Prosti delec v 3D

Če je delec prost, je $V=0$.

$$\hat{H}\psi = E\psi$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \cancel{V}$$

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

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

$$\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial\psi}{\partial z^2}\right)+\frac{2mE}{\hbar^2}\psi = 0 \quad /:\psi\ ; \quad k^2=\frac{2mE}{\hbar^2}$$

$$\frac{1}{\psi}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial\psi}{\partial z^2}\right)+k^2=0$$

$$\Downarrow$$

$$\boxed{\psi = X(x)\,Y(y)\,Z(z)}$$

$$\left.\begin{aligned}\frac{\partial^2\psi}{\partial x^2} &= YZ\ddot{X}\\ \frac{\partial^2\psi}{\partial y^2} &= XZ\ddot{Y}\\ \frac{\partial^2\psi}{\partial z^2} &= XY\ddot{Z}\end{aligned}\right\}$$

$$\frac{1}{XYZ}\left(YZ\ddot{X}+X\cdot Z\cdot\ddot{Y}+X\cdot Y\ddot{Z}\right)+k^2=0$$

$$\frac{\ddot{X}}{X}+\frac{\ddot{Y}}{Y}+\frac{\ddot{Z}}{Z}+k^2=0$$

$\downarrow$ konst. $\downarrow$ konst. $\downarrow$ konst. – določimo te vrednosti:

$$\frac{\ddot{X}}{X}=-k^2 \qquad \frac{\ddot{Y}}{Y}=-k^2 \qquad \frac{\ddot{Z}}{Z}=-k^2$$

$$X=A\cdot e^{ik_x x} \qquad Y=B\cdot e^{ik_y y} \qquad Z=C\cdot e^{ik_z z}$$

$$\psi = X\cdot Y\cdot Z = Ae^{ik_x x}\cdot Be^{ik_y y}\cdot Ce^{ik_z z} = ABCe^{i(k_x x+k_y y+k_z z)}$$

$$\boxed{\vec{k}=(k_x,k_y,k_z)} \qquad \boxed{\vec{r}=x,y,z}$$

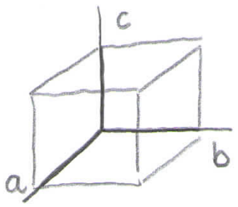
$$\boxed{\psi = D\cdot e^{i\vec{k}\vec{r}}}$$

$$\boxed{E=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2(k_x^2+k_y^2+k_z^2)}{2m}}$$

$$\underline{k^2=k_x^2+k_y^2+k_z^2}$$

Če je valovanje samo eno, gledamo v 1D. Ko imamo več valovanj v različnih smereh, moramo obravnavati 3D.

Delec v 3D neskončni pot. jami



$$V = \begin{cases} 0, & (0 \le x \le a) \wedge (0 \le y \le b) \wedge (0 \le z \le c) \\ \infty, & \text{drugače} \end{cases}$$

$$\frac{\ddot{X}}{X} + \frac{\ddot{Y}}{Y} + \frac{\ddot{Z}}{Z} + k^2 = 0$$

v 1D:

$$\frac{\psi''}{\psi} = k^2 = 0$$

$$\psi = \sqrt{\frac{2}{a}} \sin kx$$

$$k = \frac{n\pi}{a} \qquad n \in \mathbb{N}$$

$$\frac{\ddot{X}}{X} = -k_x^2 \qquad \frac{\ddot{Y}}{Y} = -k_y^2 \qquad \frac{\ddot{Z}}{Z} = -k_z^2$$

$$k_x = \frac{n_x \pi}{a} \quad n \in \mathbb{N} \qquad k_y = \frac{n_y \pi}{b} \qquad k_z = \frac{n_z \pi}{c}$$

$$X = \sqrt{\frac{2}{a}} \sin k_x k \qquad Y = \sqrt{\frac{2}{b}} \sin k_y y \qquad Z = \sqrt{\frac{2}{c}} \sin k_z z$$

gibanja v smereh x, y, z so med seboj NEODVISNA

$$\psi = X \cdot Y \cdot Z$$

$$\psi = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{b}}\sqrt{\frac{2}{c}} \sin k_x x \cdot \sin k_y y \cdot \sin k_z z$$

$$k^2 = k_x^2 + k_y^2 + k_z^2$$

$$k^2 = \left(\frac{n_x \pi}{a}\right)^2 + \left(\frac{n_y \pi}{b}\right)^2 + \left(\frac{n_z \pi}{c}\right)^2$$

$$\pi^2 \left(\left(\frac{n_x}{a}\right)^2 + \left(\frac{n_y}{b}\right)^2 + \left(\frac{n_z}{c}\right)^2 \right) = k^2$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{h^2 \pi^2 \left(\left(\frac{n_x}{a}\right)^2 + \left(\frac{n_y}{b}\right)^2 + \left(\frac{n_z}{c}\right)^2 \right)}{4\pi^2 \, 2m}$$

$$n_x, n_y, n_z \in \mathbb{N}$$

$$\boxed{E_{n_x, n_y, n_z} = \frac{h^2}{8m} \left(\left(\frac{n_x}{a}\right)^2 + \left(\frac{n_y}{b}\right)^2 + \left(\frac{n_z}{c}\right)^2 \right)}$$

$\boxed{a=b=c}$ v obliki KOCKE

$$E_{n_x, n_y, n_z} = \frac{h^2 (n_x^2 + n_y^2 + n_z^2)}{8 m a^2}$$

n_x	n_y	n_z	E	št. stanj
1	1	1	$\frac{3h^2}{8ma^2}$	1
1	1	2	$\frac{6h^2}{8ma^2}$	3
1	2	1	-ll-	
2	1	1	-ll-	
1	2	2	$\frac{9h^2}{8ma^2}$	3
2	1	2	-ll-	
2	2	1	-ll-	

3 ← degeneracija tega nivoja (npr. 2. nivoja je 3)