Kolikšna je verjetnost, da najdemo delec pri harm. oscilatorju v klasično prepovedanem območju za osnovno stanje?

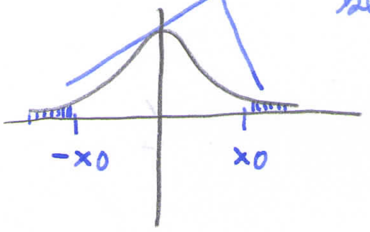
$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) \qquad \omega = \sqrt{\frac{k}{m}}$$

$$E_0 = \frac{1}{2}\hbar\omega \quad \text{- osnovno stanje} = W_{pr} = \frac{k x_0^2}{2}$$

$$\frac{1}{2}\hbar\omega = \frac{k x_0^2}{2} \sim \text{največji odmik}$$

$$x_0 = \sqrt{\frac{\hbar\omega}{k}}$$

prepovedano območje za klasičen delec => vendar ne za KV. DELEC



$$\psi_0 = \sqrt[4]{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{m\omega}{2\hbar}x^2}$$

$$P\left((x<-x_0) \wedge (x>x_0)\right) = \underline{2P(x>x_0)} \quad \text{- verjetnost}$$

$$2P(x>x_0) = 2\int_{x_0}^{\infty} \psi^*\psi\, dx =$$

$$= 2\int_{x_0}^{\infty} \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{m\omega}{\hbar}x^2} dx = \qquad +\frac{m\omega}{\hbar}x^2 = y^2$$

$$x = y\sqrt{\frac{\hbar}{m\omega}}$$

$$= \frac{2}{\sqrt{\pi}}\int^{\infty} e^{-y^2} dy \qquad dx = \sqrt{\frac{\hbar}{m\omega}}\, dy$$

$$y = \sqrt{\frac{m\omega}{\hbar}}\cdot x = \sqrt{\frac{m\omega}{\hbar}}\cdot\sqrt{\frac{\hbar\omega}{k}} =$$

$$= \sqrt{\frac{\cancel{m\omega}}{\cancel{\hbar}}\cdot\frac{\cancel{\hbar\omega}}{\cancel{\omega^2 m}}} = \underline{1}$$

$$= \underline{\frac{2}{\sqrt{\pi}}\int_{1}^{\infty} e^{-y^2} dy} = \frac{2}{\sqrt{\pi}}\int_{1}^{\infty} e^{-y^2} dy =$$

$$= \frac{2}{\sqrt{\pi}}\left(\frac{\sqrt{\pi}}{2} - \int_0^1 e^{-y^2} dy\right) =$$

$$\int_0^{\infty} e^{-y^2} dy = \int_0^1 e^{-y^2} dy + \int_1^{\infty} e^{-y^2} dy = \underline{\frac{\sqrt{\pi}}{2}}, \text{ iz Bronštejna}$$

$$= 1 - \frac{2}{\sqrt{\pi}}\int_0^1 \left(1 - y^2 + \frac{y^4}{2} - \frac{y^6}{6} \dots\right) dy =$$

$$= 1 - \frac{2}{\sqrt{\pi}}\left[y - \frac{y^3}{3} + \frac{y^5}{10} - \frac{y^7}{42} + \dots\right]\Big|_0^1 = 1 - \frac{2}{\sqrt{\pi}}\left[1 - \frac{1}{3} + \frac{1}{10} - \frac{1}{42} + \dots\right] =$$

$$= 0{,}162 = \boxed{16{,}2\,\%} \quad \text{da najdemo delec zunaj}$$

Delec je v neskončni pot. jami. $U=0$ $0<x<a$, $U=\infty$ $x>a$, $x<0$.

