginvigrunum saman í fylki

$$V = \begin{pmatrix} a & c & b \\ ib & -ia & ic \\ -c & -b & a \end{pmatrix}$$

þá sést að $V^\dagger V = \mathbb{1}$ — í grunninum $\{|i)\}$

og $V^\dagger H V = \breve{H}$ — í grunninum $\{|i\rangle\}$

því er V einota ummyndun milli grunnanna

Finnum væntigildi H í $\{|i\rangle\}$

$$\langle 1|H|1\rangle = 1E, \quad \langle 2|H|2\rangle = 2E, \quad \langle 3|H|3\rangle = 3E$$

(1) Ein rafeind innilokuð í kúlu með geisla a

Bylgjuföllin eru

$$\psi_{n\ell m}(r,\theta,\varphi) = A_{n\ell}\, j_\ell\left(\frac{\beta_{n\ell} r}{a}\right) Y_{\ell m}(\theta,\varphi)$$

Eigingildi H eru

$$E_{n\ell} = \frac{\hbar^2}{2ma^2}\beta_{n\ell}^2 = E_1 \beta_{n\ell}^2$$

$$ka = \sqrt{\frac{2ma^2}{\hbar^2}E} = \sqrt{\frac{E}{E_1}} = \beta_{n\ell}$$: n-ta núllstöð kúlu Bessel falls ℓ

$n = 1, 2, \ldots\ldots$

Viljum finna ástönd sambærileg við 1s, 2s og 2p-ástönd vetnisatóms.

1s í vetni engin núllstöð, $l=0,\ m=0$

hér er þá ein núllstöð á jaðri sambærilegt ástand, $l=0,\ m=0$, $n=1$

2s í vetni ein núllstöð, $l=0,\ m=0$

hér eru þá tvær núllst., ein á jaðri $n=2,\ l=0,\ m=0$

2p í vetni engin núllstöð, $l=1$, $m=-1,0,+1$, $n=2$

hér er þá ein núllstöð, á jaðri $n=1$, $l=1$, $m=-1,0,+1$, og önnur í $x=0$

1s

$$\psi_{100}(r,\theta,\varphi) = A_{10}\, j_0\left(\frac{\beta_{10} r}{a}\right) Y_{00}(\theta,\varphi)$$

$$j_0\left(\frac{\beta_{10} r}{a}\right) = \frac{\sin\left(\frac{\beta_{10} r}{a}\right)}{\left(\frac{\beta_{10} r}{a}\right)}$$

Fallið $\sin(x)/x$ hefur enga núllstöð í $x=0$, fyrsta núllstöðin er $x=\pi$. Setjum á jaðar

$\rightarrow r=a$ og $\beta_{10}=\pi$

$$\rightarrow E_{10} = E_1 \pi^2, \quad E_1 = \frac{\hbar^2}{2ma^2}$$

2s

$$\psi_{200}(r,\theta,\varphi) = A_{20}\, j_0\left(\frac{\beta_{20} r}{a}\right) Y_{00}(\theta,\varphi)$$

Sama r-fall næsta núllstöð

$$r=a \rightarrow \beta_{20} = 2\pi$$

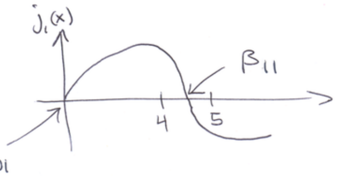
$$\rightarrow E_{20} = E_1 (2\pi)^2 = 4\cdot E_{10}$$

2p

$$\psi_{110}(r,\theta,\varphi) = A_{11}\, j_1\left(\frac{\beta_{11} r}{a}\right) Y_{1m}(\theta,\varphi)$$

$m=-1,0,+1$

$$j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}$$



$r=a$ og $\beta_{11} = 4.4934$

$$\rightarrow E_{11m} = E_1 \beta_{11}^2$$

Þannig að — 2s og 2p hafa mism. orku

2s: $E_{20} = 4\cdot E_{10}$

2p: $E_{11m} = E_1 \beta_{11}^2 = \frac{E_{10}}{\pi^2}\beta_{11}^2 \approx 2.0457\cdot E_{10}$

Fyrir vetnisatóm fékkst

$$E_n = -\frac{R_y}{n^2}$$

$E_1 = -R_y$ 1s

$E_2 = -\frac{R_y}{4}$ 2s, 2p

4.26 (6)

a) Sannreyna fyrir

$$[S_x, S_y] = i\hbar S_z \qquad S_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$[S_y, S_z] = i\hbar S_x \qquad S_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

$$[S_z, S_x] = i\hbar S_y \qquad S_y = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$

Ég reyni octave

sz = [1/2, 0 ; 0, -1/2]

sx = [0, 1/2 ; 1/2, 0]

sy = [0, -i/2 ; i/2, 0]

$$sx*sy - sy*sx = \begin{pmatrix} i/2 & 0\\ 0 & -i/2\end{pmatrix} = i S_z$$

$$\rightarrow [S_x, S_y] = i\hbar S_z$$

(7)

$$sy*sz - sz*sy = \begin{pmatrix} 0 & i/2\\ i/2 & 0\end{pmatrix} = i S_x$$

$$\rightarrow [S_y, S_z] = i\hbar S_x$$

$$sz*sx - sx*sz = \begin{pmatrix} 0 & 1/2\\ -1/2 & 0\end{pmatrix} = i S_y$$

$$\rightarrow [S_z, S_x] = i\hbar S_y$$

b) sýna að

$$\sigma_j \sigma_k = \delta_{jk} + i\sum_l \epsilon_{jkl}\sigma_l$$

(8)

