ÚLOHA 1 : POTENCIÁL NABITEJ MRIEŽKY

NÁJDITE STACIONÁRNE STAVY ČASTICE V 1D POPÍSANEJ HAMILTONIÁNOM:

$$H\psi(q) = -\psi''(q) + |q|\psi(q) = \mathcal{E}\psi(q)$$

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a) ZVOLÍME SI VHODNÚ TRIEDU FUNKCIÍ A POMOCOU VARIAČNÉHO PRINCÍPU NÁJDEME ENERGIU ZÁKLADNÉHO STAVU:

NAPR: GAUSSOVKA $\psi(q) = e^{-\alpha q^2}$

EN. ZÁKL. STAVU NÁJDEME POMOCOU VARIAČNÉHO PR. AKO:

$$\mathcal{E}_0 = E[|\psi_n\rangle] = \frac{1}{\langle\psi_n|\psi_n\rangle}\langle\psi_n|\hat{H}|\psi_n\rangle$$

KDE $|\psi_n\rangle = \psi(q) = e^{-\alpha q^2}$

NORMA JE POTOM $\langle\psi_0|\psi_0\rangle = \int_{-\infty}^{\infty} e^{-2\alpha q^2}\,dq = \sqrt{\frac{\pi}{2\alpha}}$

POTOM $$\mathcal{E}_0 = \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty} e^{-\alpha q^2}\left[-\frac{d^2}{dq^2}e^{-\alpha q^2} + |q|e^{-\alpha q^2}\right]dq$$

$$= \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}\left[(1-2\alpha q^2)\,2\alpha e^{-2\alpha q^2} + |q|e^{-2\alpha q^2}\right]dq$$

- $\int_{-\infty}^{\infty} q^2 e^{-2\alpha q^2}\,dq = \frac{1}{2}\frac{\sqrt{\pi}}{(2\alpha)^{3/2}}$

- $\int_{-\infty}^{\infty} |q| e^{-2\alpha q^2}\,dq = \int_0^{\infty} q e^{-2\alpha q^2}\,dq - \int_{-\infty}^{0} q e^{-2\alpha q^2}\,dq$

$$= \frac{1}{4\alpha} + \frac{1}{4\alpha} = \frac{1}{2\alpha}$$

$$\Rightarrow \mathcal{E} = \sqrt{\frac{2\alpha}{\pi}}\left[\sqrt{2\alpha\pi} - \frac{(2\alpha)^2}{2}\frac{\sqrt{\pi}}{(2\alpha)^{3/2}} + \frac{1}{2\alpha}\right]$$

$$= 2\alpha - \frac{2\alpha}{2} + \frac{1}{\sqrt{2\pi\alpha}} = \alpha + \frac{1}{\sqrt{2\pi}}\alpha^{-1/2}$$

ABY SME ENERGIU ZÁKLADNÉHO STAVU SKUTOČNE MINIMALIZOVALI:

$$\frac{\partial \mathcal{E}}{\partial \alpha} = 1 - \frac{1}{2\sqrt{2\pi}}\,\alpha^{-3/2} = 0 \iff \alpha^{3/2} = \frac{1}{2\sqrt{2\pi}}$$

$$\iff \alpha = \frac{1}{2\sqrt[3]{\pi}}$$

POTOM ENERGIA ZÁKL. STAVU PO DOSADENÍ ZA α VYCHÁDZA

$$\boxed{\mathcal{E}_0 = \frac{3}{2}\pi^{-\frac{1}{3}} \doteq 1{,}024}$$