$\psi = N x(x-a)$ Za koliko % se energija (izračunana) razlikuje od prave? Ali je ta funkcija lastna funkcija Ham. operatorja?

$$E = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \qquad \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$\langle\psi|\psi\rangle = N^2\int_0^a x^2(x-a)^2dx = N^2\int_0^a x^2(x^2-2ax+a^2) = N^2\int_0^a (x^4-2x^3a+a^2x^2)dx =$$

$$= N^2\left(\frac{x^5}{5}-2a\frac{x^4}{4}+a^2\frac{x^3}{3}\right)\Big|_0^a = N^2\left(\frac{a^5}{5}-\frac{2a^5}{4}+\frac{a^5}{3}\right) = 1 =$$

$$= N^2\frac{12a^5-30a^5+20a^5}{60} = 1 =$$

$$= N^2\frac{+2a^5}{60} = 1$$

$$N^2 = \left(\frac{a^5}{30}\right)^{-1}$$

$$\underline{\underline{N = \sqrt{\frac{30}{a^5}}}}$$

$$\left(\sqrt{\frac{30}{a^5}}\,x(x-a)\right)'' =$$

$$= \left(\sqrt{\frac{30}{a^5}}(x-a)+\sqrt{\frac{30}{a^5}}x\right)' =$$

$$= \sqrt{\frac{30}{a^5}}+\sqrt{\frac{30}{a^5}} = \underline{\underline{2\sqrt{\frac{30}{a^5}}}}$$

$$\langle\psi|\hat{H}|\psi\rangle = \int_0^a \sqrt{\frac{30}{a^5}}\,x(x-a)\left(\frac{-\hbar^2}{2m}\,2\cdot\sqrt{\frac{30}{a^5}}\right)dx =$$

$$= \frac{-\hbar^2}{\cancel{2}m}\cdot\frac{30\cdot\cancel{2}}{a^5}\int_0^a x(x-a) =$$

$$= \frac{-\hbar^2 30}{ma^5}\int_0^a (x^2-xa)\,dx =$$

$$= \frac{-\hbar^2 30}{ma^5}\left(\frac{x^3}{3}-\frac{x^2}{2}a\right)\Big|_0^a =$$

$$= \frac{-\hbar^2 30}{ma^5}\left(\frac{a^3}{3}-\frac{a^3}{2}\right) = \frac{-\hbar^2 30}{ma^5}\left(-\frac{1}{6}a^3\right) =$$

$$= \boxed{\frac{1\hbar^2 5}{ma^2}}$$ izračunana

nadaljevanje

$\frac{\hbar^2}{8ma} = 0,125 \frac{\hbar^2}{ma^2}$ — določena E – formula!!

$\frac{0,002}{0,127} = 0,0157 = \boxed{1,6\,\%}$ razlikuje se za 1,6 %.

$\frac{\hbar^2 5}{4\pi^2 ma^2} = 0,127 \frac{\hbar^2}{ma^2}$ – izračunana E

$\psi = \sqrt{\frac{30}{a^5}}\, x(x-a)$ $\qquad \frac{\partial}{\partial x}\psi$

$\hat{H}\psi = E\psi \qquad \hat{H}\psi = \frac{-\hbar^2}{2m} 2 \sqrt{\frac{30}{a^5}} = -\frac{\hbar^2}{m}\sqrt{\frac{30}{a^5}}$

$\phi_1 = \psi_1 = x(x-a)$
$\phi_2 = \psi_2 = x^2(x-a)^2$ } iz predavanja

$H_{ij} = \langle \phi_i | \hat{H} | \phi_j \rangle$

$S_{ij} = \langle \phi_i | \phi_j \rangle$

$$\begin{vmatrix} H_{11} - S_{11}E & H_{12} - S_{12}E \\ H_{12} - ES_{12} & H_{22} - S_{12}E \end{vmatrix} = 0$$

1) $S_{11} = \int_0^a x^2 (x-a)^2 dx = \frac{30}{a^5}$

$$S_{22} = \int_0^a x^4 (x-a)^4 dx = \int_0^a (x^4 (x^4 - 4ax^3 + 6x^2a^2 - 4a^3x + a^4) dx =$$

$$= \int_0^a (x^8 - 4x^7a + 6x^6a^2 - 4x^5a^3 + x^4a^4) dx =$$

$$= \frac{x^9}{9} - \frac{4x^8}{8}a + \frac{6x^7}{7}a^2 - \frac{4x^6}{6}a^3 + \frac{x^5}{5}a^4 \Big|_0^a = \frac{a^9}{630}$$

$$S_{12} = \int_0^a x^3(x-a)^3 dx = \int_0^a x^3(x^3 - 3x^2a + 3xa^2 - a^3) dx =$$

$$= \int_0^a (x^6 - 3x^5a + 3x^4a^2 - x^3a^3) dx =$$

$$= \frac{x^7}{7} - \frac{3x^6}{6}a + \frac{3x^5}{5}a^2 - \frac{x^4}{4}a^3 \Big|_0^a =$$

$$= a^7\left(\frac{1}{7} - \frac{1}{2} + \frac{3}{5} - \frac{1}{4}\right) = \frac{a^7}{140}$$

