The Electronic Wavefunction

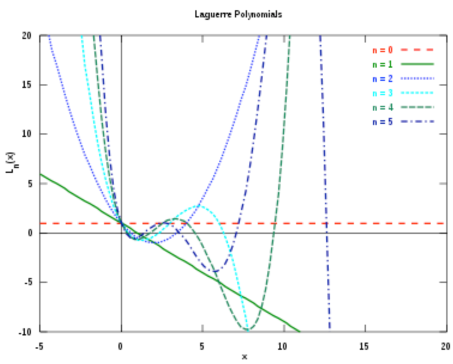
- the electronic component is determined for given nuclear coordinates, and has radial, angular and spin components which produce the principle (n) and angular quantisation (l and m_l)

$$\psi_{el} = R_n(r)Y_{l,m_l}(\theta,\phi)s_{s,m_s}(\sigma)$$
$$H_{el} = T_e + V_{ne} + V_{ee}$$

  - NOTE these are not the same angular components as discussed for the *nuclear* wavefunction (I used capital Greek letters) and these are for the *electronic* wavefunction (I use small Greek letters)
  - the eigenfunctions of the *electronic angular* Schrödinger equation are again spherical harmonic functions, Y(θ,ϕ) these are in-fact the functional forms of the s, p and d orbitals. You have seen these in your Maths lectures with Kim Jelfs.
  - the eigenfunctions of the *electronic radial* Schrödinger equation R(r) are **associated Laguerre** functions, the exact form of these is beyond the scope of this course: http://en.wikipedia.org/wiki/Laguerre_polynomials
  - the associated Laguerre polynomials are solutions to Laguerre's differential equation, they are also linked by a recursion relation

$$xy'' = (\nu + 1 - x)y' + \lambda y = 0$$
$$L_n^k(x) = \frac{e^x x^{n-k}}{n!}\frac{d^n}{dx^n}\left(e^{-x}x^{n+k}\right)$$
$$L_n^k(x) = L_n^{k+1}(x) - L_{n-1}^{k+1}(x)$$

n	$L_n(x)$
0	1
1	$-x+1$
2	$\frac{1}{2}(x^2-4x+2)$
3	$\frac{1}{6}(-x^3+9x^2-18x+6)$
4	$\frac{1}{24}(x^4-16x^3+72x^2-96x+24)$
5	$\frac{1}{120}(-x^5+25x^4-200x^3+600x^2-600x+120)$
6	$\frac{1}{720}(x^6-36x^5+450x^4-2400x^3+5400x^2-4320x+720)$



source http://en.wikipedia.org/wiki/Laguerre_polynomials

  - the spin of the electron σ(s) which can be a (m_s=+1/2) or b (m_s=-1/2), should not be ignored and is very important in determining allowed transitions.