KVANTRÖV 6

Kap. 10 Vågpaketsrörelse & superposition av stat. tillst.

$$\Psi_n(x,t) = \Psi_n(x)\, e^{-\frac{i}{\hbar}(E_n t)}$$

statisk   mult. för att få tidsberoende!

S.E. linjär ⇒ linjär superposition av lösningar till S.E. är också lösn.

$$\Psi(x,0) = c_1\Psi_1(x) + c_2\Psi_2(x) + \dots + c_n\Psi_n(x) = \sum_{i=1}^{n} c_i\Psi_i(x)$$

$$\Psi \text{ norm.} \Rightarrow 1 = \int dV\, \Psi^*(x,0)\Psi(x,0) = \sum_{i=1}^{n}\sum_{j=1}^{n} c_i^* c_j \int dV\, \Psi_i^*(x)\Psi_j^*(x) =$$

$$= \left\{ \int dV\, \Psi_i^*\Psi_j = \delta_{ij} \right\} = \sum_{i=1}^{n} c_i^* c_i \underbrace{\int dV\, |\Psi(x)|^2}_{=1}$$

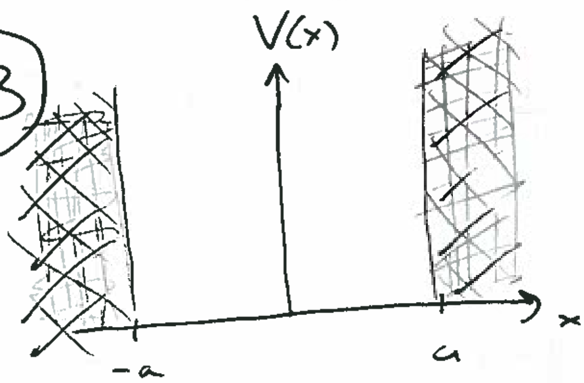
$$\text{dvs} \quad \sum_{i=1}^{n} |c_i|^2 = 1 \quad \Rightarrow \Psi(x,t) = \sum_{i=1}^{n} c_i \Psi_i(x)\, e^{-\frac{i}{\hbar}Et}$$

$$\hat{H} = \sum_{i=1}^{n} |c_i|^2 E_i$$

"vikt"

$|c_i|^2$ = sannolikhet att partikeln befinner sig i tillståndet i.

X 3



Vid viss tidpunkt:

$$\Psi(x) = A\left[1 + 4\cos\left(\frac{\pi}{a}x\right)\right] \sin\left(\frac{2\pi x}{a}\right)$$

Vilka möjliga E vid en mätning och med vilka sannolikheter?

Skriv $\Psi(x)$ som superposition av kända egenfunktioner:

$$\begin{cases} \Psi_n(x) = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{2a}\right) & \text{jämna } n \\ \Psi_n(x) = \frac{1}{\sqrt{a}} \cos\left(\frac{n\pi x}{2a}\right) & \text{udda } n \end{cases}$$

(kända lösningar till potentialgropsproblem)

...

... Skriv $\psi(x)$ som linj. komb. av dessa! Jämför m. när vi skriver ψ i termer av ψ_n...

$$\psi(x) = A\left[\sin\left(\frac{2\pi x}{a}\right) + 4\underbrace{\cos\frac{\pi x}{a}\sin\frac{2\pi x}{a}}_{=2\cos\frac{\pi x}{a}\sin\frac{\pi x}{a}}\right] = A\left(\sin\frac{2\pi x}{a} + 8\underbrace{\cos^2\frac{\pi x}{a}}_{=1-\sin^2\frac{\pi x}{a}}\sin\frac{\pi x}{a}\right) =$$

$$= A\left(\sin\frac{2\pi x}{a} + 8\sin\frac{\pi x}{a} - 8\sin^3\frac{\pi x}{a}\right) = \left\{\sin^3 x = \frac{1}{4}\left(3\sin x - \sin(3x)\right)\right\} =$$

$$= A\left[\sin\frac{2\pi x}{a} + 8\sin\frac{\pi x}{a} - 8\frac{1}{4}\left(3\sin\frac{\pi x}{a} - \sin\frac{3\pi x}{a}\right)\right] =$$

$$= A\left[\sin\frac{4\pi x}{2a} + 2\sin\frac{2\pi x}{2a} + 2\sin\frac{6\pi x}{2a}\right]$$ udda funktion