H_{11} = energija $\rightarrow$ ✓

$\downarrow$
že izračunana,
prejšnja naloga

$$N^2 H_{11} = \frac{\hbar^2 5}{ma^2} \qquad N = \sqrt{\frac{30}{a^5}}$$

$$H_{11} = \frac{5\hbar^2}{ma^2 N^2} = \frac{5\hbar^2 a^5}{ma^3 30} = \underline{\underline{\frac{\hbar^2 a^3}{6m}}}$$

$$H_{21} = \int_0^a \overbrace{x^2(x-a)^2}^{\phi_2}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\overbrace{x(x-a)}^{\phi_1}\,dx =$$

$$= \int_0^a \left(x^2(x-a)^2\left(-\frac{\hbar^2}{2m}\right)\cdot 2\right)dx = \int_0^a \left(x^2(x-a)^2\left(-\frac{\hbar^2}{m}\right)\right)dx =$$

$$= \frac{-\hbar^2}{m}\int_0^a \left(x^4 - 2x^3 a + x^2 a^2\right)dx =$$

$$= -\frac{\hbar^2}{m}\left(\frac{x^5}{5} - \frac{2x^4}{4}a + \frac{x^3}{3}a^2\right)\Big|_0^a =$$

$$= -\frac{\hbar^2}{m}\left(\frac{a^5}{5} - \frac{2}{4}a^5 + \frac{a^5}{3}\right) =$$

$$= \frac{-\hbar^2}{m}a^5\left(\frac{1}{5} - \frac{1}{2} + \frac{1}{3}\right) = \underline{\underline{\frac{\hbar^2 a^5}{30m}}}$$

$$H_{22} = \int_0^a \underbrace{x^2(x-a)^2}_{\phi_2}\left(-\frac{\hbar^2}{2m}\frac{\partial}{\partial x^2}\right)\underbrace{x^2(x-a)^2}_{\phi_2}dx$$

$$\left(x^4 - 2x^3a + x^2a^2\right)'' = \cancel{4}\ \underline{12x - 12xa + 2a^2}$$

$$= \frac{-\hbar^2}{\cancel{2}m}\int_0^a \left(x^4 - 2x^3a + x^2a^2\right)\left(\overset{6}{\cancel{12}}x^2 - \overset{6}{\cancel{12}}xa + \overset{1}{\cancel{2}}a^2\right)dx =$$

$$= \frac{-\hbar^2}{m}\int_0^a \left(x^4 - 2x^3a + x^2a^2\right)\left(6x^2 - 6xa + a^2\right)dx =$$

$$= \frac{-\hbar^2}{m}\int_0^a \Big(6x^6 - 6x^5a + x^4a^2 - 12x^5a + 12x^4a^2 - 2x^3a^3 + 6x^4a^2 - 6x^3a^3 + x^2a^4\Big)dx =$$

$$= -\frac{\hbar^2}{m}\left(\frac{6x^7}{7} - \frac{18x^6}{6}a + \frac{19x^5}{5}a^2 - \frac{8x^4}{4}a^3 + \frac{x^3}{3}a^4\right)\Big|_0^a$$

$$= \underline{\underline{\frac{\hbar^2 a^7}{105m}}}$$

DETERMINANTA !

