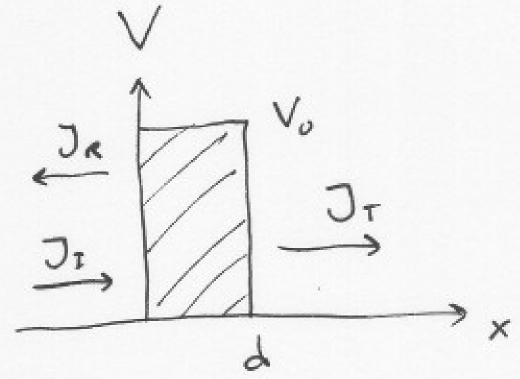
KVANTRÖV 4

VI 6



metall | oxid | metall

Infallande elektron med kinetisk energi

$E = 2{,}0$ eV

$V_0 = 5{,}0$ eV

$d = 2{,}0$ nm

Sökt: Tunnlingssannolikhet $T = \dfrac{J_T}{J_I}$

(J = sannolikhetsströmtäthet, se IV 5)

J för planvåg: $J = \frac{\hbar k}{m}|\psi|^2$, från IV 5.

TOSE: $\partial_x^2 \psi(x) + \dfrac{2m(E-V)}{\hbar^2}\psi(x) = 0$

$x<0,\ V=0:\ \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$ $\qquad k_1 = \dfrac{\sqrt{2mE}}{\hbar}$

$0<x<d,\ V=V_0:\ \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$ $\qquad k_2 = \dfrac{\sqrt{2m(E-V_0)}}{\hbar}$

$x>d,\ V=0:\ \psi_3(x) = Fe^{ik_1x} + \cancel{Ge^{-ik_1x}}$

$V_0 > E$ och konventionen säger att vi vill ha reella vågtal:

$k_2 = \dfrac{\sqrt{2m(E-V_0)}}{\hbar} = \dfrac{i\sqrt{2m(V_0-E)}}{\hbar}$. Def. reellt $\varkappa \equiv -ik_2$

$= \dfrac{\sqrt{2m(V_0-E)}}{\hbar}$

$\Rightarrow \psi_2(x) = Ce^{-\varkappa x} + De^{\varkappa x}$

...

$$J = \frac{\hbar k}{m}|\psi|^2 \qquad \left(\text{"}v\text{"} = \frac{p}{m} = \frac{\hbar k}{m}\right)$$

Här: $J_I = \frac{\hbar k_1}{m}\left|Ae^{ik_1x}\right|^2 = \frac{\hbar k_1}{m}|A|^2$

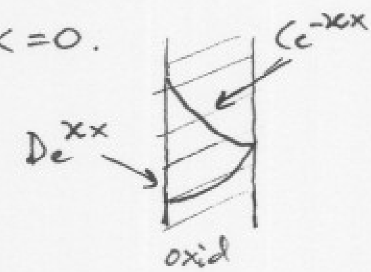
$$J_R = \frac{\hbar k_1}{m}\left|Be^{-ik_1x}\right|^2 = \frac{\hbar k_1}{m}|B|^2 \qquad \Rightarrow T = \frac{J_T}{J_I} = \left|\frac{F}{A}\right|^2$$

$$J_T = \frac{\hbar k_1}{m}\left|Fe^{ik_1x}\right|^2 = \frac{\hbar k_1}{m}|F|^2$$

Skarvningsproblem

OBS först att den exponentiellt växande termen $De^{\varkappa x}$ är reflektionen från den avtagande vågfknen i oxiden. Den kommer alltså att vara mycket liten vid $x=0$.

$\Rightarrow$ stryk D vid $x=0$!



- Vid $x=0$:

$$\left.\begin{aligned} \psi_1(0) = \psi_2(0) &\Rightarrow A+B = C \\ \psi_1'(0) = \psi_2'(0) &\Rightarrow ik_1(A-B) = -\varkappa C \end{aligned}\right\} \Rightarrow \begin{aligned} &B = C-A \\ &ik_1(2A-C) = -\varkappa C \end{aligned}$$

$$\Leftrightarrow \frac{C}{A} = \frac{2ik_1}{ik_1-\varkappa} \qquad (*)$$

- Vid $x=d$:

$$\left.\begin{aligned} \psi_2(d) = \psi_3(d) &\Rightarrow Ce^{-\varkappa d} + De^{\varkappa d} = Fe^{ik_1d} \\ \psi_2'(d) = \psi_3'(d) &\Rightarrow \varkappa\left(De^{\varkappa d} - Ce^{-\varkappa d}\right) = ik_1Fe^{ik_1d} \end{aligned}\right\}$$

