POLITECHNIKA GDAŃSKA

Chemia teoretyczna

Wybrane wyprowadzenia

Wykład 5. Postulaty mechaniki kwantowej, nieoznaczoność

Operator energii $\hat{E}$:

$$\Psi = \mathrm{e}^{\mathrm{i}(kx-\omega t)}$$

$$\frac{\partial \Psi}{\partial t} = -\mathrm{i}\omega \mathrm{e}^{\mathrm{i}(kx-\omega t)} = -\mathrm{i}\omega\Psi$$

$$E = h\nu = \hbar\omega$$

$$\omega = \frac{E}{\hbar}$$

$$\frac{\partial \Psi}{\partial t} = -\mathrm{i}\frac{E}{\hbar}\Psi$$

$$-\frac{\hbar}{\mathrm{i}}\frac{\partial \Psi}{\partial t} = E\Psi$$

$$E\Psi = \mathrm{i}\hbar\frac{\partial \Psi}{\partial t}$$

$$\hat{E} = \mathrm{i}\hbar\frac{\partial}{\partial t}$$

Równanie Schrödingera niezależne od czasu:

$$\hat{H}\Psi = \mathrm{i}\hbar\frac{\partial}{\partial t}\Psi$$

$$\Psi(q,t) = \psi(q)\cdot\varphi(t)$$

$$\hat{H}\psi\varphi = \mathrm{i}\hbar\frac{\partial}{\partial t}\psi\varphi$$

$$\varphi\hat{H}\psi = \mathrm{i}\hbar\psi\frac{\partial\varphi}{\partial t} \;|:\psi\varphi$$

$$\frac{1}{\psi}\hat{H}\psi = \frac{\mathrm{i}\hbar}{\varphi}\frac{\partial\varphi}{\partial t}$$

$$\frac{\mathrm{i}\hbar}{\varphi}\frac{\partial\varphi}{\partial t} = C$$

$$\frac{\partial\varphi}{\partial t} = \frac{C}{\mathrm{i}\hbar}\varphi \;|\cdot -\mathrm{i}^2$$

$$\frac{\partial\varphi}{\partial t} = -\frac{\mathrm{i}C}{\hbar}\varphi$$

$$\frac{\partial\varphi}{\partial t} = -\frac{\mathrm{i}C}{\hbar}\varphi$$

$$\varphi = \mathrm{e}^{-\frac{\mathrm{i}C}{\hbar}t}$$

$$\varphi = \mathrm{e}^{\mathrm{i}(kx-\omega t)}$$

$$x = 0$$

$$\mathrm{e}^{-\mathrm{i}\frac{C}{\hbar}t} = \mathrm{e}^{-\mathrm{i}\omega}$$

$$\frac{C}{\hbar} = \omega$$

$$E = h\nu = h\frac{\omega}{2\pi} = \hbar\omega$$

$$C = E$$

$$\varphi = \mathrm{e}^{-\frac{\mathrm{i}E}{\hbar}t}$$

$$\Psi = \varphi\psi = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\psi$$

$$\hat{H}\Psi = \mathrm{i}\hbar\frac{\partial}{\partial t}\Psi$$

$$\hat{H}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\psi = \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\psi$$

$$\hat{H}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\psi = \mathrm{i}\hbar\left(-\frac{\mathrm{i}}{\hbar}E\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\right)\psi$$

$$\hat{H}\psi = \mathrm{i}\hbar\left(-\frac{\mathrm{i}}{\hbar}E\right)\psi$$

$$\hat{H}\psi = -\mathrm{i}^2 E\psi$$

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

Wykład 7. Cząstka w jednowymiarowej studni potencjału

Operator energii kinetycznej:

$$T = \frac{mv^2}{2}$$

$$\vec{p} = m\vec{v}$$

$$T = \frac{p^2}{2m}$$

$$\vec{p} \leftarrow \hat{p} = -\mathrm{i}\hbar\nabla$$

$$\hat{T} = \frac{1}{2m}(-\mathrm{i}\hbar\nabla)^2 = \mathrm{i}^2\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\nabla^2$$

