3.1

$$\hat{H} = \frac{\vec{p}^2}{2m} + V(\vec{r})$$

$$-i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \hat{H}\psi(\vec{r},t)$$

$$= -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t)$$

$$\psi(\vec{r},t) = e^{-\frac{iEt}{\hbar}}\psi_E(\vec{r})$$

$$\hat{H}\psi_E(\vec{r}) = E\psi_E(\vec{r})$$

3.2

$$\psi_{\vec{p}}(\vec{r}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$$

$$[\hat{p}_i, \hat{H}] = 0$$

$$e^{\frac{i}{\hbar}p_x x}\quad e^{\frac{i}{\hbar}p_y y}\ \ldots$$

$$\vec{p}\,\psi_{\vec{p}}(\vec{r}) = \vec{p}\,\psi_{\vec{p}}(\vec{r})$$

$$\int d^3r\, \psi^*_{\vec{p}'}(\vec{r})\psi_{\vec{p}}(\vec{r}) = \delta(\vec{p}-\vec{p}')$$

$$= \delta(p_x - p_x')\delta(p_y - p_y')\delta(p_z - p_z')$$

3.3 Box. $x \in [0, L_x]$

$y \in [0, L_y]$

$z \in [0, L_z]$

Pot. energie $= +\infty$ buiten box

1-D: $\chi(x) = \sqrt{\frac{2}{L_x}}\sin kx$

$\chi(0) = \chi(L_x) = 0$

$\Rightarrow k = \frac{\pi}{L}n,\ n = 1, 2, \ldots$

$$\left\{ \begin{array}{l} \psi_{\vec{k}}(\vec{r}) = \left(\frac{8}{V}\right)^{\frac{1}{2}}(\sin k_x x)(\sin k_y y)\sin(k_z z) \\ k_x = \frac{\pi}{L_x}n_x,\ k_y = \frac{\pi}{L_y}n_y,\ k_z = \frac{\pi}{L}n_z \end{array}\right.$$

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

3.4 Centrale potentiaal

$$\left(\vec{a}\times(\vec{b}\times\vec{c})\right) = (\vec{a}\cdot\vec{c})\vec{b} - (\vec{a}\cdot\vec{b})\vec{c}$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(r) \rightarrow \text{invariant onder rotatie}$$

$$[\hat{L}_i, V(r)] = 0$$

$\rightarrow$ Laplaciaan in sferische coördinaten?

$$\vec{L}^2 = (\vec{r}\times\vec{p})^2 = p^2r^2 - (\vec{r}\cdot\vec{p})^2$$

$$(\underbrace{\vec{r}}_{a}\times\vec{p})\cdot(\underbrace{\vec{r}}_{b}\times\underbrace{\vec{p}}_{c}) = \vec{r}\cdot(\vec{p}\times(\vec{r}\times\vec{p}))$$

$$= \vec{r}\cdot\left((\vec{p}^2)\vec{r} - (\vec{p}\cdot\vec{r})\vec{p}\right)$$

$$= p^2r^2 - (\vec{r}\cdot\vec{p})^2$$

$$\vec{p}^2 = \frac{1}{r^2}(\vec{r}\cdot\vec{p})^2 + \frac{1}{r^2}\vec{L}^2$$

$$= \underbrace{\left(\frac{\vec{r}}{r}\cdot\vec{p}\right)}_{p_r}{}^2 + \frac{\vec{L}^2}{r^2}$$

$\cancel{\hat{p}_r = -i\hbar\frac{\partial}{\partial r}}$: Niet Hermitisch

$$\left[\int_0^\infty dr\, r^2\varphi(r)\left(-i\hbar\frac{\partial}{\partial r}\right)\chi(r)\right]^*$$

$$\overset{?}{=} \int_0^\infty dr\, r^2\left(-i\hbar\frac{\partial}{\partial r}\right)\chi(r)$$

$$\rightarrow i\hbar\int dr\, r^2\varphi(r)\frac{\partial}{\partial r}\chi(r)$$

$$= -i\hbar\int_0^\infty dr\left(\frac{\partial}{\partial r}r^2\varphi(r)\right)\chi(r) + \cancel{i\hbar\, r^2\varphi\chi\Big|_0^\infty}$$