Munum að

$$S_x = \frac{\hbar}{2}\sigma_x$$

$$S_y = \frac{\hbar}{2}\sigma_y$$

$$S_z = \frac{\hbar}{2}\sigma_z$$

Nota octave aftur

Byrja að sannreyna að

$$(\sigma_i)^2 = 1 \quad \text{fyrir } i = x, y, z$$

$$\epsilon_{iil} = 0$$

$$\sigma_x\sigma_y = \begin{pmatrix} i & 0\\ 0 & -i\end{pmatrix} = i\sigma_z \qquad \sigma_y\sigma_x = \begin{pmatrix} -i & 0\\ 0 & i\end{pmatrix} = -i\sigma_z$$

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

$$\sigma_y\sigma_z = \begin{pmatrix} 0 & i\\ i & 0\end{pmatrix} = i\sigma_x \qquad \sigma_z\sigma_y = \begin{pmatrix} 0 & -i\\ -i & 0\end{pmatrix} = -i\sigma_x$$

passar við $\sigma_j\sigma_k = \delta_{jk} + i\sum_l \epsilon_{jkl}\sigma_l$

(1) (1)

Athugum $|n, n-1, m\rangle$ - ástand vetnisatóms

Samkvæmt fyrirlestri og bók er almenna bylgjufallið

$$\psi_{nlm}(r) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]}}\; e^{-\frac{r}{na}}\left(\frac{2r}{na}\right)^l L^{2l+1}_{n-l-1}\left(\frac{2r}{na}\right) Y_{lm}(\theta,\phi)$$

Ef $l = n-1$, (hæsta leyfilega l-gildi ástands með n)

þá er Laguerre $L^{2n-1}_0\left(\frac{2r}{na}\right) = 1$

því $2l+1 = 2n-1$ og $n-l-1 = 0$

Ég nota aðra skilgreiningu á Laguerre en bókin, $L^\alpha_n(x) = e^x \frac{x^{-\alpha}}{n!}\frac{d^n}{dx^n}(e^{-x}x^{n+\alpha})$

$$\psi_{n,n-1,m}(r) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{1}{2n[(2n-1)!]}}\; e^{-\frac{r}{na}}\left(\frac{2r}{na}\right)^{n-1} Y_{n-1,m}(\theta,\phi)$$

sjá http://en.wikipedia.org/Laguerre_polynomials eða Lebedev. N.N., Dover

a) Athugum stöðlunina

(2)

$$\int_0^\infty r^2 dr\, d\Omega\, \left|\psi_{n,n-1,m}(\vec r)\right|^2$$

$$= \left(\frac{2}{na}\right)^3 \frac{1}{2n\left[(2n-1)!\right]} \int_0^\infty r^2 dr\; e^{-\frac{2r}{na}} \left(\frac{2r}{na}\right)^{2n-2}$$

$$= \left(\frac{2}{na}\right)^3 \frac{n^3a^3}{2n\left[(2n-1)!\right]\,8} \int_0^\infty \left(\frac{2r}{na}\right)^2 d\left(\frac{2r}{na}\right) e^{-\frac{2r}{na}} \left(\frac{2r}{na}\right)^{2n-2}$$

$$= \frac{1}{2n\left[(2n-1)!\right]} \int_0^\infty du\; u^{2n} e^{-u} = \frac{\Gamma(2n+1)}{2n\left[(2n-1)!\right]} = 1$$

(3)

b) Reiknið væntigildin fyrir $\langle r\rangle$ og $\langle r^2\rangle$

$$\langle r^p\rangle = \int_0^\infty r^{2+p} dr\, d\Omega\, \left|\psi_{n,n-1,m}(\vec r)\right|^2$$

$$= \left(\frac{2}{na}\right)^3 \frac{1}{2n\,(2n-1)!} \int_0^\infty r^{2+p}\, dr\; e^{-\frac{2r}{na}} \left(\frac{2r}{na}\right)^{2n-2}$$

$$= \left(\frac{2}{na}\right)^3 \frac{n^3a^3}{2n\,(2n-1)!\cdot 8} \frac{(na)^p}{2^p} \int_0^\infty d\left(\frac{2r}{na}\right) e^{-\frac{2r}{na}} \left(\frac{2r}{na}\right)^{2n} \left(\frac{2r}{na}\right)^p$$

$$= \left(\frac{na}{2}\right)^p \frac{1}{(2n)!} \int_0^\infty du\; e^{-u}\, u^{2n+p}$$

(4)

$$\langle r\rangle = \left(\frac{na}{2}\right) \frac{1}{(2n)!} \int_0^\infty du\; e^{-u}\, u^{2n+1} = \frac{na}{2} \frac{\Gamma(2n+2)}{(2n)!}$$

$$= \frac{na}{2}(2n+1) = na\left(n+\frac{1}{2}\right)$$

$$\langle r^2\rangle = \left(\frac{na}{2}\right)^2 \frac{1}{(2n)!} \int_0^\infty du\; e^{-u}\, u^{2n+2} = \left(\frac{na}{2}\right)^2 \frac{\Gamma(2n+3)}{(2n)!}$$

$$= \left(\frac{na}{2}\right)^2 (2n+1)(2n+2) = (na)^2\left(n+\frac{1}{2}\right)(n+1)$$

---

c) $$\sigma_r = \sqrt{\langle r^2\rangle - \langle r\rangle^2} = na\sqrt{\left\{\left(n+\tfrac{1}{2}\right)(n+1) - \left(n+\tfrac{1}{2}\right)^2\right\}}$$

(5)

$$\sigma_r = (na)\sqrt{\left(n+\tfrac{1}{2}\right)}\cdot\frac{1}{\sqrt{2}}$$

$$\longrightarrow \sigma_r/\langle r\rangle = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{n+\frac{1}{2}}} = \frac{1}{\sqrt{2n+1}}$$