$$\Rightarrow \quad \Rightarrow \varkappa\left(-2Ce^{-\varkappa d} + Fe^{ik_1d}\right) = ik_1Fe^{ik_1d}$$

$$\Leftrightarrow Fe^{ik_1d}(ik_1-\varkappa) = -2\varkappa Ce^{-\varkappa d} \Leftrightarrow F = -\frac{2\varkappa}{ik_1-\varkappa}Ce^{-\varkappa d-ik_1d}$$

$$\overset{(*)}{\Rightarrow} F = -\frac{2\varkappa}{ik_1-\varkappa}\left(\frac{2ik_1}{ik_1-\varkappa}\right)Ae^{-\varkappa d-ik_1d} = -\frac{4ik_1\varkappa}{(ik_1-\varkappa)^2}Ae^{-\varkappa d-ik_1d}$$

$$\Rightarrow T = \left|\frac{F}{A}\right|^2 = \left|-\frac{4ik_1\varkappa}{(ik_1-\varkappa)^2}e^{-\varkappa d-ik_1d}\right|^2 = \frac{16k_1^2\varkappa^2}{(k_1^2+\varkappa^2)^2}e^{-2\varkappa d}$$

...

Faktorn $e^{-2\varkappa d}$ kallas "barriärpenetreringsfaktor"

och faktorn $\frac{16k_1^2\varkappa^2}{(k_1^2+\varkappa^2)^2}$ kallas "förfaktor" och brukar

vara av storleksordningen 1.

Vi har:
$$\left.\begin{array}{l} d = 2\cdot 10^{-9}\,m \\ E = 2\,eV \\ V_0 = 5\,eV \\ m = 9{,}1\cdot 10^{-31}\,kg \\ \hbar = 1{,}05\cdot 10^{-34}\,Js \end{array}\right\} \Rightarrow \begin{array}{l} k_1 = 7{,}2\cdot 10^{9}\,m^{-1} \\ \varkappa = 8{,}9\cdot 10^{9}\,m^{-1} \end{array}$$

$$\Rightarrow e^{-2\varkappa d} = 4\cdot 10^{-16} \quad \text{och} \quad \frac{16k_1^2\varkappa^2}{(\varkappa^2+k_1^2)^2} = 3{,}8$$

$$\Rightarrow T \sim 10^{-15} \qquad (T \approx 1{,}5\cdot 10^{-15})$$

Approximationen att strunta i $De^{\varkappa x}$ vid $x=0$ brukar vara OK då $\varkappa d \gg 1$. Vi har $\varkappa d = 17{,}8$

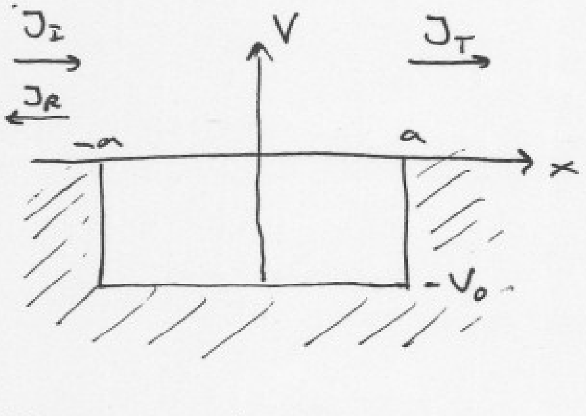
Om vi tar med $De^{\varkappa x}$ vid $x=0$ får vi att

$$T = \left(\left| \frac{1}{2ik_1}\left(-\frac{2\varkappa}{ik_1-\varkappa}e^{-ik_1d-\varkappa d}\right)^{-1}\left[(ik_1-\varkappa)-(ik_1+\varkappa)e^{-2\varkappa d}\right] + (ik_1+\varkappa)e^{ik_1d-\varkappa d} \right|^2 \right)^{-1}$$

$$= 1{,}32\cdot 10^{-15}$$

(VI 7)

$$V(x) = \begin{cases} 0 & |x| > a \\ -V_0 & |x| < a \end{cases} \qquad (V_0 > 0)$$



