PHY310 - MATHEMATICAL METHODS FOR PHYSICISTS I

Odd Term 2019
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LECTURE 12

August 29, 2019

SPECIAL FUNCTIONS 12

Topics: Laguerre polynomials, Associated Laguerre polynomials.

Laguerre polynomials

Schroedinger equation for the one-electron atom

The most important application of the Laguerre polynomials is in the solution of the Schroedinger equation for the one-electron atom. The equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi_{nlm}(r,\theta,\phi) - \frac{Ze^2}{4\pi\epsilon_0 r}\psi_{nlm}(r,\theta,\phi) = E_n\psi_{nlm}(r,\theta,\phi), \tag{1}$$

where $Z = 1$ for hydrogen, 2 for ionized helium etc.

Separating the wavefunction into radial and angular parts

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi), \tag{2}$$

where $R_{nl}(r)$ and $Y_l^m(\theta,\phi)$ are the radial and angular parts of the wavefunction, respectively.

The radial part, $R \equiv R_{nl}(r)$, satisfies the equation

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{Ze^2}{4\pi\epsilon_0 r}R + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}R = E_nR, \tag{3}$$

with $n \geq 1$ and $l = 0, 1, 2, \cdots n-1$.

For bound states, we must have a finite value for R at the origin $r = 0$, and $R \to 0$ as $r \to \infty$.

Rescaling r to the dimensionless radial variable ρ, we get

$$\rho \;\; = \;\; \alpha r \tag{4}$$

with

$$\alpha^2 = -\frac{8mE}{\hbar^2}, \quad E < 0, \quad \text{and} \quad \lambda = \frac{mZe^2}{2\pi\epsilon_0\alpha\hbar^2}, \tag{5}$$

the radial equation becomes

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{d\chi(\rho)}{d\rho}\right) + \left(\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2}\right)\chi(\rho) = 0, \tag{6}$$

where $\chi(\rho) = R(\rho/\alpha)$.

Noting that

$$\frac{1}{\rho^2}\frac{d}{d\rho}\rho^2\frac{d\chi}{d\rho} = \frac{1}{\rho}\frac{d^2}{d\rho^2}(\rho\chi), \tag{7}$$

we can write down the above equation

$$\frac{1}{\rho}\frac{d^2}{d\rho^2}(\rho\chi) + \left(\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2}\right)\chi = 0. \tag{8}$$

That is,

$$\frac{d^2}{d\rho^2}(\rho\chi) + \left(\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2}\right)(\rho\chi) = 0. \tag{9}$$

A solution to the above equation is

$$\rho\chi(\rho) = e^{-\rho/2}\rho^{l+1}L^{2l+1}_{\lambda-l-1}(\rho). \tag{10}$$

The functions $L^k_n(x)$ are called *associated Laguerre polynomials.*

In our physical problem we must have

$$\lim_{r\to\infty} R(r) = 0. \tag{11}$$

This tells us that we must restrict the parameter λ to integer values $n = 1, 2, 3, \cdots$. Note that for nonintegral values n Laguerre functions would diverge as $\rho^n e^\rho$. This restriction on λ has the effect of quantizing the energy

$$E_n = -\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{Z^2 m}{2\hbar^2}\frac{1}{n^2}. \tag{12}$$

Upon using this result for E_n we have

$$\alpha = \frac{me^2}{2\pi\epsilon_0\hbar^2}\frac{Z}{n} = \frac{2Z}{na_0}, \quad \rho = \frac{2Z}{na_0}r, \tag{13}$$

where

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} \tag{14}$$

is the Bohr radius.

Laguerre polynimials

Laguerre's differential equation is given by

$$xy'' + (1-x)y' + ny = 0, \tag{15}$$

where n is an integer.

The solutions to this differential equation are called Laguerre polynomials. They can be expressed as a series

$$L_n(x) = \sum_{m=0}^{n} (-1)^m \frac{n!}{(n-m)!} \frac{x^m}{m!m!}. \tag{16}$$

From this we can write down the first few Laguerre polynomials

$$\begin{aligned} L_0(x) &= 1, && (17)\\ L_1(x) &= -x+1, && (18)\\ 2!L_2(x) &= x^2-4x+2, && (19)\\ 3!L_3(x) &= -x^3+9x^2-18x+6. && (20) \end{aligned}$$

Rodrigues' representation and generating function

It has a Rodrigues' representation

$$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} \left(x^n e^{-x} \right). \tag{21}$$

The generating function is

$$\phi(x,t) = \frac{e^{-xt/(1-t)}}{(1-t)} = \sum_{n=0}^{\infty} L_n(x) t^n, \quad |t| < 1. \tag{22}$$

We have

$$\phi(0,t) = \frac{1}{(1-t)} = \sum_{n=0}^{\infty} t^n = \sum_{n=0}^{\infty} L_n(0) t^n. \tag{23}$$

From this equation we obtain special values of Laguerre polynomials

$$L_n(0) = 1. \tag{24}$$

Recursion relations and orthogonality

They also satisfy recursion relations

$$\begin{aligned} (n+1)L_{n+1}(x) &= (2n+1-x)L_n(x) - nL_{n-1}(x), && (25)\\ xL_n'(x) &= nL_n(x) - nL_{n-1}(x). && (26) \end{aligned}$$