$\langle r\rangle \sim n^2 a$ —> fjarlægð rafeindar vex sem n^2

en $\dfrac{\sigma_r}{\langle r\rangle} = \dfrac{1}{\sqrt{2n+1}}$ þýðir að bylgjufallið þrengist með vaxandi n

—> stefnir á klassíska braut

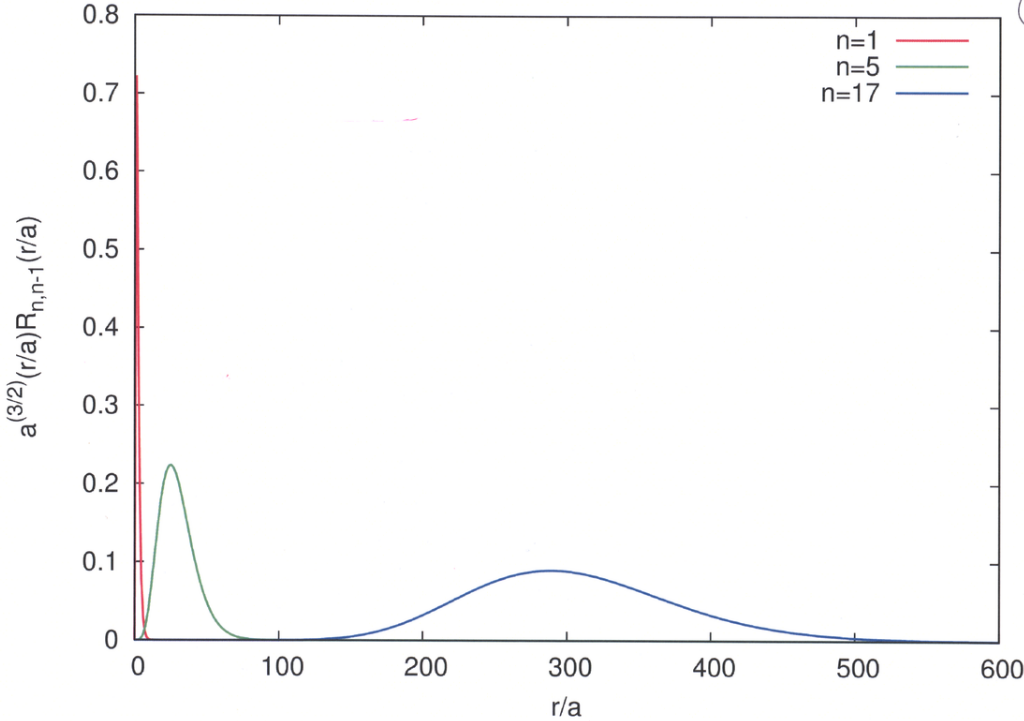
d) Teikna fyrir $n = 1,\ 5,\ 17$

$$R_{n,n-1}(r) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{1}{2n(2n-1)!}}\; e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^{n-1}$$

$$R_{n,n-1}\left(\frac{r}{a}\right) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{1}{2n(2n-1)!}}\; e^{-\frac{1}{n}\left(\frac{r}{a}\right)} \left(\frac{r}{a}\right)^{n-1}\cdot\left(\frac{2}{n}\right)^{n-1}$$

$$a^{3/2}\left(\frac{r}{a}\right)R_{n,n-1}\left(\frac{r}{a}\right) = \left(\frac{2}{n}\right)^{n-1}\sqrt{\left(\frac{2}{n}\right)^3\frac{1}{2n(2n-1)!}}\; e^{-\frac{1}{n}\left(\frac{r}{a}\right)}\left(\frac{r}{a}\right)^n$$

$$a^{3/2}\left(\frac{r}{a}\right)R_{n,n-1}\left(\frac{r}{a}\right) = F(n)\; e^{-\frac{1}{n}\left(\frac{r}{a}\right)}\left(\frac{r}{a}\right)^n$$



② Finna fylkja-útsetningu S_y og S_z fyrir eind með spuna 3/2 í grunni eiginástanda S_z

S_z hefur eiginástöndin

$$\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle \quad \left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle \quad \left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle \quad \left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle$$

Notum (4.136): $S_\pm|s,m\rangle = \hbar\sqrt{s(s+1)-m(m\pm1)}\,|s,m\pm1\rangle$

og $S_y = \frac{1}{2i}(S_+ - S_-)$

$$S_+\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle = 0$$

$$S_+\left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle = \hbar\sqrt{\tfrac{3}{2}\cdot\tfrac{5}{2}-\tfrac{1}{2}\cdot\tfrac{3}{2}}\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle = \sqrt{3}\,\hbar\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle$$

$$S_+\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle = 2\hbar\left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle \qquad S_-\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle = \sqrt{3}\,\hbar\left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle$$

$$S_+\left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle = \sqrt{3}\,\hbar\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle \qquad S_-\left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle = 2\hbar\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle$$

$$S_-\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle = \sqrt{3}\,\hbar\left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle \qquad S_-\left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle = 0$$

$$\rightarrow S_+ = \hbar\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$S_- = \hbar\begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

$$S_y = \frac{1}{2i}(S_+ - S_-) = \frac{\hbar}{2i}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & 0 & 2 & 0 \\ 0 & -2 & 0 & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & 0 \end{pmatrix}$$

(10)

Eigingildi S_y

Reynt með octave getur

$+\frac{\hbar}{2}\cdot 3$ eins og við mátti búast

$+\frac{\hbar}{2}\cdot 1$

$-\frac{\hbar}{2}\cdot 1$

$-\frac{\hbar}{2}\cdot 3$

(1)

þrístiga kerfi með $H_0 = E_0\{|1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3|\}$