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

Normalizacja:

$$\int \sin^2 ax \,\mathrm{d}x = \frac{x}{2} - \frac{\sin 2ax}{4a}$$

$$\int_0^L \psi^2 \,\mathrm{d}x = 1$$

POLITECHNIKA GDAŃSKA

$$\psi^2 = c_1^2 \sin^2\left(\frac{n\pi x}{L}\right)$$

$$c_1^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) \mathrm{d}x$$

$$c_1^2 \left[\frac{x}{2} - \frac{\sin\frac{2n\pi x}{L}}{\frac{4n\pi}{L}}\right]_0^L$$

$$c_1^2 \left[\frac{x}{2} - \frac{L\sin\frac{2n\pi x}{L}}{4n\pi}\right]_0^L$$

$$c_1^2 \frac{L}{2} = 1$$

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

Energie stanów stacjonarnych:

$$[\sin ax]' = a\cos ax$$

$$[\sin ax]'' = -a^2 \sin ax$$

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left[\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)\right] = E\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left[\sin\left(\frac{n\pi}{L}x\right)\right] = E\sin\left(\frac{n\pi}{L}x\right)$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left[\sin\left(\frac{n\pi}{L}x\right)\right] = E\sin\left(\frac{n\pi}{L}x\right)$$

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

$$E = \left(\frac{h}{2\pi}\right)^2 \frac{n^2\pi^2}{2mL^2}$$

$$E = \frac{h^2 n^2}{8mL^2}$$

POLITECHNIKA GDAŃSKA

Wykład 9. Oscylator harmoniczny

Równanie Schrödingera:

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

$$(\hat{T} + \hat{V})\psi = E\psi$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{kx^2}{2}\right)\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{k}{2}x^2\psi = E\psi$$

Próbne rozwiązanie szczególne:

$$\left[\mathrm{e}^{f(x)}\right]' = f'(x)\mathrm{e}^{f(x)}$$

$$\psi_0 = N_0\mathrm{e}^{-ax^2}$$

$$\frac{\mathrm{d}\psi_0}{\mathrm{d}x} = N_0(-2ax)\mathrm{e}^{-ax^2} = -2ax\psi_0$$

$$\frac{\mathrm{d}^2\psi_0}{\mathrm{d}x^2} = -2a[x\psi_0]' = -2a(\psi_0 + x\psi_0') = -2a(\psi_0 - 2ax^2\psi_0) = (-2a + 4a^2x^2)\psi_0$$

Powrót do równania Schrödingera:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{k}{2}x^2\psi = E\psi$$

$$-\frac{\hbar^2}{2m}(-2a + 4a^2x^2)\psi_0 + \frac{k}{2}x^2\psi_0 = E_0\psi_0$$

$$-\frac{\hbar^2}{2m}(-2a + 4a^2x^2) + \frac{k}{2}x^2 = E_0$$

$$\frac{a\hbar^2}{m} - \frac{2a^2\hbar^2}{m}x^2 + \frac{k}{2}x^2 = E_0$$

Stan stacjonarny:

$$E_0 = const.$$

$$\frac{a\hbar^2}{m} - \frac{2a^2\hbar^2}{m}x^2 + \frac{k}{2}x^2 = E_0$$

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

$$4a^2\hbar^2 = km$$

$$a = \sqrt{\frac{km}{4\hbar^2}} = \frac{\sqrt{km}}{2\hbar}$$

Normalizacja:

$$\int_0^\infty \mathrm{e}^{-Cx^2}\,\mathrm{d}x = \frac{\sqrt{\pi}}{2\sqrt{C}}$$

$$\int_0^\infty |\psi|^2\,\mathrm{d}x = 1$$

$$\psi_0 = N_0 \mathrm{e}^{-ax^2}$$

$$\psi_0^2 = N_0^2 \mathrm{e}^{-2ax^2}$$

$$\int_0^{\infty} N_0^2 \mathrm{e}^{-2ax^2}\,\mathrm{d}x = N_0^2 \int_0^{\infty} \mathrm{e}^{-2ax^2}\,\mathrm{d}x = N_0^2 \frac{\sqrt{\pi}}{2\sqrt{2a}}$$

