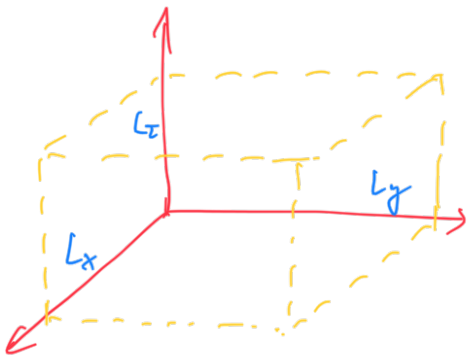
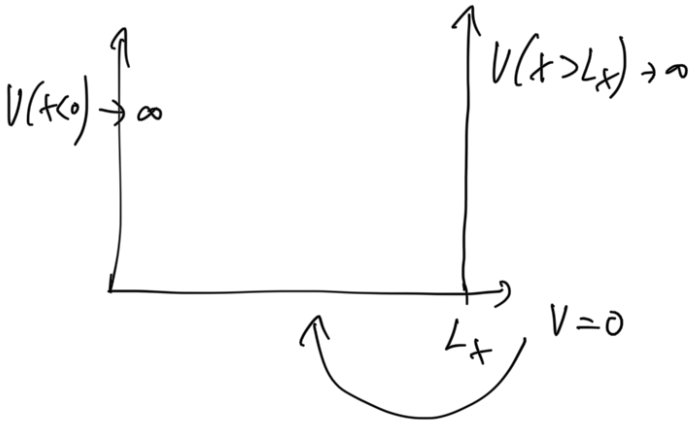
Částice v nekonečně hluboké potenciálové jámě





Schrödingerova rovnice

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z)=E\,\psi(x,y,z)$$

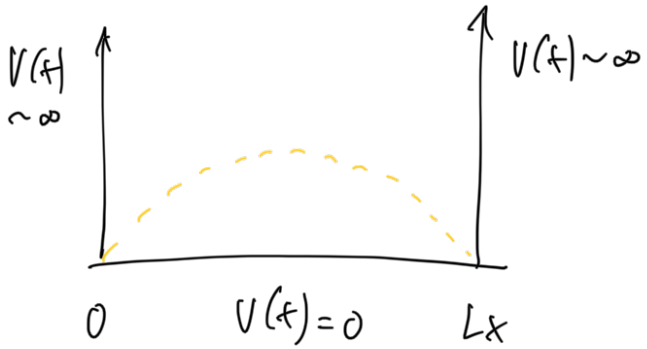
Separace proměnných

$$\psi(x,y,z)=\psi_x(x)\,\psi_y(y)\,\psi_z(z)$$

$$\frac{\partial^2}{\partial x^2}\psi(x,y,z)=\psi_y(y)\,\psi_z(z)\,\frac{\partial^2}{\partial x^2}\psi_x(x)$$

Jednorozměrný problém

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_x(x)=E\,\psi_x(x)$$



$\sin\left(\frac{\pi}{L_x} n x\right)$ $\qquad \frac{\hbar^2}{2m}\left(\frac{\pi}{L_x}\right)^2 n^2 \sin\left(\frac{\pi}{L_x} n x\right) = E \sin\left(\frac{\pi}{L_x} n x\right)$

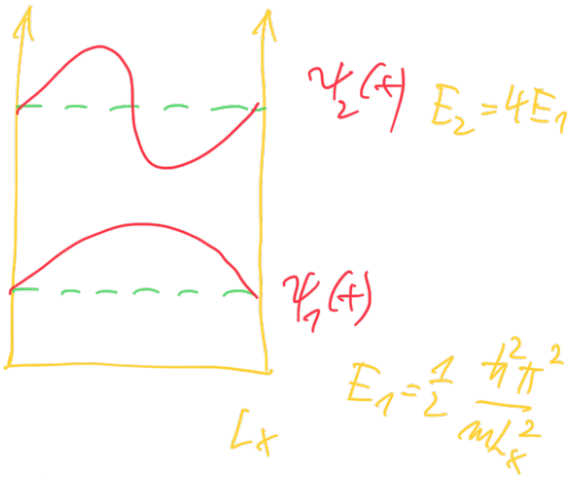
$n = 1, \dots, \infty$

$\psi_n(x) = \frac{1}{\sqrt{2}} \sin\left(\frac{\pi}{L_x} n x\right)$

$$E_n = \frac{1}{2} \frac{\hbar^2 \pi^2 n^2}{m L_x^2}$$

$n = 1$

$$E_1 = \frac{1}{2} \frac{\hbar^2 \pi^2}{m L_x^2}$$



Př: Dipólový moment $d_{21} = \langle 2 | \hat{\mu} | 1 \rangle$

$\hat{\mu} = e \hat{x}$

$$d_{21} = e \int_0^{L_x} \psi_2(x) \cdot \psi_1(x) = \frac{e}{2} \int_0^{L_x} dx \sin\left(\frac{2\pi}{L_x} x\right) \cdot \sin\left(\frac{\pi}{L_x} x\right)$$