1) $\rightarrow$ þrefalt orkustig með $E_1 = E_2 = E_3 = E_0$

Ef við veljum framsetningu eiginástandanna sem

$$\begin{pmatrix}1\\0\\0\end{pmatrix},\ \begin{pmatrix}0\\1\\0\end{pmatrix} \text{ og } \begin{pmatrix}0\\0\\1\end{pmatrix}$$

þá fæst fylkið fyrir H_0 í þessum grunni

$$H_0 = E_0\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}$$

(2)

Kerfið er truflað með $\lambda H'$ þ.s.

$$H' = E_0\left\{-|1\rangle\langle 1| + i|1\rangle\langle 3| + |2\rangle\langle 2| - i|3\rangle\langle 1|\right\}$$

sem í sama grunni útsett sem

$$H' = E_0\begin{pmatrix}-1 & 0 & i\\ 0 & 1 & 0\\ -i & 0 & 0\end{pmatrix}$$

þannig að

$$H = H_0 + \lambda H' = E_0\begin{pmatrix}1-\lambda & 0 & i\lambda\\ 0 & 1+\lambda & 0\\ -i\lambda & 0 & 1\end{pmatrix}$$

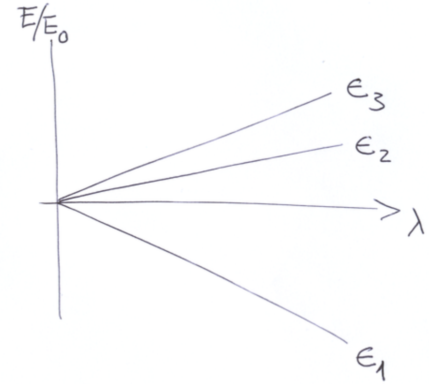
(3)

2) Finna nákvæmt orkuróf, Eigingildi H

$$\epsilon_3 = E_0(1+\lambda)$$

$$\epsilon_2 = E_0\left(1 + \frac{\lambda}{2}(\sqrt{5}-1)\right)$$

$$\epsilon_1 = E_0\left(1 - \frac{\lambda}{2}(\sqrt{5}+1)\right)$$



tökum eftir að nákvæma lausnin er línuleg í λ

(4)

3) Nota 1. stigs truflun t.p.a. finna ϵ_i, eigingildi H

Hér er ekki hægt að nota truflunarröð fyrir einfölld ástönd því þá fengjust óendanlegir liðir. Hér þarf að nota truflun á þrefölduð ástandi

Notum grunn eiginástanda H_0, $\{|i\rangle\}$ til þess að útsetja $\lambda H'$

$$\lambda H' = E_0 \begin{pmatrix} -1 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

eigingildi þessa eru

$$E_0 \lambda$$
$$E_0 \frac{\lambda}{2}(\sqrt{5}-1)$$
$$-E_0 \frac{\lambda}{2}(\sqrt{5}+1)$$

(5)

4) Þannig að 1. stigs truflun 3-falds ástands hér gefur réttu lausnina, þar sem hún inniheldur ekki hærri veldi af λ en 1. stigs!

---

(2) Einvíður hreintóna sveifill með róf $E_n = \hbar\omega(n+1/2)$ truflaður með

$$H' = \lambda \hbar\omega \left(\frac{x}{a}\right)^p \quad , \quad \lambda << 1$$

Finna grunnástand ásamt samsvarandi 1. stigs truflun þegar $p = 3, 4$

(6)

$p = 4$ er auðvelt, því fyrr í haust reiknuðum við fyrir kerfið

$$\langle x^4 \rangle = a^4 \left\{\frac{3}{2}n^2 + \frac{3}{2}n + \frac{3}{4}\right\}$$

$$\rightarrow \quad \epsilon_n = E_n + \lambda\hbar\omega\left\{\frac{3}{2}n^2 + \frac{3}{2}n + \frac{3}{4}\right\}$$

$$= \hbar\omega\left\{\frac{3\lambda}{2}n^2 + n\left(1 + \frac{3\lambda}{2}\right) + \frac{1}{2} + \frac{3\lambda}{4}\right\}$$

$$\rightarrow \quad \epsilon_0 = \hbar\omega\left\{\frac{1}{2} + \frac{3\lambda}{4}\right\}$$

(7)

Hvað þá með $\langle x^3 \rangle$?

$$\langle x^3 \rangle = \langle n | x^3 | n \rangle = 0$$

Það þarf 2. stigs truflun til þess að finna áhrif x^3!

---

x^2 þrengir mættið, en „smá" x^3 leiðrétting mætti skekkir það aðeins án þess að þrengja eða víkka.

(1)

(1) Hreintóna sveifill með ástönd $|n\rangle$ og $E_n=\hbar\omega(n+\frac{1}{2})$ er truflaður með $\lambda H' = \lambda\hbar\omega\left(\frac{x}{a}\right)^4$

Finnum orku grunnástandsins með λ^2 leiðréttingu.

$$\epsilon_0 = E_0 + \langle 0|\lambda H'|0\rangle + \lambda^2\sum_{n=1}^{\infty}\frac{|\langle n|H'|0\rangle|^2}{E_0-E_n}$$

Í síðasta skammti fékkst

$$E_0 + \langle 0|\lambda H'|0\rangle = \hbar\omega\left\{\frac{1}{2}+\frac{3\lambda}{4}\right\}$$

$$\langle n|H'|0\rangle = \hbar\omega\langle n|\left(\frac{x}{a}\right)^4|0\rangle$$

$$= \frac{\hbar\omega}{4}\langle n|(a_+ + a_-)^4|0\rangle$$

Munum að

$$x = \frac{a}{\sqrt{2}}(a_+ + a_-)$$

$$p = \frac{i\hbar}{\sqrt{2}a}(a_+ - a_-)$$

$$a_-|n\rangle = \sqrt{n}\,|n-1\rangle$$

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

(2)

$$= \frac{\hbar\omega}{4}\left\{\delta_{n,4}\cdot\sqrt{24} + \delta_{n,0} + \delta_{n,0}\sqrt{4} + \delta_{n,2}\left(\sqrt{18}+\sqrt{8}+\sqrt{2}\right)\right\}$$