$$\int_0^{\infty} |\psi|^2\,\mathrm{d}x = 1$$

$$N_0^2 \frac{\sqrt{\pi}}{2\sqrt{2a}} = 1$$

$$N_0^2 = \frac{2\sqrt{2a}}{\sqrt{\pi}}$$

$$\psi_0 = \sqrt[4]{\frac{8a}{\pi}}\,\mathrm{e}^{-ax^2}$$

$$a = \frac{\sqrt{km}}{2\hbar}$$

Energia poziomu zerowego:

$$\frac{a\hbar^2}{m} - \frac{2a^2\hbar^2}{m}x^2 + \frac{k}{2}x^2 = E_0$$

$$E_0 = \frac{a\hbar^2}{m} = \frac{\frac{\sqrt{km}}{2\hbar}\hbar^2}{m} = \frac{\hbar\sqrt{km}}{2m} = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$$

$$E_0 = \frac{1}{2}\hbar\omega = \frac{1}{2}h\nu$$

Wykład 10. Cząstka na okręgu

Rozwiązanie równania Schrödingera dla cząstki na okręgu:

$$-\frac{\hbar^2}{2I}\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}\psi = E\psi$$

$$\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}\psi = -\frac{2IE}{\hbar^2}\psi$$

$$\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}\psi = -m_l^2\psi$$

$$\psi = N\mathrm{e}^{\mathrm{i}m_l\varphi}$$

Warunek brzegowy i normalizacja:

$$\psi(\varphi) = \psi(\varphi + 2\pi)$$

$$N\mathrm{e}^{\mathrm{i}m_l\varphi} = N\mathrm{e}^{\mathrm{i}m_l(\varphi+2\pi)}$$

$$\mathrm{e}^{\mathrm{i}m_l\varphi} = \mathrm{e}^{\mathrm{i}m_l\varphi}\mathrm{e}^{\mathrm{i}m_l 2\pi}$$

$$\left(\mathrm{e}^{\pi\mathrm{i}}\right)^{2m_l} = 1$$

$$(-1)^{2m_l} = 1$$

$$m_l \in \mathbb{Z}$$

$$\int_0^{2\pi} |\psi|^2 \, \mathrm{d}\varphi = 1$$

$$\int_0^{2\pi} \psi^* \, \psi \, \mathrm{d}\varphi = \int_0^{2\pi} N\mathrm{e}^{-\mathrm{i}m_l\varphi} N\mathrm{e}^{\mathrm{i}m_l\varphi} \, \mathrm{d}\varphi = N^2 \int_0^{2\pi} \mathrm{d}\varphi = N^2 \cdot 2\pi$$

$$N = \frac{1}{\sqrt{2\pi}}$$

Ostatecznie:

$$\psi = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}m_l\varphi}$$

lub

$$\psi = \frac{1}{\sqrt{2\pi}} (\cos m_l\varphi + \mathrm{i} \sin m_l\varphi)$$

gdzie:

$$m_l = 0, \pm 1, \pm 2, \pm 3, \ldots$$

Wykład 11. Cząstka w dwuwymiarowej studni potencjału

Normalizacja funkcji falowej w prostokątnej nieskończonej studni potencjału:

$$\iint_\Omega |\psi|^2 \, \mathrm{d}\tau = 1$$

$$\int_0^{L_y} \int_0^{L_x} \psi^2 \, \mathrm{d}x \, \mathrm{d}y = 1$$

$$\psi = N \sin\left(\frac{n_x \pi}{L_x} x\right) \sin\left(\frac{n_y \pi}{L_y} y\right)$$

$$\psi^2 = N^2 \sin^2\left(\frac{n_x \pi}{L_x} x\right) \sin^2\left(\frac{n_y \pi}{L_y} y\right)$$