$n=4 \qquad n=2 \qquad n=6 \qquad \leftarrow (n \text{ i } \psi_n(x))$

Energiegenvärden (fr. kap. 4): $E_n = \dfrac{n^2\pi^2\hbar^2}{2m(2a)^2}$

$$\Rightarrow E_4 = \frac{2\pi^2\hbar^2}{ma^2},\quad E_2 = \frac{\pi^2\hbar^2}{2ma^2},\quad E_6 = \frac{9\pi^2\hbar^2}{2ma^2}$$

Dessa är de möjliga energierna vid mätning!

Sannolikheter $\quad \psi(x) = \sum_{i=1}^{n} c_i \psi_i(x)$ egenfkner m. $E = E_i$ och slh. $|c_i|^2$

3

$$\text{Norm.: } 1 = \int|\psi|^2 dx = A^2\int_{-a}^{a}dx\left(\sin^2\frac{2\pi x}{a} + 4\sin^2\frac{\pi x}{a} + 4\sin^2\frac{2\pi x}{a}\right) = \ldots =$$

$$= A^2 \cdot 9a \iff A = \frac{1}{3\sqrt{a}}$$

$$\psi(x) = \sum_{i=1}^{n} c_i\psi_i(x) = \frac{1}{3}\left[2\frac{1}{\sqrt{a}}\sin\left(2\frac{\pi x}{2a}\right) + \frac{1}{\sqrt{a}}\sin\left(4\frac{\pi x}{2a}\right) + 2\frac{1}{\sqrt{a}}\sin\left(6\frac{\pi x}{2a}\right)\right]$$

$$= \frac{2}{3}\psi_2(x) + \frac{1}{3}\psi_4(x) + \frac{2}{3}\psi_6(x)$$

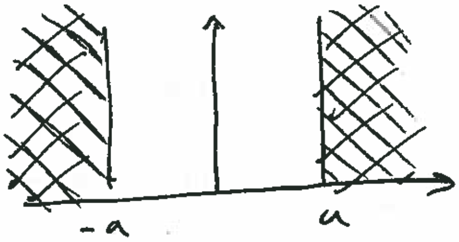
$$\Rightarrow c_2 = \frac{2}{3},\quad c_4 = \frac{1}{3},\quad c_6 = \frac{2}{3}$$

sannolikheterna!

$$\Rightarrow |c_2|^2 = \frac{4}{9},\quad |c_4|^2 = \frac{1}{9},\quad |c_6|^2 = \frac{4}{9} \qquad \left(\sum_i |c_i|^2 = 1,\ \text{OK!}\right)$$

X13

$V(x)$:



Vid $t=0$: $\Psi(x,0) = N \sin^3\left(\frac{2\pi x}{a}\right)$

Beräkna $\Psi(x,t)$!

Skriv $\Psi(x,0)$ som linj. komb. av lösningar:

$$\Psi(x,0) = N \sin^3\left(\frac{2\pi x}{a}\right) = \frac{N}{4}\left(3 \sin \frac{2\pi x}{a} - \sin \frac{6\pi x}{a}\right) =$$

$$= \frac{N}{4}\left(3\sqrt{a}\,\Psi_4(x) - \sqrt{a}\,\Psi_{12}(x)\right)$$

Norm.: $$1 = \int_{-a}^{a} dx\, \Psi^* \Psi = \left(\frac{3N\sqrt{a}}{4}\right)^2 \underbrace{\int dx\, \Psi_4^* \Psi_4}_{=1} + \left(\frac{-N\sqrt{a}}{4}\right)^2 \underbrace{\int dx\, \Psi_{12}^* \Psi_{12}}_{=1} =$$

$$= \frac{N^2 a}{16}(9+1) \Leftrightarrow N = \sqrt{\frac{16}{10a}} = \sqrt{\frac{8}{5a}}$$