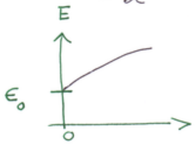
$\cdot|a_+a_+a_+a_+|\cdot$ $\cdot|a_-a_+a_-a_+|\cdot$ $\cdot|a_-a_-a_+a_+|\cdot$ $\cdot|a_-a_+a_+a_+|\cdot\sqrt{18}$, $\cdot|a_+a_-a_+a_+|\cdot\sqrt{8}$, $\cdot|a_+a_+a_-a_+|\cdot\sqrt{2}$

$$= \frac{\hbar\omega}{4}\left\{\delta_{n,4}\cdot\sqrt{24} + \delta_{n,0}(1+\sqrt{4}) + \delta_{n,2}\left(\sqrt{18}+\sqrt{8}+\sqrt{2}\right)\right\}$$

$$\epsilon_0 = \hbar\omega\left[\frac{1}{2}+\frac{3\lambda}{4}\right] + \lambda^2\left(\frac{\hbar\omega}{4}\right)^2\left\{\frac{24}{E_0-E_4}+\frac{72}{E_0-E_2}\right\}$$

$$= \hbar\omega\left\{\frac{1}{2}+\frac{3\lambda}{4}\right\} + \lambda^2\frac{\hbar\omega}{16}\left\{\frac{24}{-4}+\frac{72}{-2}\right\}$$

$$= \hbar\omega\left\{\frac{1}{2}+\lambda\frac{3}{4}-\lambda^2\frac{21}{8}\cdots\right\}$$



(2b)

Brillouin-Wigner

$$\epsilon_0 = \hbar\omega\left\{\frac{1}{2}+\frac{3\lambda}{4}\right\} + \lambda^2\left(\frac{\hbar\omega}{4}\right)^2\left[\frac{24}{\epsilon_0-\hbar\omega(4+\frac{1}{2})}+\frac{72}{\epsilon_0-\hbar\omega(2+\frac{1}{2})}\right]$$

$$\frac{\epsilon_0}{\hbar\omega} = \left[\frac{1}{2}+\frac{3\lambda}{4}\right] + \left(\frac{\lambda}{4}\right)^2\left[\frac{24}{\frac{\epsilon_0}{\hbar\omega}-\frac{9}{2}}+\frac{72}{\frac{\epsilon_0}{\hbar\omega}-\frac{5}{2}}\right]$$

Reynum lausn á ~~þessari~~ jöfnu fyrir gefin gildi á λ

Ekki ~~bætt~~ um í dæmi, en til gamans

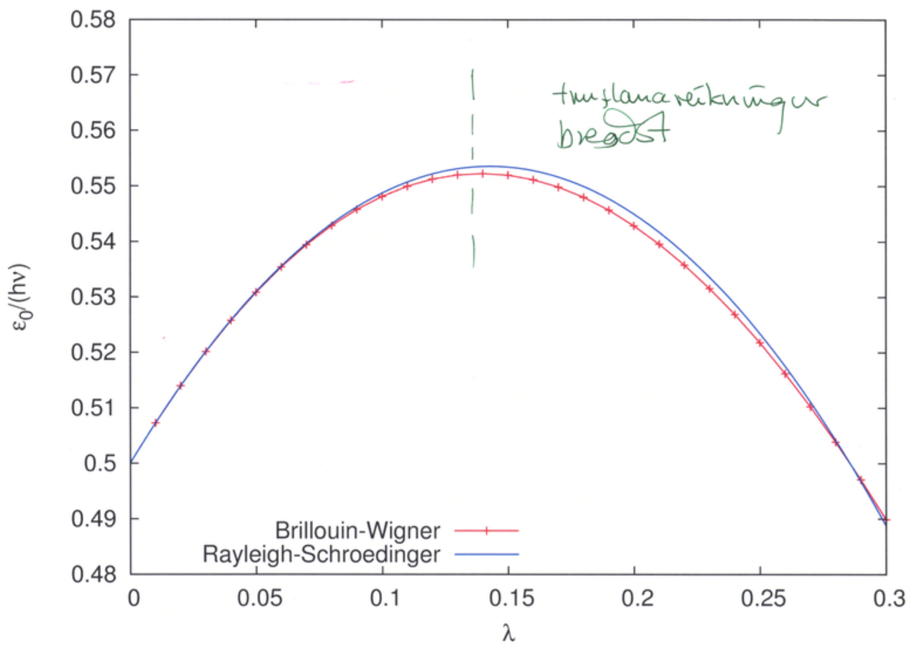
Plús leysa $H_0+\lambda H'$ í grunni 128 lægstu ástanda notandi