$$\int_0^{L_y} \int_0^{L_x} N^2 \sin^2\left(\frac{n_x \pi}{L_x} x\right) \sin^2\left(\frac{n_y \pi}{L_y} y\right) \mathrm{d}x \, \mathrm{d}y$$

$$N^2 \int_0^{L_y} \sin^2\left(\frac{n_y \pi}{L_y} y\right) \int_0^{L_x} \sin^2\left(\frac{n_x \pi}{L_x} x\right) \mathrm{d}x \, \mathrm{d}y$$

$$N^2 \int_0^{L_x} \sin^2\left(\frac{n_x \pi}{L_x} x\right) \mathrm{d}x \int_0^{L_y} \sin^2\left(\frac{n_y \pi}{L_y} y\right) \mathrm{d}y$$

$$N^2 \frac{L_x}{2} \frac{L_y}{2}$$

$$N^2 \frac{L_x}{2} \frac{L_y}{2} = 1$$

$$N = \frac{2}{\sqrt{L_x L_y}}$$

$$\psi = \frac{2}{\sqrt{L_x L_y}} \sin\left(\frac{n_x \pi}{L_x} x\right) \sin\left(\frac{n_y \pi}{L_y} y\right)$$

$$n_x, n_y \in \mathbb{N}_+$$

Rozdzielanie zmiennych w równaniu Schrödingera dla cząstki w okrągłej nieskończonej studni potencjału:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right]\psi = E\psi$$

$$\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right]R\Phi = -\frac{2mE}{\hbar^2}R\Phi$$

$$\frac{1}{R\Phi}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right]R\Phi = -\lambda$$

$$\frac{1}{R\Phi}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)R\Phi + \frac{1}{R\Phi}\frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}R\Phi = -\lambda$$

$$\frac{1}{R}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)R + \frac{1}{\Phi}\frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\Phi = -\lambda$$

$$\frac{r}{R}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)R + \frac{1}{\Phi}\frac{\partial^2}{\partial \varphi^2}\Phi = -\lambda r^2$$

$$\frac{r}{R}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)R + \lambda r^2 = m_l^2 = -\frac{1}{\Phi}\frac{\partial^2}{\partial \varphi^2}\Phi$$

Przekształcenie równania funkcji radialnej do postaci równania różniczkowego Bessela:

$$\frac{r}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}}{\mathrm{d}r}\right)R + \lambda r^2 = m_l^2$$

$$\frac{r}{R}\left(r\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\mathrm{d}}{\mathrm{d}r}\right)R + \lambda r^2 = m_l^2$$

$$r^2\frac{\mathrm{d}^2R}{\mathrm{d}r^2} + r\frac{\mathrm{d}R}{\mathrm{d}r} + \lambda r^2 R = m_l^2 R$$

$$r^2\frac{\mathrm{d}^2R}{\mathrm{d}r^2} + r\frac{\mathrm{d}R}{\mathrm{d}r} + (\lambda r^2 - m_l^2)R = 0$$

$$R = N_1 J_{m_l}(\sqrt{\lambda} r) + N_2 Y_{m_l}(\sqrt{\lambda} r)$$

Wykład 12. Rotator sztywny

Laplasjan we współrzędnych sferycznych:

$$\nabla^2 = \Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \varphi^2}$$

$$= \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \varphi^2}\right]$$

$$r = const. \Rightarrow \frac{\partial}{\partial r}\psi = 0$$

$$\nabla^2 = \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] = \frac{1}{r^2}\Lambda^2$$

Rozdzielanie funkcji falowej:

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi = E\psi$$

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\Lambda^2\psi = E\psi$$

$$\psi(r,\theta,\varphi) = R(r)\Theta(\theta)\Phi(\varphi)$$

$$\psi(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$$

$$-\frac{\hbar^2}{2I}\Lambda^2\Theta\Phi = E\Theta\Phi$$

Rozdzielanie zmiennych:

$$-\frac{\hbar^2}{2I}\Lambda^2\Theta\Phi = E\Theta\Phi$$

$$\frac{1}{\Theta\Phi}\Lambda^2\Theta\Phi = -\frac{2EI}{\hbar^2}$$

$$\frac{1}{\Theta\Phi}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\Theta\Phi = -\frac{2EI}{\hbar^2}$$