$$\int d^3r\, \underbrace{\Phi^*(\vec{r})\hat{\vec{p}}\chi(\vec{r})}_{\varphi(r)Y_{\ell' m'}(\theta,\varphi)|\chi(r)Y_{\ell m}(\theta,\varphi)} = \left[\int_0^\infty dr\, r^2\varphi(r) - i\hbar\frac{\partial}{\partial r}\chi(r)\right]$$

$$\left[\times\int d\Omega\, Y^*_{\ell' m'}(\Omega)Y_{\ell m}(\Omega)\right]$$

Klassiek $p_r = \frac{\vec{r}}{r}\cdot\vec{p} = \frac{1}{2}\left(\frac{\vec{r}}{r}\cdot\vec{p} + \vec{p}\cdot\frac{\vec{r}}{r}\right)$

$$\left(\begin{array}{l} \text{Q.M.}: A = A^\dagger,\ B = B^\dagger \\ (AB)^\dagger = B^\dagger A^\dagger = BA \\ \frac{1}{2}(AB + BA) \end{array}\right)$$

$$\hat{p}_r = \frac{1}{2}\left(\frac{\vec{r}}{r}\cdot\vec{p} + \vec{p}\cdot\frac{\vec{r}}{r}\right)$$

$$= \frac{1}{2}\left(2\frac{\vec{r}}{r}\hat{\vec{p}} + \left[\hat{\vec{p}}, \frac{\vec{r}}{r}\right]\right)$$

$$\left[\hat{\vec{p}}\cdot,\frac{\vec{r}}{r}\right] = \sum_i\left[\hat{p}_i, \frac{r_i}{r}\right] = -\frac{2i\hbar}{r}$$

$$\hat{p}_r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

$$\Rightarrow \left[\int_0^\infty dr\, r^2\varphi(r)(-i\hbar)\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\chi(r)\right]^*$$

$$= i\hbar\left[-\int_0^\infty dr\left(\frac{\partial}{\partial r}r^2\varphi\right)\chi(r) + \int_0^\infty dr\, r^2\varphi(r)\frac{1}{r}\chi(r)\right)$$

$$= i\hbar\left[-\int_0^\infty dr\, \cancel{2}r\varphi\chi + \left(r^2\frac{\partial}{\partial r}\varphi\right)\chi + r^2\varphi(r)\frac{1}{r}\chi\right]$$

$$= \int_0^\infty dr\, r^2\left[-i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\varphi(r)\right]\chi(r)$$

$$\left[p_i, \frac{r_i}{r}\right] = -i\hbar\left[\frac{\partial}{\partial r_i}, \frac{r_i}{r}\right]$$

$$= -i\hbar\frac{\partial}{\partial r_i}\left(\frac{r_i}{r}\right)$$

$$= -i\hbar\left(\frac{1}{r} - \frac{r_i}{r^2}\underbrace{\frac{\partial}{\partial r_i}\left(\frac{1}{\sqrt{x^2+y^2+z^2}}\right)}_{L\rightarrow\frac{r_i}{r}}\right)$$

$$= -i\hbar\left(\frac{1}{r} - \frac{r_i^2}{r^3}\right)$$

$$\sum_i = -i\hbar\left(\frac{3}{r} - \frac{1}{r}\right)$$

$$[r, \hat{p}_r] = i\hbar = \left[r, -i\hbar\left(\frac{\partial}{\partial r} + \cancel{\frac{1}{r}}\right)\right]$$

$$\hat{p}_r^2 = (-i\hbar)^2\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial}{\partial r}\frac{1}{r}\right)$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \cancel{\frac{1}{r^2}} + \frac{2}{r}\frac{\partial}{\partial r} - \cancel{\frac{1}{r^2}}\right)$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)$$

$$\vec{p}^2 = \hat{p}_r^2 + \frac{\vec{L}^2}{r^2} \rightarrow \hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\vec{L}^2}{2mr^2} + V(r)$$

$$[\hat{H}, \hat{L}_i] = 0 \rightarrow \hat{H}, \hat{L}^2, \hat{L}_z$$

$$\langle r\theta\varphi|E\ell m\rangle = R_{E\ell}(r)Y_{\ell m}(\theta,\varphi)$$

$\rightarrow$ radiale golffunctie

$$\left\{-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + V(r)\right\}R_{E\ell}(r)$$

$$= E_\ell R_{E\ell}(r) \rightarrow (2\ell+1)\text{-voudig}$$