$$\langle n|\frac{x}{a}|m\rangle = \frac{1}{2}\sqrt{n+m+1}\,\delta_{|n-m|,1}$$

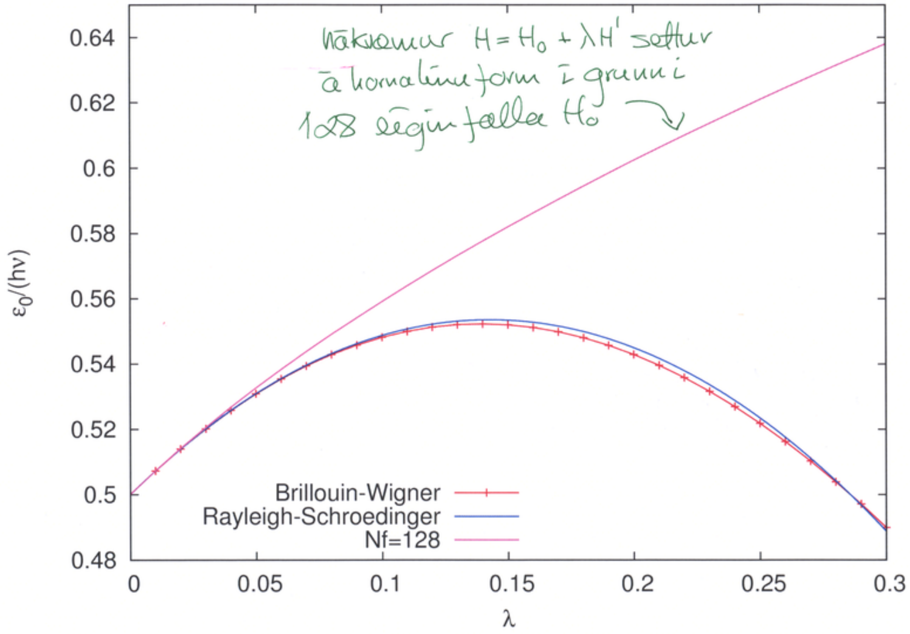
og

$$\langle n|\frac{x^4}{a^4}|m\rangle = \sum_{lpq}\langle n|\frac{x}{a}|l\rangle\langle l|\frac{x}{a}|p\rangle\langle p|\frac{x}{a}|q\rangle\langle q|\frac{x}{a}|m\rangle$$

(2c)

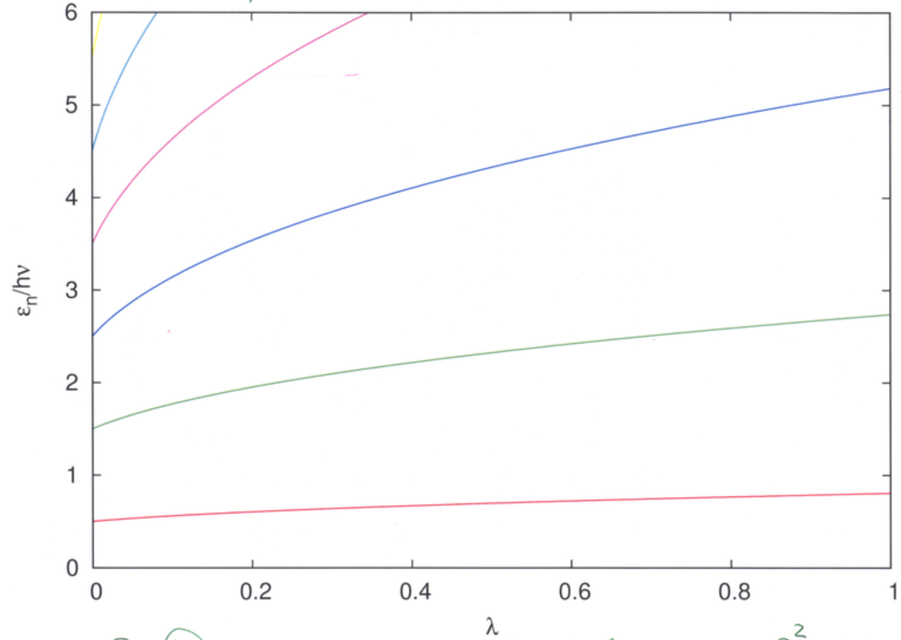


2d



2f

Orkuróf $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \lambda\hbar\omega\left(\frac{x}{a}\right)^4$



Fundið í grunni 128 eiginfalla $H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$

3

② H-atóm lokað inni í kúlu með geisla $a \gg a_B$
Hvernig er hægt að reikna $\Delta E = E_{2s} - E_{1s}$?

Kúlan hefur mætti

$$V_{sp}(r) = \begin{cases} 0 & \text{ef } r < a \\ \infty & \text{ef } r \geq a \end{cases}$$

V_{sp} er aldrei lítil truflun, verðum að snúa við dæminu: Hugsum okkur rafeind í kúlu sem er trufluð með

$$V_{coul}(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

$$a_B = \frac{4\pi\epsilon_0\hbar^2}{me^2} \quad \rightarrow \quad V_{coul}(r) = -\frac{e^2}{4\pi\epsilon_0}\,\frac{a}{r}\,\frac{me^2}{4\pi\epsilon_0\hbar^2}$$

4

$$V_{coul}(r) = -2Ry\cdot\left(\frac{a}{r}\right), \quad Ry = \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}$$

Ef við byrjum með kúlu

$$\psi_{1s}(\vec{r}) = A_{10}\, j_0\left(\frac{\pi r}{a}\right) Y_{00}(\theta,\varphi)$$

$$j_0(x) = \frac{\sin(x)}{x}$$

og

$$\psi_{2s}(\vec{r}) = A_{20}\, j_0\left(\frac{2\pi r}{a}\right) Y_{00}(\theta,\varphi)$$

$$E_{1s} = E_1\pi^2$$

$$E_{2s} = E_1(2\pi)^2$$

(5)