$$\frac{1}{\Theta\Phi}\left[\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{\partial^2}{\partial\varphi^2}\right]\Theta\Phi = -\lambda\sin^2\theta$$

$$\frac{1}{\Theta\Phi}\left[\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{\partial^2}{\partial\varphi^2}\right]\Theta\Phi = -\lambda\sin^2\theta$$

$$\frac{1}{\Theta\Phi}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta\Phi + \frac{1}{\Theta\Phi}\frac{\partial^2}{\partial\varphi^2}\Theta\Phi = -\lambda\sin^2\theta$$

$$\frac{1}{\Theta}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta + \frac{1}{\Phi}\frac{\partial^2}{\partial\varphi^2}\Phi = -\lambda\sin^2\theta$$

$$\frac{1}{\Theta}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta + \lambda\sin^2\theta = -\frac{1}{\Phi}\frac{\partial^2}{\partial\varphi^2}\Phi$$

$$\frac{1}{\Theta}\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\right)\Theta + \lambda\sin^2\theta = m_l^2 = -\frac{1}{\Phi}\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}\Phi$$

$$\frac{1}{\Theta}\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\right)\Theta + \lambda\sin^2\theta = m_l^2$$

$$-\frac{1}{\Phi}\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}\Phi = m_l^2$$

Wykład 13. Atom wodoru i jony wodoropodobne

Równanie Schrödingera w jednostkach atomowych:

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

$$(\hat{T} + \hat{V})\psi = E\psi$$

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}\right)\psi = E\psi$$

$$\left(-\frac{1}{2}\nabla^2 - \frac{Z}{r}\right)\psi = E\psi$$

Równanie Schrödingera we współrzędnych sferycznych:

$$-\frac{1}{2}\nabla^2\psi - \frac{Z}{r}\psi = E\psi$$

$$\nabla^2 = \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \Lambda^2\right]$$

$$-\frac{1}{2r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \Lambda^2\right]\psi - \frac{Z}{r}\psi = E\psi$$

$$\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \Lambda^2\right]\psi + 2Zr\psi = 2Er^2\psi$$

Rozdzielanie funkcji falowej:

$$\psi(r,\theta,\varphi) = R(r)\Theta(\theta)\Phi(\varphi)$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R\Theta\Phi + \Lambda^2 R\Theta\Phi + 2ZrR\Theta\Phi = 2Er^2R\Theta\Phi$$

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R + \frac{1}{\Theta\Phi}\Lambda^2\Theta\Phi + 2Zr = 2Er^2$$

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R + 2Zr - 2Er^2 = \lambda = -\frac{1}{\Theta\Phi}\Lambda^2\Theta\Phi$$

Rozwiązaniami równania sferycznego są harmoniki sferyczne!

Funkcję radialną wygodnie jest uzależnić od bezwymiarowej wielkości $\rho = \frac{2Z}{na_0}r$. Jest ona wtedy dana wzorem:

$$R_{n,l}(\rho) = N_{n,l}\,\rho^l\,\mathrm{e}^{-\frac{\rho}{2}}\,L_{n-l-1}^{2l+1}(\rho)$$

gdzie N to stała normalizacyjna wyznaczona z warunku:

$$\int_0^\infty r^2R^2\,\mathrm{d}r = 1$$

L_{n-l-1}^{2l+1} to stowarzyszony wielomian Laguerre'a:

$$L_{n-l-1}^{2l+1}(\rho) = (-1)^{2l+1}\frac{\mathrm{d}^{2l+1}}{\mathrm{d}\rho^{2l+1}}L_{n+l}(\rho)$$

podczas gdy wielomiany Laguerre'a dane są jako:

$$L_{n+l}(\rho) = \frac{\mathrm{e}^{\rho}}{(n+l)!}\frac{\mathrm{d}^{n+l}}{\mathrm{d}\rho^{n+l}}\mathrm{e}^{-\rho}\rho^{n+l}$$