$$(H_{11}-S_{11}E)(H_{22}-ES_{22})-(H_{12}-ES_{12})^2=0$$

$$\left(\frac{\cancel{\hbar^2}\cancel{a^3}\cancel{m}}{6\cancel{m}}-E\cdot\frac{a^{\cancel{5}\,2}m}{30}\right)\left(\frac{\cancel{\hbar^2}\cancel{a^7}\cancel{m}}{105\cancel{m}}-E\cdot\frac{a^{\cancel{9}\,2}m}{630}\right)-\left(\frac{\cancel{\hbar^2}\cancel{a^5}\cancel{m}}{30\cancel{m}}-E\cdot\frac{a^{\cancel{7}\,2}m}{140}\right)^2=0\;\Big|\;\cdot m^2,\;:\hbar^4, a^{10}$$

$$\left(\frac{1}{6}-E\frac{a^2m}{30\hbar^2}\right)\left(\frac{1}{105}-E\cdot\frac{a^2m}{630\hbar^2}\right)-\left(\frac{1}{30}-E\frac{a^2m}{140\hbar^2}\right)^2=0$$

$$\boxed{x=\frac{Ea^2m}{\hbar^2}}\qquad\left(\frac{1}{6}-\frac{x}{30}\right)\left(\frac{1}{105}-\frac{x}{630}\right)-\left(\frac{1}{30}-\frac{x}{140}\right)^2=0$$

$$\frac{1}{6\cdot105}-\frac{x}{6\cdot630}-\frac{x}{30\cdot105}+\frac{x^2}{30\cdot630}-\left(\frac{1}{900}-\frac{\cancel{2}x}{30\cdot\cancel{140}\,70}+\frac{x^2}{140^2}\right)=0$$

$$\frac{1}{630}-\frac{x}{3780}-\frac{x}{3150}+\frac{x^2}{18900}-\frac{1}{900}+\frac{x}{2100}-\frac{x^2}{19600}=0$$

$$\frac{1}{2100}-x\frac{1}{9450}+x^2\frac{1}{529200}=0$$

$$x^2-56x+252=0$$

$$x_{1,2}=\frac{56\pm\sqrt{56^2-4\cdot252}}{2}=$$

$$x_1=51{,}065\ldots=\underline{2\cdot(14+\sqrt{133})}$$

$$x_2=4{,}935\ldots=\underline{\underline{2\cdot(14-\sqrt{133})}}\quad\text{- najnižja vrednost:}$$

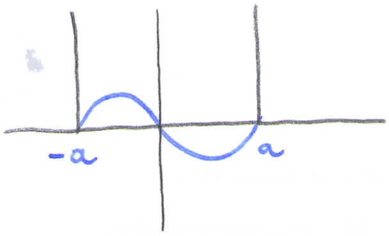
$$\boxed{x_2=4{,}93487}$$

$$E=\frac{x\cdot\hbar^2}{a^2m}=\frac{\boxed{4{,}93487}\cdot(6{,}63\cdot10^{-34})^2\to\hbar^2}{\boxed{4\pi^2}\cdot a^2m}=\underline{\underline{0{,}12500184\frac{h^2}{a^2m}}}\quad\text{- variacijska metoda}$$

$E=0{,}125$ - po Schrödingerju

$$0{,}12500184-0{,}125=\underline{0{,}00000184}$$

$$\frac{\Delta E}{E_{\text{prava}}}=\frac{0{,}00000184}{\frac{1}{8}}=0{,}00001472=\underline{\underline{0{,}001472\,\%}}$$



$$\psi_1 = x(x-a)(x+a) = x(x^2-a^2)$$

$$E = \frac{\langle \psi_1 | \hat{H} | \psi_1 \rangle}{\langle \psi_1 | \psi_1 \rangle}$$

$$\langle \psi_1 | \psi_1 \rangle = \int_{-a}^{a} \psi_1^2 \, dx = \int_{-a}^{a} x^2 (x^2-a^2)^2 \, dx =$$

$$= \int_{-a}^{a} (x^6 - 2x^4a^2 + x^2a^4) \, dx =$$

$$= \frac{x^7}{7} - \frac{2x^5}{5}a^2 + \frac{x^3}{3}a^4 \Big|_{-a}^{a} =$$

$$= \frac{a^7}{7} - \frac{2a^7}{5} + \frac{a^7}{3} - \left(\frac{-a^7}{7} - \frac{2a^7}{5} + \frac{-a^7}{3} \right) =$$

$$= 2a^7 \left(\frac{1}{7} - \frac{2}{5} + \frac{1}{3} \right) = \underline{\frac{16}{105} a^7}$$