Normierung

$$1 = \int_0^a r^2 dr \left| j_0\left(\frac{\pi r}{a}\right)\right|^2 |A_{10}|^2 = \int_0^a r^2 dr \, \frac{\sin^2\left(\frac{\pi r}{a}\right)}{\left(\frac{\pi r}{a}\right)^2} |A_{10}|^2$$

$$\left(\frac{a}{\pi}\right)^3 |A_{10}|^2 \int_0^\pi du \, \sin^2 u = \left(\frac{a}{\pi}\right)^3 |A_{10}|^2 \frac{\pi}{2}$$

$$\rightarrow \quad A_{10} = \sqrt{\frac{2\pi^2}{a^3}}$$

$$1 = \int_0^a r^2 dr \left| j_0\left(\frac{2\pi r}{a}\right)\right|^2 |A_{20}|^2 = \int_0^a r^2 dr \, \frac{\sin^2\left(\frac{2\pi r}{a}\right)}{\left(\frac{2\pi r}{a}\right)^2} |A_{20}|^2$$

$$= \left(\frac{a}{2\pi}\right)^3 |A_{20}|^2 \int_0^{2\pi} du \, \sin^2 u = \left(\frac{a}{2\pi}\right)^3 |A_{20}|^2 \pi$$

$$\rightarrow \quad A_{20} = \sqrt{\frac{8\pi^2}{a^3}}$$

(6)

Rechnung

$$\langle 1s | V_{Coul} | 1s \rangle = -\frac{2\pi^2}{a^3} \cdot 2R_y \cdot \int_0^a r^2 dr \, \frac{\sin^2\left(\frac{\pi r}{a}\right)}{\left(\frac{\pi r}{a}\right)^2} \, \frac{a}{r}$$

$$= -4R_y \int_0^a \left(\frac{\pi r}{a}\right) d\left(\frac{\pi r}{a}\right) \frac{\sin^2\left(\frac{\pi r}{a}\right)}{\left(\frac{\pi r}{a}\right)^2}$$

$$= \int_0^\pi du \, \frac{\sin^2 u}{u} \quad = -4R_y \cdot \frac{1}{2}\left\{-\mathrm{Ci}(2\pi) + \gamma + \ln(2\pi)\right\}$$

$$\simeq -4R_y \cdot 1.21883$$

(7)

$$\langle 2s | V_{Coul} | 2s \rangle = -\frac{8\pi^2}{a^3} \, 2R_y \cdot \int_0^a r^2 dr \, \frac{\sin^2\left(\frac{2\pi r}{a}\right)}{\left(\frac{2\pi r}{a}\right)^2} \, \frac{a}{r}$$

$$= -4R_y \cdot \int_0^a \left(\frac{2\pi r}{a}\right) d\left(\frac{2\pi r}{a}\right) \frac{\sin^2\left(\frac{2\pi r}{a}\right)}{\left(\frac{2\pi r}{a}\right)}$$

$$= -4R_y \int_0^{2\pi} du \, \frac{\sin^2(u)}{u} \quad \simeq -4R_y \cdot 1.55718$$

$$\rightarrow \quad \epsilon_{1s} = E_1 \pi^2 - 4R_y \cdot 1.21883$$

$$\epsilon_{2s} = E_1 (2\pi)^2 - 4R_y \cdot 1.55718$$

(8)

$$\left.\begin{aligned} E_1 &= \frac{\hbar^2}{2ma^2} \\ R_y &= \frac{\hbar^2}{2ma_B^2} \end{aligned}\right\} \rightarrow \quad \begin{aligned} \epsilon_{1s} &= E_1\left\{\pi^2 - 4\frac{R_y}{E_1} \, 1.21883\right\} \\ \epsilon_{2s} &= E_1\left\{(2\pi)^2 - 4\frac{R_y}{E_1} \, 1.55718\right\} \end{aligned}$$

$$\frac{R_y}{E_1} = \frac{a^2}{a_B^2}$$

$$\rightarrow \quad \epsilon_{1s} = E_1\left\{\pi^2 - 4\left(\frac{a^2}{a_B^2}\right) 1.21883\right\}$$

$$\epsilon_{2s} = E_1\left\{(2\pi)^2 - 4\left(\frac{a^2}{a_B^2}\right) 1.55718\right\}$$

(9)

$$\Delta E^0 = E_{2s} - E_{1s} = E_1\left\{(2\pi)^2 - \pi^2\right\} = E_1\pi^2\cdot 3$$

$$\Delta E \approx \mathcal{E}_{2s} - \mathcal{E}_{1s} = \Delta E^0 - E_1 4\left(\frac{a}{a_B}\right)^2 0.3384$$

$$= E_1\pi^2 3 - E_1 4\left(\frac{a}{a_B}\right)^2 0.3384$$

$$= 3E_1\pi^2\left\{1 - \left(\frac{a}{a_B}\right)^2\frac{4\cdot 0{,}3384}{3\pi^2}\right\}$$

$$\approx 3E_1\pi^2\left\{1 - 0{,}0457\left(\frac{a}{a_B}\right)^2\right\}$$

(1)

(9.4) Kerfinu er lýst með

$$i\hbar d_t \bar{C}(t) = H'\bar{C}(t) \qquad H' = \begin{pmatrix} H'_{aa} & H'_{ab}e^{-i\omega_0 t} \\ H'_{ba}e^{i\omega_0 t} & H'_{bb} \end{pmatrix}$$

eða með

$$\bar{C}(t) = \bar{C}(0) + \frac{1}{i\hbar}\int_0^t ds\, H'(s)\,\bar{C}(s)$$

a)

Gerum ráð fyrir því að $C_a(0) = 1$, $C_b(0)$, $\bar{C}(0) = \begin{pmatrix}1\\0\end{pmatrix}$

