

HYDROGEN ATOM - LAGUERRE POLYNOMIALS EXAMPLE

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.12.

The radial function for the hydrogen atom wave function can be written in terms of associated Laguerre polynomials L_n^k .

$$R_{nl}(r) = \frac{1}{r} \rho^{l+1} e^{-\rho} L_{n-l-1}^{2l+1}(2\rho) \quad (1)$$

Although there is a formula giving the associated Laguerre polynomials in terms of ordinary Laguerre polynomials, which are in turn given in terms of derivatives, it is easier to work out the associated Laguerre polynomials using the explicit series formula:

$$L_p^q(x) = c_0 \sum_{j=0}^p \frac{(-1)^j (p+q)!}{(p-j)!(q+j)!j!} x^j \quad (2)$$

This formula gives the polynomial up to an overall normalization constant c_0 .

For example, when $n = 5$ and $l = 2$, we get

$$L_{n-l-1}^{2l+1}(2\rho) = L_2^5(2\rho) \quad (3)$$

$$= 7!c_0 \sum_{j=0}^2 \frac{(-2)^j}{(2-j)!(5+j)!j!} \rho^j \quad (4)$$

$$= 7!c_0 \left(\frac{1}{2!5!} - \frac{2}{6!}\rho + \frac{4}{7!2!}\rho^2 \right) \quad (5)$$

$$= c_0 (21 - 14\rho + 2\rho^2) \quad (6)$$

We can also use the recursion formula for $n = 5$ and $l = 2$ which is

$$c_{j+1} = \frac{2(j-2)}{(j+1)(j+6)} c_j \quad (7)$$

We get

$$c_1 = -\frac{2}{3}c_0 \quad (8)$$

$$c_2 = -\frac{1}{7}c_1 = \frac{2}{21}c_0 \quad (9)$$

This agrees with the values above.

The radial function in this case is (since $\rho = r/5a$)

$$R_{52}(r) = \frac{r^2}{(5a)^3} e^{-r/5a} \left(1 - \frac{2}{15a}r + \frac{2}{525a^2}r^2 \right) c_0 \quad (10)$$

Normalizing gives

$$c_0 = \sqrt{\frac{56}{125a}} \quad (11)$$