Sökt: E för transmissionsresonans

$(J_T = J_I)$

TOSE: $\psi''(x) + k^2\psi = 0$, $k = \frac{\sqrt{2m(E-V)}}{\hbar}$

$x < -a, V=0$: $\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$

$|x| < a, V=-V_0$: $\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$

$x > a, V=0$: $\psi_3(x) = E'e^{ik_1x}$

$k_1 = \frac{\sqrt{2mE}}{\hbar}$

$k_2 = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

Nu: skarva som i VI 6 : $\psi_1(-a) = \psi_2(-a)$

$\psi_1'(-a) = \psi_2'(-a)$

$\psi_2(a) = \psi_3(a)$, $\psi_2'(a) = \psi_3'(a)$

... Långa räkningar ...

$$\Rightarrow T = \frac{|E|^2}{|A|^2} = \frac{1}{1 + \frac{(k_1^2 - k_2^2)^2}{4k_1^2k_2^2}\sin^2(2k_2a)}$$

Vill veta när $T=1$. $\Rightarrow \frac{k_1^2-k_2^2}{4k_1k_2}\sin(2k_2a) = 0$

Två lösningar: 1) $k_1^2 - k_2^2 = 0 \Leftrightarrow k_1 = k_2$ (positiva)

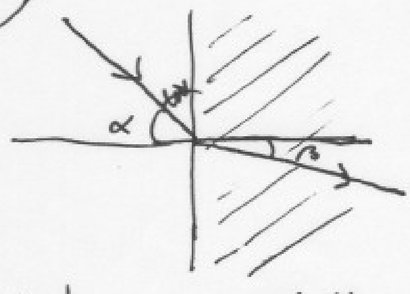
2) $\sin(2k_2a) = 0 \Leftrightarrow 2k_2a = n\pi \Leftrightarrow k_2 = \frac{n\pi}{2a}$

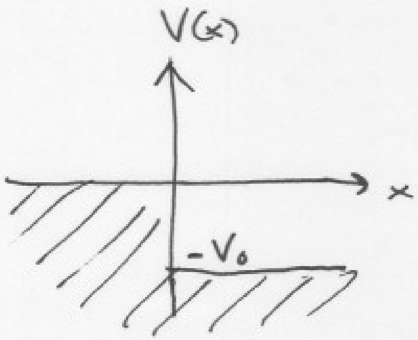
1) $k_1 = k_2 \Leftrightarrow E = E + V_0 \Leftrightarrow V_0 = 0$ (tråkig lösn.)

2) $k_2 = \frac{n\pi}{2a} = \frac{\sqrt{2m(E+V_0)}}{\hbar} \Leftrightarrow E = \frac{\pi^2\hbar^2}{8ma^2}n^2 - V_0$

OBS: $E > 0 \Rightarrow n > \sqrt{\frac{8ma^2V_0}{\pi^2\hbar^2}}$

VI 8





$n \equiv \frac{\sin\alpha}{\sin\beta} = \frac{\lambda_0}{\lambda_{metall}}$

Sökt: β, givet $\alpha = 45°$

$\left\{\begin{array}{l} E = 10\,eV \\ V_0 = 12\,eV \end{array}\right.$

TOSE: $\psi''(x) + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$

$\Leftrightarrow \psi''(x) + k^2\psi(x) = 0$, $k = \frac{\sqrt{2m(E-V)}}{\hbar}$

$x<0, V=0: \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$ $k_1 = \frac{\sqrt{2mE}}{\hbar}$

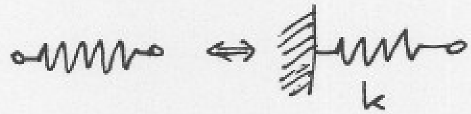
$x>0, V=-V_0: \psi_2(x) = Ce^{ik_2x}$ $k_2 = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

$$\ldots \quad \lambda = \frac{2\pi}{k} \Rightarrow \lambda_0 = \frac{h}{\sqrt{2mE}}, \quad \lambda_{metall} = \frac{h}{\sqrt{2m(E+V_0)}}$$

$$\sin\beta = \sin\alpha \frac{\lambda_{metall}}{\lambda_0} = \sin\alpha \sqrt{\frac{E}{E+V_0}} = \frac{\sin\alpha}{\sqrt{1+\frac{V_0}{E}}}$$

Här: $\alpha = 45°$, $\frac{V_0}{E} = \frac{12}{10} \Rightarrow \beta = \arcsin 0{,}48 = \underline{\underline{28°}}$

VII 1   Harmonisk oscillator



k

(fjäderkonstant)