The orthogonality relation satisfied by Laguerre polynomials is

$$\int_0^\infty dx\ e^{-x} L_m(x) L_n(x) = \delta_{mn}. \tag{27}$$

We can define orthogonalized Laguerre functions by

$$\phi_n(x) = e^{-x/2} L_n(x), \tag{28}$$

and they satisfy the equation

$$x\phi_n''(x) + \phi_n'(x) + \left(n + \frac{1}{2} - \frac{x}{4}\right)\phi_n(x) = 0. \tag{29}$$

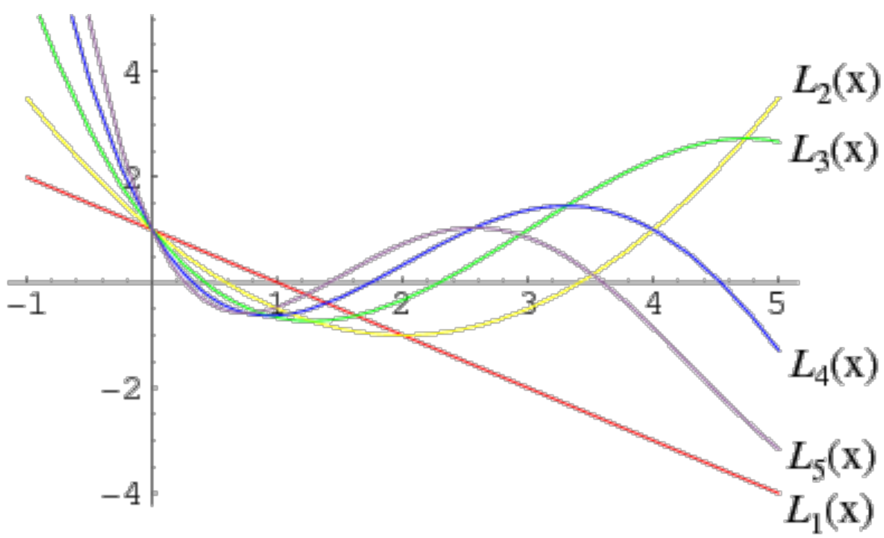

Figure 1: The first few Laguerre polynomials. (Source: Weisstein, Eric W. "Laguerre Polynomial." From MathWorld – A Wolfram Web Resource. http://mathworld.wolfram.com/LaguerrePolynomial.html.)

Associated Laguerre polnomials

Earlier we saw that in quantum mechanics we need the associated Laguerre polynomials. They are defined by

$$L_n^k(x) = (-1)^k \frac{d^k}{dx^k} L_{n+k}(x). \tag{30}$$

In a series form we write it as

$$L_n^k(x) = \sum_{m=0}^{n} (-1)^m \frac{(n+k)!}{(n-m)!(k+m)!m!} x^m, \quad k > -1. \tag{31}$$

We can write down a generating function for associated Laguerre polynomials by differentiating the Laguerre generating function k times. We get

$$\frac{e^{-xt/(1-t)}}{(1-t)^{k+1}} = \sum_{n=0}^{\infty} L_n^k(x) t^n, \quad |t| < 1. \tag{32}$$

Recurrence relations can be derived from this generating function.

By differentiating Laguerre's equation k times we arrive at the differential equation for associated Laguerre polynomials

$$x \frac{d^2}{dx^2} L_n^k(x) + (k+1-x) \frac{d}{dx} L_n^k(x) + n L_n^k(x) = 0. \tag{33}$$

This equation appears when we study the bound states of one-electron atoms.

The orthogonality relation satisfied by the associated Laguerre polynomials is

$$\int_0^{\infty} e^{-x} dx \; x^k L_n^k(x) L_m^k(x) = \frac{(n+k)!}{n!} \delta_{mn}. \tag{34}$$

We can introduce a new function by letting

$$\psi_n^k(x) = e^{-x^2/2} x^{k/2} L_n^k(x). \tag{35}$$

This function satisfies the differential equation

$$x \frac{d^2}{dx^2} \psi_n^k(x) + \frac{d}{dx} \psi_n^k(x) + \left(-\frac{x}{4} + \frac{2n+k+1}{2} - \frac{k^2}{4x} \right) \psi_n^k(x) = 0. \tag{36}$$

The functions $\psi_n^k(x)$ are sometimes called *Laguerre functions*.

Let us define

$$\Phi_n^k(x) = e^{-x/2} x^{(k+1)/2} L_n^k(x). \tag{37}$$

Substituting this in the associated Laguerre equation gives another useful form of the differential equation

$$\frac{d^2}{dx^2} \Phi_n^k(x) + \left(-\frac{1}{4} + \frac{2n+k+1}{2x} - \frac{k^2-1}{4x^2} \right) \Phi_n^k(x) = 0. \tag{38}$$

This is equation has the same form we encountered earlier when we looked at the bound states of one-electron atom

$$\frac{d^2}{d\rho^2}(\rho\chi) + \left(\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2} \right)(\rho\chi) = 0. \tag{39}$$