Känner vågfkn. vid stat. tillst. $\Rightarrow$ tidsberoende gm. att $\times e^{-\frac{i}{\hbar}E_n t}$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2} \Rightarrow E_4 = \frac{2\pi^2 \hbar^2}{ma^2}, \quad E_{12} = \frac{18\pi^2\hbar^2}{ma^2}$$

$$\Psi(x,t) = \sqrt{\frac{8}{5}} \cdot \frac{1}{4}\left(3\Psi_4(x)\, e^{-i/\hbar}\right.$$

X 15

$\omega = \omega_{t<0} = \sqrt{\frac{k}{m}}$

$\tilde{\omega} = \omega_{t>0} = \sqrt{\frac{k}{\beta m}} = \frac{\omega}{\sqrt{\beta}}$

massändring vid $t=0$:

$m \to \beta m$

(harm. osc.)

Sökt: Sannolikhet för gr.tillst. då $t>0$ om vi har gr. tillst. då $t=0$

Känt: $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$

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

Vågfn för gr. tillst.: $\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right) e^{-\frac{m\omega}{2\hbar}x^2}$

$t<0$: Gr.-tillst.: $\psi(x,t) = \psi_0(x) e^{-\frac{i}{\hbar}E_0 t}$

$t>0$: $\tilde{\psi}(x,t) = \sum_{i=0}^{\infty} \tilde{c}_i \tilde{\psi}_i(x) e^{-\frac{i}{\hbar}\tilde{E}_i t}$

$\tilde{\psi}_0(x) = \left(\frac{\beta m\tilde{\omega}}{\hbar\pi}\right)^{1/4} e^{-\frac{\beta m\tilde{\omega}}{2\hbar}x^2}$

$\Rightarrow$ Vi söker $|\tilde{c}_0|^2$! ψ kontinuerlig i tiden

$\Rightarrow \psi(x,0) = \tilde{\psi}(x,0)$

$\Rightarrow \psi_0(x)e^0 = \sum_{i=0}^{\infty} \tilde{c}_i \tilde{\psi}_i(x) e^0$ Mult. m. $\tilde{\psi}_0^*$ och integrera:

$\Rightarrow \int dx\, \tilde{\psi}_0^* \psi_0 = \int dx\, \tilde{\psi}_0^* \sum_{i=0}^{\infty} \tilde{c}_i \tilde{\psi}_i = \sum_i \tilde{c}_i \underbrace{\int \tilde{\psi}_0^* \tilde{\psi}_i \, dx}_{\delta_{0,i}} = \tilde{c}_0$

$\Rightarrow |\tilde{c}_0|^2 = \left|\int dx\, \tilde{\psi}_0^* \psi_0\right|^2 = \left|\int_{-\infty}^{\infty} dx \left(\frac{\beta m\tilde{\omega} m\omega}{\hbar^2\pi^2}\right)^{1/4} e^{-x^2\left(\frac{\beta m\tilde{\omega}+m\omega}{2\hbar}\right)}\right|^2 =$

$= \ldots = \frac{2\beta^{1/4}}{1+\beta^{1/2}}$

X20 Ehrenfest: $\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\langle[A,H]\rangle$

Visa virialteoremet: $2\langle T\rangle = \langle \mathbf{r}\cdot\nabla V(\mathbf{r})\rangle$

(gäller för partikel i potentialfält $V(\mathbf{r})$)

$$\langle \mathbf{r}\cdot\mathbf{p}\rangle = \int \psi^*(\mathbf{r},t)\,\mathbf{r}\cdot\mathbf{p}\,\psi(\mathbf{r},t)\,dV = \left\{\psi(\mathbf{r},t) = \psi_n(\mathbf{r})e^{-\frac{i}{\hbar}E_n t}\right\}$$

$$= \int \psi_n^*(\mathbf{r})\,\mathbf{r}\cdot\mathbf{p}\,\psi_n(\mathbf{r})\,\underbrace{e^{+i/\hbar E_n t - i/\hbar E_n t}}_{=1} \quad \left(\begin{array}{c}\text{dvs}\\ \text{tidsoberoende!}\end{array}\right)$$

$$\Rightarrow \frac{d}{dt}\langle \mathbf{r}\cdot\mathbf{p}\rangle = 0 \xRightarrow{\text{Ehrenfest}} \langle[\mathbf{r}\cdot\mathbf{p},\hat{H}]\rangle = 0$$