Klassiskt: $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$, $E = \frac{1}{2}m(v^2 + \omega^2x^2)$

(Allmänt: $\frac{1}{2}k(x-x_0)^2 - V_0$)

(dvs $\omega = \sqrt{\frac{k}{m}}$) $E_{kin.}$ $E_{pot.} = V(x)$

Kvant: $E_n = \hbar\omega(n+\frac{1}{2})$ $(n = 0, 1, \ldots)$

$$\psi_n(y) = A_n H_n(y) e^{-\frac{1}{2}y^2}, \quad y = \sqrt{\frac{m\omega}{\hbar}}\,x$$

hermitepolynom

$$A_n = \left(\frac{\sqrt{\alpha}}{\sqrt{\pi}\,2^n n!}\right)^{1/2} \quad \text{(normeringsfaktor)}$$

Uppgift: $F = -kx$ (k = fjäderkonstant)

Visa att $\psi_1(x) = Ae^{-\alpha x^2}$ (i)

och $\psi_2(x) = Bxe^{-\beta x^2}$ (ii)

är egenfunktioner till $\hat{H}$.

Kraft: $F = -\frac{\partial}{\partial x}V(x) \Rightarrow V(x) = \frac{1}{2}kx^2$

$$\Rightarrow \text{SE}: \hat{H}\psi = E\psi \Leftrightarrow \left(-\frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2}kx^2\right)\psi = E\psi$$

$\ldots$

... Derivator: $\psi_1'(x) = -2\alpha x \psi_1 \Rightarrow \psi_1''(x) = (-2\alpha + 4\alpha^2 x^2)\psi_1$

$$\psi_2'(x) = B\left(e^{-\beta x^2} - 2\beta x^2 e^{-\beta x^2}\right)$$

$$\Rightarrow \psi_2''(x) = B\left(-2\beta x - 4\beta x - 2\beta x^2(-2\beta x^2)\right)e^{-\beta x^2} =$$

$$= B\left(-6\beta x + 4\beta^2 x^3\right)e^{-\beta x^2} = \left(-6\beta + 4\beta^2 x^2\right)\psi_2(x)$$

<u>Insättning i TOSE:</u>

(i) $\hat{H}\psi_1(x) = \left[-\frac{\hbar^2}{2m}\left(-2\alpha + 4\alpha^2 x^2\right) + \frac{1}{2}kx^2\right]\psi_1(x) = E_1\psi_1(x)$

För $E_1 =$ konst. energiegenvärde krävs $-\frac{\hbar^2}{2m}(4\alpha^2 x^2) + \frac{1}{2}kx^2 = 0$

ober. av x!

$$\Leftrightarrow \frac{2\alpha^2\hbar^2}{m} = \frac{1}{2}k \Leftrightarrow \alpha = \frac{\sqrt{km}}{2\hbar}$$

$$\Rightarrow E_1 = \frac{2\alpha\hbar^2}{2m} = \frac{\alpha\hbar^2}{m} = \frac{\sqrt{km}\,\hbar^2}{2\hbar m} = \sqrt{\frac{k}{m}}\frac{\hbar}{2} = \frac{1}{2}\hbar\omega$$

Normering: $1 = \int_{-\infty}^{\infty}|\psi(x)|^2 dx = A^2\int_{-\infty}^{\infty} e^{-2\alpha x^2}dx = A^2\sqrt{\frac{\pi}{2\alpha}}$

$$\Rightarrow A = \left(\frac{2\alpha}{\pi}\right)^{1/4} = \left(\frac{mk}{\pi^2\hbar^2}\right)^{1/8}$$

(ii) $\hat{H}\psi_2(x) = \left[-\frac{\hbar^2}{2m}\left(-6\beta + 4\beta^2 x^2\right) + \frac{1}{2}kx^2\right]\psi_2(x) = E_2\psi_2(x)$

Sätt $-\frac{\hbar^2}{2m}(4\beta^2 x^2) + \frac{1}{2}kx^2 = 0 \Leftrightarrow$ som i (i): $\beta = \alpha = \frac{\sqrt{km}}{2\hbar}$

$$\Rightarrow E_2 = \frac{3\beta\hbar^2}{m} = \frac{3\hbar}{2}\sqrt{\frac{k}{m}} = \hbar\omega\left(1 + \frac{1}{2}\right)$$