$$\langle \psi_1 | \hat{H} | \psi_1 \rangle = \int_{-a}^{a} \psi_1 \hat{H} \psi_1 \, dx = \int_{-a} x(x^2-a^2) \left(-\frac{\hbar^2}{2m} \frac{\partial}{\partial x^2} (x(x^2-a^2)) \right) dx =$$

$$= \frac{-\hbar^2}{2m} \int_{-a}^{a} x(x^2-a^2) \, 6x \, dx = \frac{-\hbar^2}{2m} \int_{-a} (6x^4 - 6x^2a^2) \, dx =$$

$$\boxed{(x^3 - xa^2)'' = (3x^2 - a^2)' = \underline{6x}}$$

$$= \frac{-3\hbar^2}{m} \int_{-a}^{a} (x^4 - x^2a^2) \, dx =$$

$$= \frac{-3\hbar^2}{m} \left(\frac{x^5}{5} - \frac{x^3}{3}a^2 \right) \Big|_{-a}^{a} =$$

$$= \frac{-3\hbar^2}{m} \left(\frac{2a^5}{5} - \frac{2a^5}{3} \right) =$$

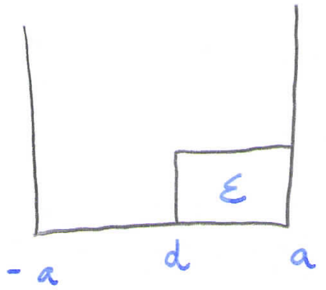
$$= \frac{-3\hbar^2 a^5}{m} \left(\frac{2}{5} - \frac{2}{3} \right) =$$

$$= \underline{\frac{4\hbar^2 a^5}{5m}}$$

$$E = \frac{\frac{4\hbar^2 a^5}{5m}}{\frac{16}{105} a^{7}} = \underline{\frac{21}{4} \frac{h^2}{4\pi^2 m a^2}} = \boxed{0{,}133 \frac{h^2}{ma^2}}$$

$$E_2 = \frac{n^2 h^2}{8m(2a)^2} = \boxed{0{,}125 \frac{h^2}{ma^2}}$$

$$\frac{0{,}008}{0{,}125} = \boxed{6{,}4\,\%}$$



Kolikšen je popravek energije 1. reda?

$$E_0 = \frac{h^2}{32 m a^2}, \quad \psi_0 = \sqrt{\frac{1}{a}}\cos\frac{\pi x}{2a} \quad \Bigg\}\ \text{osnovno stanje}$$

$$V' = H' = \begin{cases} \varepsilon, & d < x < a \\ 0, & \text{drugod} \end{cases}$$

$$E_0' = \langle \psi_0 | H' | \psi_0 \rangle = \underbrace{\int_{-a}^{d} \dots}_{\substack{0,\ \text{saj} \\ \text{je } V=0}} + \int_{d}^{a} \sqrt{\frac{1}{a}}\cos\frac{\pi x}{2a}\, \varepsilon\, \sqrt{\frac{1}{a}}\cos\frac{\pi x}{2a}\, dx =$$

$$= \frac{\varepsilon}{a}\int_{d}^{a} \cos^2\frac{\pi x}{2a}\, dx = \frac{\varepsilon}{a}\left(\frac{x}{2} + \frac{\sin \cancel{2}\cdot\frac{\pi}{\cancel{2}a}x}{\cancel{4}\cdot\frac{\pi}{\cancel{2}a}2}\right)\Bigg|_{d}^{a} =$$

$$= \frac{\varepsilon}{a}\left(\frac{x}{2} + \frac{\sin\frac{\pi x}{a}}{\frac{2\pi}{a}}\right)\Bigg|_{d}^{a} =$$

$$= \frac{\varepsilon}{a}\left(\frac{a}{2} + 0 - \frac{d}{2} - a\,\frac{\sin\frac{\pi d}{a}}{2\pi}\right) =$$

$$= \underline{\underline{\varepsilon\left(\frac{a-d}{2a} - \frac{\sin\frac{\pi d}{a}}{2\pi}\right)}} \quad \text{popravek energije}$$

Če je ε majhen, je to DOBER POPRAVEK.