<u>Kommutatorer</u>: $[\mathbf{r}\cdot\mathbf{p},\mathbf{p}^2] = \mathbf{p}[\mathbf{r}\cdot\mathbf{p},\mathbf{p}] + [\mathbf{r}\cdot\mathbf{p},\mathbf{p}]\mathbf{p}$,

där $[\mathbf{r}\cdot\mathbf{p},\mathbf{p}] = \mathbf{r}\underbrace{[\mathbf{p},\mathbf{p}]}_{=0} + \underbrace{[\mathbf{r},\mathbf{p}]}_{=i\hbar}\mathbf{p} = i\hbar\mathbf{p}$

$$\Rightarrow [\mathbf{r}\cdot\mathbf{p},\mathbf{p}^2] = \mathbf{p}\,i\hbar\mathbf{p} + i\hbar\mathbf{p}\mathbf{p} = 2i\hbar\,\mathbf{p}^2 \qquad \left(\text{X}10: [p,f(x)] = -i\hbar\frac{\partial f}{\partial x}\right)$$

Dessutom: $[\mathbf{r}\cdot\mathbf{p},V(\mathbf{r})] = \underbrace{[\mathbf{r},V(\mathbf{r})]}_{=0} + \mathbf{r}\underbrace{[\mathbf{p},V(\mathbf{r})]}_{=i\hbar\nabla V(\mathbf{r})} = i\hbar\,\mathbf{r}\nabla V(\mathbf{r})$

$$\Rightarrow 0 = \frac{d}{dt}\langle \mathbf{r}\cdot\mathbf{p}\rangle \overset{\text{Ehrenfest}}{=} \frac{1}{i\hbar}\langle[\mathbf{r}\cdot\mathbf{p},\underbrace{\frac{\mathbf{p}^2}{2m}+V(\mathbf{r})}_{=\hat{H}}]\rangle = \frac{1}{i\hbar}\left\langle\frac{1}{2m}2i\hbar\mathbf{p}^2 - i\hbar\mathbf{r}\nabla V(\mathbf{r})\right\rangle$$

$$= \left\langle\frac{\mathbf{p}^2}{m} - \mathbf{r}\nabla V(\mathbf{r})\right\rangle = \int\psi^*\left(\frac{\mathbf{p}^2}{m} - \mathbf{r}\nabla V(\mathbf{r})\right)\psi\,dV$$

$$\Leftrightarrow \int\psi^*\frac{\mathbf{p}^2}{m}\psi\,dV - \int\psi^*\mathbf{r}\nabla V(\mathbf{r})\psi\,dV = 0$$

$$\Leftrightarrow 2\left\langle\frac{\mathbf{p}^2}{2m}\right\rangle = \langle \mathbf{r}\cdot\nabla V(\mathbf{r})\rangle \quad \text{, V.S.V. !}$$

XI 1 a) Uppskatta g.t. tillst. för H-atomen med var.-metoden

$\psi = Ne^{-\alpha r^2}$. Strategi:

① Normering
② Beräkna $\hat{H}\psi$
③ Beräkna $\langle \hat{H} \rangle = \int dV \psi^* \hat{H} \psi$
④ Minimera $\langle \hat{H} \rangle$ m.a.p α

$\Rightarrow E_0 \leq \min_\alpha \langle \hat{H} \rangle$

① $1 = \int dV \psi^* \psi = N^2 \int_0^\infty 4\pi r^2 dr\, e^{-2\alpha r^2} =$

$= 4\pi N^2 \frac{1}{2^2(2\alpha)} \sqrt{\frac{\pi}{2\alpha}} \Leftrightarrow N^2 = \left(\frac{2\alpha}{\pi}\right)^{3/2}$