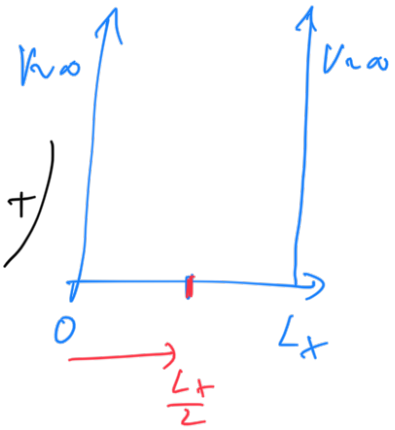
$$= \frac{e}{2} \int_0^{L_x} dx \; \frac{e^{i\frac{3\pi}{L_x}x} + e^{-i\frac{3\pi}{L_x}x} - e^{i\frac{\pi}{L_x}x} - e^{-i\frac{\pi}{L_x}x}}{-4} x$$

$$= -\frac{4 e L_x^2}{9\pi^2}$$

Obecná výšková pánička

$$\psi_n(x) = \frac{1}{\sqrt{2}} \sin\left(n \frac{\pi}{L_x} x\right)$$

$$d_{nm} = \frac{2}{L} \int_0^{L_x} dx \, \sin\left(n \frac{\pi}{L_x} x\right) (x - x_0) \sin\left(m \frac{\pi}{a} x\right)$$

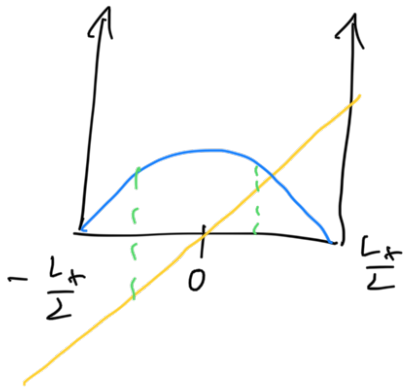


x

lichá funkce

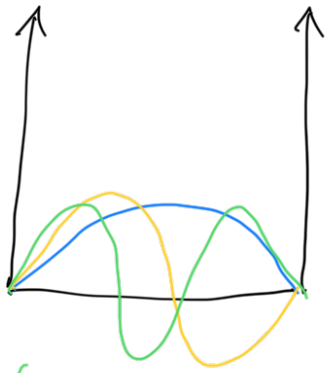
$\psi_1(x)$

sudá funkce



$$\int_{-\frac{L_x}{2}}^{\frac{L_x}{2}} f_{sudá}(x) \, f_{lichá}(x) = 0$$

$$\int_{-\frac{L_x}{2}}^{\frac{L_x}{2}} f_{sudá}(x) \, f_{lichá}(x) \neq 0$$



lichá, lichá

sudá fce	lichá fce
n	n
1	2
3	4
5	6

$+ f_{sudá} \rightarrow f_{lichá}$

$+ f_{lichá} \rightarrow f_{sudá}$

Dovolené přechody

$0 \to 1$ $\quad 1 \to 2$

$0 \to 3$ $\quad 1 \to 4$

Zakázané přechody

$0 \to 2$ $\quad 1 \to 3$

$0 \to 4$ $\quad 1 \to 5$

Operátor parity

$\hat{P}$ $\qquad \hat{P}\,\psi(+) = \psi(-+)$

$x \to -x$

$\hat{P}\,\psi_{\text{sudá}}(+) = \psi_{\text{sudá}}(+)$ ← vlastní číslo 1

$\hat{P}\,\psi_{\text{lichá}}(+) = -\psi_{\text{lichá}}(+)$ ← vlastní číslo −1

$\hat{P}\,V(+)\,\psi(+) = V(-+)\,\psi(-+) = V(+)\,\psi(-+) \equiv V(+)$

$V(+)\,\hat{P}\,\psi(+) \to [\hat{V}, \hat{P}] = 0$

$\hat{P}\,\frac{\partial^2}{\partial +^2} \to$ také komutuje

$$[\hat{H}, \hat{P}] = 0$$

⇒ společné vlastní vektory