Í fyrirlestri var 1. stigs lausn leidd út:

$$\bar{C}^{(1)}(t) = \bar{C}(0) + \frac{1}{i\hbar}\int_0^t ds\, H'(s)\,\bar{C}(0)$$

$$= \left[1 + \frac{1}{i\hbar}\int_0^t ds\, H'(s)\right]\bar{C}(0)$$

(2)

$$\begin{pmatrix} C_a(t) \\ C_b(t) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{i\hbar}\int_0^t ds \begin{pmatrix} H'_{aa}(s) \\ H'_{ba}(s)e^{i\omega_0 s} \end{pmatrix}$$

eða

$$C_a(t) = 1 + \frac{1}{i\hbar}\int_0^t ds\, H'_{aa}(s)$$

$$C_b(t) = \frac{1}{i\hbar}\int_0^t ds\, H'_{ba}(s)e^{i\omega_0 s}$$

$$|C_a|^2 = \left[1 - \frac{1}{i\hbar}\int_0^t ds\, H'_{aa}(s)\right]\left[1 + \frac{1}{i\hbar}\int_0^t dz\, H'_{aa}(z)\right]$$

$$= 1 + \left\{\frac{1}{\hbar}\int_0^t ds\, H'_{aa}(s)\right\}^2 = 1 + o\left((H')^2\right)$$

(3)

$$|C_b|^2 = o\left((H')^2\right)$$

$$\rightarrow |C_a|^2 + |C_b|^2 = 1 + o\left((H')^2\right)$$

b) skoðum

$$d_a(t) \equiv U_a(t)\,C_a(t)$$
$$d_b(t) \equiv U_b(t)\,C_b(t)$$

þar sem

$$U_a(t) = \exp\left\{-\frac{1}{i\hbar}\int_0^t ds\, H'_{aa}(s)\right\}$$

$$U_b(t) = \exp\left\{-\frac{1}{i\hbar}\int_0^t ds\, H'_{bb}(s)\right\}$$

{ tíma þróun vegna H'_{aa} og H'_{bb}, hér er henni haldið aðgreindri frá tímaþróun vegna H'_{ab} og H'_{ba} }

(4)

$$\dot{d}_a(t) = \dot{U}_a(t)\, C_a(t) + U_a(t)\, \dot{C}_a(t)$$

$$= U_a(t)\left[-\frac{1}{i\hbar} H'_{aa}(t)\, C_a(t) + \dot{C}_a(t)\right]$$

og $$\dot{C}_a(t) = \frac{1}{i\hbar}\left(H'_{aa}(t)\, C_a(t) + H'_{ab}(t)\, e^{-i\omega_0 t} C_b(t)\right)$$

$$\to \dot{d}_a(t) = U_a(t)\left\{H'_{ab}(t)\, e^{-i\omega_0 t} C_b(t)\right\}\frac{1}{i\hbar}$$

$$= U_a(t)\, H'_{ab}(t)\, e^{-i\omega_0 t}\, U_b^*(t)\, d_b(t)\, \frac{1}{i\hbar}$$

$$= U_a(t)\, H'_{ab}(t)\, U_b^*(t)\, e^{-i\omega_0 t}\, d_b(t)\, \frac{1}{i\hbar}$$

$$= \exp\left\{-\frac{1}{i\hbar}\int_0^t ds\left(H'_{aa}(s) - H'_{bb}(s)\right)\right\} e^{-i\omega_0 t} H'_{ab}\, d_b(t)\, \frac{1}{i\hbar} \quad (**)$$

(5)

$$\dot{d}_b(t) = \dot{U}_b(t)\, C_b(t) + U_b(t)\, \dot{C}_b(t)$$

$$= U_b(t)\left\{-\frac{1}{i\hbar} H'_{bb}(t)\, C_b(t) + \dot{C}_b(t)\right\}$$

$$\dot{C}_b(t) = \frac{1}{i\hbar}\left(H'_{ba}\, e^{i\omega_0 t} C_a(t) + H'_{bb}\, C_b\right)$$

$$\to \dot{d}_b(t) = U_b(t)\left\{H'_{ba}\, e^{i\omega_0 t} C_a(t)\right\}\frac{1}{i\hbar}$$

$$= U_b(t)\, H'_{ba}\, U_a^*(t)\, e^{i\omega_0 t}\, d_a(t)\, \frac{1}{i\hbar}$$

$$= \exp\left\{-\frac{1}{i\hbar}\int_0^t ds\left(H'_{bb}(s) - H'_{aa}(s)\right)\right\} e^{-i\omega_0 t} H'_{ba}\, d_a(t)\, \frac{1}{i\hbar} \quad (*)$$

(6)

c) Lausnir f. d_a og d_b

Upphafsskilyrði $C_a(0) = 1$, $C_b(0) = 0$

$U_a(0) = 1$ og $U_b(0) = 1$ $\to$ $d_a(0) = 1$, $d_b(0) = 0$

líka núllta stigs lausn (engin víxlverkun a og b)

Fyrsta stigs nálgun

$\to$ nota í (**)

$$\to \dot{d}_a(t) = 0 \to d_a(t) = 1 \to U_a(t)\, C_a(t) = 1$$

$$\to C_a(t) = U_a^*(t) = \exp\left\{\frac{1}{i\hbar}\int_0^t ds\, H'_{aa}(s)\right\}$$

(7)

Notum (*)

$$\dot{d}_b(t) = U_b(t)\, H'_{ba}\, U_a^*(t)\, e^{i\omega_0 t}\cdot 1 \cdot \frac{1}{i\hbar}$$

$$\to d_b(t) = \frac{1}{i\hbar}\int_0^t ds\, U_b(s)\, H'_{ba}\, U_a^*(s)\, e^{i\omega_0 s}$$

$$\to C_b(t) = \frac{1}{i\hbar}\, U_b^*(t)\int_0^t ds\, U_b(s)\, H'_{ba}\, U_a^*(s)\, e^{i\omega_0 s}$$

þetta þarf ~~að~~ gera ~~að~~ 1. stig truflun í H'_{ab} $\quad U_a \to 1$, $U_b \to 1$

$$\to C_b(t) \simeq \frac{1}{i\hbar}\int_0^t ds\, H'_{ba}(s)\, e^{i\omega_0 s}$$

til þess að fá réttan samanburð við lausn í bókinni