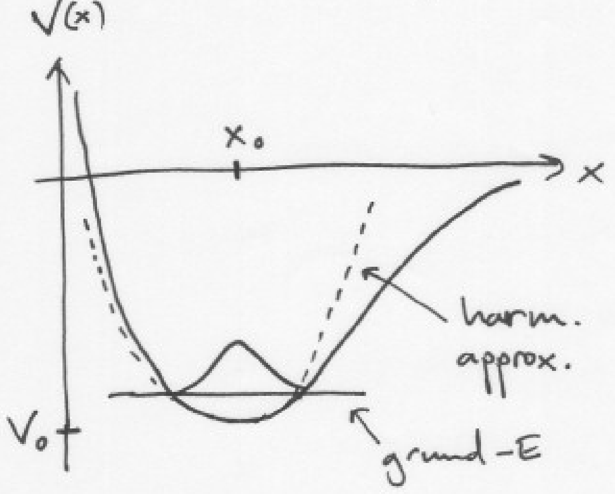
Ser att med $E_n = \hbar\omega(n + \frac{1}{2})$, så är E_2 egentligen E_1, dvs 1:a exciterande tillståndets energi för harm. osc.

Norm.: $1 = \int_{-\infty}^{\infty}|\psi_2(x)|^2 dx = B^2\frac{1}{4\beta}\sqrt{\frac{\pi}{2\beta}} \Rightarrow B = \left(\frac{4}{\pi}\right)^{1/4}\left(\frac{km}{\hbar^2}\right)^{3/8}$

VII 8

Bestäm grundtillståndsenergin i harmoniska approximationen för en partikel i:

$V = V_0\left(e^{-2a(x-x_0)} - 2e^{-a(x-x_0)}\right)$



Harm. approx. ⇒ Taylorutveckling kring x_0

$f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{1}{2!}f''(x_0)(x-x_0) + \ldots$

$e^{-2a(x-x_0)} \approx 1 - 2a(x-x_0) + 2a^2(x-x_0)^2$

$e^{-a(x-x_0)} \approx 1 - a(x-x_0) + \frac{a^2}{2}(x-x_0)^2$

$\Rightarrow V(x) = V_0\left[a^2(x-x_0)^2 - 1\right] = a^2V_0(x-x_0)^2 - V_0 \quad (1)$

$V_{harm.osc.} = \frac{1}{2}k(x-x_0)^2 - V_0 \quad (2)$

$(1)=(2) \Rightarrow k = 2V_0a^2 \Rightarrow \omega = \sqrt{\frac{k}{m}} = \sqrt{\frac{2V_0a^2}{m}}$

$E_{harm.osc.} = \hbar\omega\left(n+\frac{1}{2}\right) - V_0$

Väte: $a = 20\ nm^{-1}$, $V_0 = 7\cdot 10^{9}\ J$, $x_0 = 0{,}074\ nm$, $m = 0{,}84\cdot 10^{-27}\ kg$

$\Rightarrow E_0 = \frac{1}{2}\hbar\omega - V_0 = \frac{1}{2}\hbar\sqrt{\frac{2V_0a^2}{m}} - V_0 = 0{,}27\ eV - 4{,}38\ eV =$

$= \underline{\underline{-4{,}11\ eV}}$

VII 9

Elektron m. harmosc-pot. & el-pot.

$$V(x) = \underbrace{\frac{1}{2}m\omega^2x^2}_{V_{h.o.}} + \underbrace{eEx}_{V_{el.}} = \left\{\begin{matrix}\text{kvadrat-}\\ \text{komplettera}\end{matrix}\right\} =$$

$$= \frac{1}{2}m\omega^2\left(x + \frac{eE}{m\omega^2}\right)^2 - \frac{e^2E^2}{2m\omega^2}$$

Jämför m. $V(x) = \frac{1}{2}k(x-x_0)^2 - V_0$, $\Rightarrow$

$$\Rightarrow \begin{cases} k = m\omega^2, & \text{fjäderkonst.} \\ x_0 = -\dfrac{eE}{m\omega^2}, & \text{jämviktsläge} \\ V_0 = \dfrac{e^2E^2}{2m\omega^2} & \text{-jämviktspot.} \end{cases}$$

E-spektrum: $E_n = \hbar\omega\left(n + \frac{1}{2}\right) - V_0 = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{e^2E^2}{2m\omega^2}$

VII 10

Skapelse- & förintelseoperatorer

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right), \quad a^\dagger\sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

