Schrödingerova rovnice v souřadnicové reprezentaci

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

$\leftarrow$ 1D

$$\langle \vec{r}|\hat{H}|\psi\rangle = E\langle \vec{r}|\psi\rangle$$

1D:

$$\langle x|\psi\rangle = \psi(x) \quad \Rightarrow \quad \text{P. S.} \quad E\langle x|\psi\rangle = E\,\psi(x)$$

Levá strana

$$\langle x|\hat{H}\int dx'\,|x'\rangle\langle x'|\psi\rangle = \int dx'\,\langle x|\hat{H}|x'\rangle\,\psi(x')$$

$$\langle x|\hat{H}|x'\rangle = \int dp\,\frac{p^2}{2m}\langle x|p\rangle\langle p|x'\rangle + \int dq\,V(q)\langle x|q\rangle\langle q|x'\rangle$$

$$= \int dp\,\frac{p^2}{2m}\,\frac{1}{2\pi\hbar}\,e^{\frac{i}{\hbar}px - \frac{i}{\hbar}px'} + \int dq\,V(q)\,\delta(x-q)\,\delta(x'-q)$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\int dp\,\frac{e^{\frac{i}{\hbar}p(x-x')}}{2\pi\hbar} + V(x)\,\delta(x-x')$$

$$\Rightarrow \quad \int dx'\,\langle x|\hat{H}|x'\rangle\,\psi(x') = \int dx'\,V(x)\,\delta(x-x')\,\psi(x')$$

$$+ \int dx'\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\delta(x-x')\,\psi(x')$$

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

$\Rightarrow$

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

1D - Schrödingerova rovnice

Ve 3D a 1 částice

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

Δ, D^2