

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2} - \frac{Ze^2}{4\pi\epsilon_0 r}\right)P_{n\ell}(r) = EP_{n\ell}(r). \quad (1)$$

The following dimensionless variables were defined:

$$\begin{aligned} \xi &= r/Da_0 \\ E' &= E/(Z^2\mu\hbar^2/(2m_e^2a_0^2)) \end{aligned} \quad (2)$$

In principle, E' should take the values $-1, -1/4, -1/9, \dots$. The variable ξ is on the interval $[0, 1]$. Then we get

$$\hat{H}u = -\beta^2 \left(\frac{d^2}{d\xi^2} - \frac{\ell(\ell+1)}{\xi^2} + \frac{2}{\beta\xi} \right) u = E'u \quad (3)$$

where $\beta = m_e/(Z\mu\alpha)$. The numerical solution to (3) as a linear combination of n B-splines of degree k :

$$\hat{u}(\xi) = \sum_{j=0}^{n-1} c_j B_{j,k}(\xi). \quad (4)$$

Inserting this into equation (3), multiplying by $B_{i,k}(x)$ and integrating over $(0, 1)$ yields:

$$\sum_{j=1}^{n-2} c_j \int_0^1 B_{i,k} \hat{H} B_{j,k} = E' \sum_{j=1}^{n-2} c_j \int_0^1 B_{i,k} B_{j,k} \quad (5)$$

which is a generalized eigenvalue problem of the form $A\mathbf{c} = E'B\mathbf{c}$.