$$\hat{H} = -\frac{\hbar^2}{2m}\underbrace{\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)}_{\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} = \frac{1}{r^2}\left(r^2\frac{\partial^2}{\partial r^2} + 2r\frac{\partial}{\partial r}\right)} + \frac{\hat{L}^2}{2mr^2} + V(r)$$

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

→ behoud hoekafh.

Gemeenschappelijke eigenbasis van $\hat{H}, \hat{L}^2, \hat{L}_z$?

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

$$\hat{H}|E\ell m\rangle = E|E\ell m\rangle$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\right)R_{E\ell}(r)Y_{\ell m}(\theta,\varphi) + \frac{\overbrace{\hat{L}^2}^{\hbar^2\ell(\ell+1)}}{2mr^2}R_{E\ell}(r)Y_{\ell m}(\theta,\varphi) + V(r)R_{E\ell}(r)Y_{\ell m}(\theta,\varphi) = E R_{E\ell}(r)Y_{\ell m}(\theta,\varphi)$$

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

→ $(2\ell+1)$voudig ontaard

$V(r) \to 0$ voor $r \to +\infty$

$V(r)$ voor $r \to 0$; maar niet singulierder dan $\frac{1}{r}$

$$1 = \left(\int_0^\infty dr\, r^2 (R_{E\ell}(r))^2\right)\cancel{\left(\int d\Omega\, Y^*_{\ell m}(\Omega) Y_{\ell m}(\Omega)\right)}$$

"gereduceerde golffunctie"

$$u_{E\ell}(r) = r R_{E\ell}(r)$$

$$\int_0^\infty dr\, (u_{E\ell}(r))^2 = 1$$

$$\frac{d^2}{dr^2}R_{E\ell} + \frac{2}{r}\frac{d}{dr}R_{E\ell} = \frac{1}{r^2}\frac{d}{dr}r^2\underbrace{\frac{d}{dr}\left(\frac{1}{r}u\right)}_{\frac{1}{r}u' - \frac{1}{r^2}u}$$

$$= \frac{1}{r^2}\frac{d}{dr}(ru' - u)$$

$$= \frac{1}{r^2}(ru'' + u' - u')$$

$$-\frac{\hbar^2}{2m}\left(\cancel{\frac{1}{r}}u''\right) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\frac{u}{\cancel{r}} + V(r)\frac{u}{\cancel{r}} = E\frac{u}{\cancel{r}}$$

$$-\frac{\hbar^2}{2m}u''_{E\ell} + \underbrace{\left(\frac{\hbar^2\ell(\ell+1)}{2mr^2} + V(r)\right)}_{V_{eff}(r)}u_{E\ell}(r) = E_\ell\, u_{E\ell}(r)$$

Randvoorwaarden $R_{E\ell}(0)$ is eindig, dus $u_{E\ell}(0) = 0$

Gedrag bij $r \to 0$: $V(r) = r^p(b_0 + b_1 r + \ldots)$ met $p \geq -1$; $b_0 \neq 0$

$$u_{E\ell}(r) - r^s(c_0 + c_1 r + c_2 r^2 + \ldots) \text{ met } c_0 \neq 0$$

$$-\frac{\hbar^2}{2m}\left(s(s-1)c_0 r^{s-2} + (s+1)sc_1 r^{s-1} + \ldots\right) + \frac{\ell(\ell+1)\hbar^2}{2m}\left(c_0 r^{s-2} + c_1 r^{s-1}\ldots\right) + \underbrace{r^p(b_0 + b_1 r + \ldots)\, r^s(c_0 + c_1 r + \ldots)}_{r^{p+s} \text{ en } p \geq -1} = E_\ell\, r^s\cancel{(c_0 + c_1 r + \ldots)}$$

$$s + p \geq s - 1$$

$$-s(s-1)c_0 + \ell(\ell+1)c_0 = 0$$

$$s(s-1) - \ell(\ell+1) = 0$$

$$s^2 - \ell^2 - s - \ell = 0$$

$$(s+\ell)(s-\ell-1) = 0$$

~~1) $s = -\ell$ kan niet $u \to r^{-\ell}$, $R \to r^{-\ell-1}$ → voor $r \to 0$~~

2) $s = \ell + 1 \Rightarrow u \to r^{\ell+1}$, $R \to r^\ell$

→ Reguliere oplossing

Pariteit van $\psi_{E\ell m}(r,\theta,\varphi) = R_{E\ell}(r) Y_{\ell m}(\theta,\varphi)$

$$\hat{P}: \vec{r} \to -\vec{r}$$

$$\psi_{E\ell m}(-\vec{r}) = R_{E\ell}(r) Y_{\ell m}(\pi-\theta, \varphi+\pi)$$

$$= (-1)^\ell R_{E\ell}(r) Y_{\ell m}(\theta,\varphi)$$

$$= (-1)^\ell \psi_{E\ell m}(\vec{r})$$

$$\left\{-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \frac{\ell(\ell+1)\hbar^2}{r^2\, 2m}\right\}R_{E\ell}(r) = E R_{E\ell}(r) \quad \Big|\times -\frac{2m}{\hbar^2}$$

$$\left\{\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} + k^2\right\}R_{E\ell}(r) = 0 \quad \text{met } k^2 = \frac{2mE}{\hbar^2}$$

$$E = \frac{\hbar^2 k^2}{2m}$$

(a) $\underline{\ell = 0}$ $\quad \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + k^2\right)R_{k0} = 0$

$$u_{k0} = rR_{k0} \to \boxed{u'' + k^2 u_{k0}(r) = 0}$$

$$u_{k0}(r) \sim \sin(kr) \text{ of } \cos(kr)$$

$$R_{k0}(r) \sim \frac{\sin(kr)}{r} \text{ of } \frac{\cos(kr)}{r}$$

$$R_{k0}(r) = C_{k0}\frac{\sin kr}{r}$$

Wat met $\ell > 0$?

Definieer: $R_{k\ell}(r) = r^\ell X_{k\ell}(r)$

$$R'_{k\ell} = \ell r^{\ell-1}X_{k\ell} + r^\ell X'_{k\ell}$$

$$R''_{k\ell} = \ell(\ell-1)r^{\ell-2}X_{k\ell} + 2\ell r^{\ell-1}X'_{k\ell} + r^\ell X''_{k\ell}$$

En $\boxed{R''_{k\ell} + \frac{2}{r}R'_{k\ell} - \frac{\ell(\ell+1)}{r^2}R_{k\ell} + k^2 R_{k\ell} = 0}$

$$\cancel{\ell(\ell-1)r^{\ell-2}X_{k\ell}} + 2\ell r^{\ell-1}X'_{k\ell} + r^\ell X''_{k\ell} + \frac{2}{r}\ell r^{\ell-1}X_{k\ell} + 2r^{\ell-1}X'_{k\ell} + \left(k^2 - \frac{\ell(\ell+1)}{r^2}\right)r^\ell X_{k\ell} = 0$$

$$\cancel{r^{\ell-2}X_{k\ell}(r)\left(\ell(\ell-1) + 2\ell - \ell(\ell+1)\right)}$$

$$\to r^{\ell-1}X'_{k\ell}\, 2(\ell+1) + k^2 r^\ell X_{k\ell} + r^\ell X''_{k\ell} = 0$$

$$X''_{k\ell} + \frac{2(\ell+1)}{r}X'_{k\ell} + k^2 X_{k\ell} = 0$$