Först: Bestäm $\hat{H}$. (Kolla om $\hbar\omega(\frac{1}{2} + a^\dagger a)$ är ok) $[x,p] = i\hbar$

$$a^\dagger a = \left(\frac{m\omega}{2\hbar}\right)\left(x - \frac{ip}{m\omega}\right)\left(x + \frac{ip}{m\omega}\right) = \frac{m\omega}{2\hbar}\left(x^2 + \frac{p^2}{m^2\omega^2} + \frac{i}{m\omega}[x,p]\right) =$$

$$= \frac{m\omega}{2\hbar}\left(x^2 + \frac{p^2}{m^2\omega^2} - \frac{\hbar}{m\omega}\right) = \frac{m\omega}{2\hbar}x^2 + \frac{p^2}{2m\hbar\omega} - \frac{1}{2}$$

$$\Rightarrow \hat{H} = \left(\frac{1}{2} + a^\dagger a\right)\hbar\omega = \hbar\omega\left(\frac{1}{2} - \frac{1}{2} + \frac{m\omega}{2\hbar}x^2 + \frac{p^2}{2m\hbar\omega}\right) = \frac{1}{2}m\omega^2x^2 + \frac{p^2}{2m}$$

OK!

... Kommutator:

$$[a, a^{\dagger}] = \frac{m\omega}{2\hbar}\left[\left(x+\frac{ip}{m\omega}\right)\left(x-\frac{ip}{m\omega}\right)-\left(x-\frac{ip}{m\omega}\right)\left(x+\frac{ip}{m\omega}\right)\right] =$$

$\left\{[x,x] = [p,p] = 0 \Rightarrow \text{kolla endast blandade termer}\right\}$

$$= \frac{m\omega}{2\hbar}\left[\frac{i}{m\omega}(-xp+px) - \frac{i}{m\omega}(xp-px)\right] =$$

$$= \frac{i}{2\hbar}(-2xp+2px) = \frac{i}{\hbar}[p,x] = \frac{i}{\hbar}(-i\hbar) = 1$$

dvs $[a, a^{\dagger}] = 1$ & $[a^{\dagger}, a] = 1 \Rightarrow aa^{\dagger} = 1 + a^{\dagger}a$ (*)

<u>Nu:</u> Kolla om $a^{\dagger}$ (a) är en skapelse- (förintelse-) operator genom att kolla om energinivån ökar (minskar) med 1 när den appliceras.

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

$$\hat{H}\psi_n = E_n\psi_n \Rightarrow \begin{cases} \hat{H}\psi_{n+1} = (E_n+\hbar\omega)\psi_{n+1} \\ \hat{H}\psi_{n-1} = (E_n-\hbar\omega)\psi_{n-1} \end{cases}$$

Alltså: Om $a^{\dagger}\psi_n = \psi_{n+1}$ och $a\psi_n = \psi_{n-1}$, så är:

$$\hat{H}a^{\dagger}\psi_n = (E_n+\hbar\omega)a^{\dagger}\psi_n \quad \text{och} \quad \hat{H}a\psi_n = (E_n-\hbar\omega)a\psi_n$$

Låt oss undersöka detta ...

$$\ldots \quad \hat{H} = \left(\tfrac{1}{2} + a^+ a\right)\hbar\omega$$

$$\Rightarrow \hat{H}\left(a^+\psi_n\right) = \hbar\omega\left(\tfrac{1}{2} + a^+ a\right)a^+\psi_n = \hbar\omega\left(\frac{a^+}{2} + a^+ a\, a^+\right)\psi_n =$$

$$\overset{(*)}{=} \hbar\omega\left(\frac{a^+}{2} + a^+(1 + a^+ a)\right)\psi_n = a^+\,\hbar\omega\left(\tfrac{1}{2} + 1 + a^+ a\right)\psi_n =$$

$$= \left(\hat{H} + \hbar\omega\right)a^+\psi_n = \left(E_n + \hbar\omega\right)a^+\psi_n$$

och:

$$\hat{H}\left(a\psi_n\right) = \hbar\omega\left(\tfrac{1}{2} + a^+ a\right)a\psi_n = \hbar\omega\left(\tfrac{1}{2} + a a^+ - 1\right)a\psi_n =$$

$$= \hbar\omega\left(\frac{a}{2} + a^+ a - a\right)\psi_n = a\left[\hbar\omega\left(\tfrac{1}{2} + a^+ a - 1\right)\right]\psi_n =$$

$$= \left(\hat{H} - \hbar\omega\right)a\psi_n = \left(E_n - \hbar\omega\right)a\psi_n$$

OK!