② $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r}$; $\nabla^2\psi = \Big[\Big(\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \underbrace{\frac{1}{r^2}\Big(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\big(\sin\theta\frac{\partial}{\partial\theta}\big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\Big)}_{\text{ger } 0,\ \psi \neq \psi(\theta,\varphi)}\Big)\Big]\psi =$

$= (4\alpha^2 r^2 - 6\alpha)\psi$

$\Rightarrow \hat{H}\psi = -\left[\frac{\hbar^2}{2m}(4\alpha^2 r^2 - 6\alpha) + \frac{e^2}{4\pi\varepsilon_0 r}\right]\psi$

③ $\langle \hat{H} \rangle = -4\pi N^2 \int_0^\infty r^2 dr \left[\frac{\hbar^2}{2m}(4\alpha^2 r^2 - 6\alpha) + \frac{e^2}{4\pi\varepsilon_0 r}\right] e^{-2\alpha r^2} = \ldots =$

$= \frac{3\hbar^2\alpha}{2m} - \frac{e^2}{2\pi\varepsilon_0}\sqrt{\frac{2\alpha}{\pi}}$

④ $0 = \frac{d\langle \hat{H} \rangle}{d\alpha} = \frac{3\hbar^2}{2m} - \frac{e^2}{(2\pi)^{3/2}\varepsilon_0}\frac{1}{\sqrt{\alpha}} \Rightarrow \alpha_{min} = \frac{1}{2\pi}\left(\frac{me^2}{3\hbar^2\pi\varepsilon_0}\right)^2$

(koll: $\frac{d^2\langle \hat{H} \rangle}{d\alpha^2} = \frac{1}{\alpha^{3/2}} > 0$ $\Rightarrow$ minpkt!)

$\Rightarrow E_0 \leq \min_\alpha \langle \hat{H} \rangle = -\frac{me^4}{12\hbar^2\pi^2\varepsilon_0^2} = -11{,}5\text{ eV}$

(ok, ty $E_0 = -13{,}6$ eV)

XI 2 $\quad V(r) = \frac{1}{2}kr^2 \Rightarrow$ harm. osc. (3 dim)

Ansatz: $\psi(r) = Ae^{-\alpha r}$, $H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}kr^2$

① $1 = \int d^3r\, \psi^*\psi = |A|^2 \int d^3r\, e^{-2\alpha r} = 4\pi|A|^2 \int dr\, r^2 e^{-2\alpha r} =$

$= 4\pi|A|^2 \frac{2}{(2\alpha)^3} = \frac{A^2\pi}{\alpha^3} \Leftrightarrow A^2 = \frac{\alpha^3}{\pi}$

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

$= \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi(r)) = \frac{A}{r}\frac{\partial}{\partial r}\left(e^{-\alpha r} - \alpha r e^{-\alpha r}\right) = \frac{A}{r}\left(-2\alpha e^{-\alpha r} + \alpha^2 r e^{-\alpha r}\right)$

$\Rightarrow \hat{H}\psi = -\frac{\hbar^2}{2m}\frac{A}{r}\left(-2\alpha e^{-\alpha r} + \alpha^2 r e^{-\alpha r}\right) + \frac{1}{2}kr^2 A e^{-\alpha r}$

③ $\langle\hat{H}\rangle = \int dV\, \psi^*\hat{H}\psi = A^2 \int d^3r\, e^{-\alpha r}\left(-\frac{\hbar^2}{2m}\frac{1}{r}\left(-2\alpha e^{-\alpha r} + \alpha^2 r e^{-\alpha r}\right) + \right.$

$\left. + \frac{1}{2}kr^2 e^{-\alpha r}\right) =$

$= A^2 4\pi \int dr\, r^2 e^{-2\alpha r}\left(\frac{\hbar^2}{2m}\frac{1}{r}(2\alpha - \alpha^2 r) + \frac{1}{2}kr^2\right) =$

$= A^2 4\pi \int dr\, e^{-2\alpha r}\left(\frac{\hbar^2}{m}\alpha r - \frac{\hbar^2}{2m}\alpha^2 r^2 + \frac{1}{2}kr^4\right) = \{\text{Beta}\} =$

$= A^2\left(\frac{\hbar^2\pi}{2m\alpha} + \frac{4!\,k\pi}{16\alpha^5}\right) = \frac{\alpha^2\hbar^2}{2m} + \frac{3k}{2\alpha^2}$

④ $0 = \frac{d\langle\hat{H}\rangle}{d\alpha} = \frac{\alpha\hbar^2}{m} - \frac{3k}{\alpha^3} \Rightarrow \alpha_{min} = \left(\frac{3km}{\hbar^2}\right)^{1/4}$

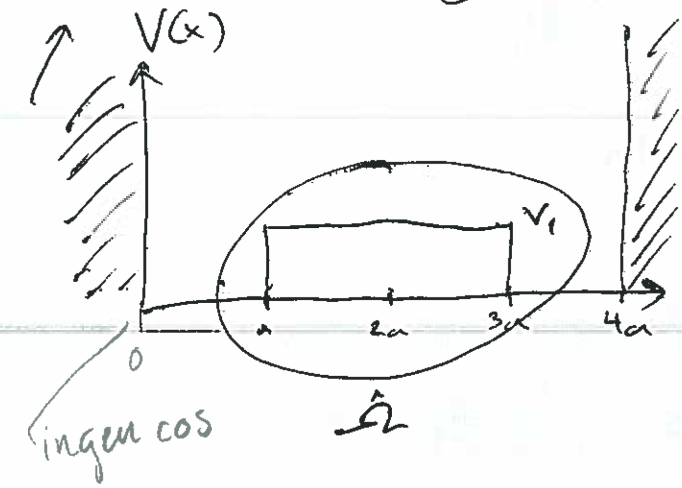
$\Rightarrow \langle\hat{H}\rangle(\alpha_{min}) = \frac{\hbar^2}{2m}\left(\frac{3km}{\hbar^2}\right)^{1/2} + \frac{3k}{2}\left(\frac{\hbar^2}{3km}\right)^{1/2} = \sqrt{3}\sqrt{\frac{k}{m}}\,\hbar = \underline{\underline{\sqrt{3}\hbar\omega \geq E_0}}$

$E_n = \hbar\omega(n_x + n_y + n_z + 3/2)$

Att jämföra med $E_0 = \frac{3}{2}\hbar\omega$: $\frac{\langle\hat{H}\rangle_{min}}{E_0} = \frac{\sqrt{3}}{3/2} = \frac{2}{\sqrt{3}} = 1,15$

(dvs 15% för stor uppskattning)

XI 5 Störningsräkning! Partikel rör sig längs x-axeln:



$V_1 << E_0$

Bestäm E m.h.a. störn. räkn.

$H\psi = E\psi$, $\hat{H} = \hat{H}^{(0)} + \hat{\Omega} =$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V^{(0)}(x) + V_1(x)$$

"partikel i låda"-pot. $\quad \hat{\Omega}$

($V_1 = 0$)

Ostörda problemet har egenfkner $\psi_n^{(0)}(x) = \frac{1}{\sqrt{2a}} \sin\left(\frac{n\pi x}{4a}\right)$

och $E_n^{(0)} = \frac{\hbar^2 \pi^2 n^2}{(4a)^2 2m}$

(lådans kant vid $x=0$ $\Rightarrow$ endast sin-fkner...)

1:a ordn. störn. räkn.: $E_n = E_n^{(0)} + \langle n | V_1 | n \rangle$, där

$$\langle n | V_1 | n \rangle = \int_{-\infty}^{\infty} \psi_n^{(0)*} V_1(x) \psi_n^{(0)} dx = V_1 \int_a^{3a} \frac{1}{2a} \sin^2\left(\frac{n\pi x}{2a}\right) dx = \ldots =$$

$$= \frac{V_1}{2} + \frac{V_1}{n\pi} \sin\left(\frac{n\pi}{2}\right)$$

$$\Rightarrow E_n = \frac{\hbar^2 \pi^2 n^2}{32 m a^2} + \frac{V_1}{2} + \frac{V_1}{n\pi} \sin\left(\frac{n\pi}{2}\right)$$