

## 21 Orthogonal Polynomials

1. We have now seen three different kinds of functions that we haven't seen earlier: (a) the Legendre polynomials, these are the solutions to the  $\theta$  part of the Hydrogen atom Schrödinger Equation, (b) the Laguerre polynomials, these are the solutions to the  $\rho$  or the radial part of the Hydrogen atom Schrödinger Equation, (c) the Hermite polynomials, these are the solutions to the harmonic oscillator that we have just studied. In addition we have also studied the Fourier functions (the sines and cosines) which we came across while solving the particle in a box problem.
2. Do all these functions have anything in common? Yes. They are eigenstates of Hermitian operators. How do we know? Consider the hydrogen atom Hamiltonian. It contains the kinetic energy and potential energy part each of which are separately Hermitian. (Remember, we proved that the kinetic and potential energy operators are both Hermitian!!) The kinetic energy operator is itself made of three parts, a  $\rho$  dependent part, a  $\theta$  dependent part and a  $\phi$  dependent part. Since  $\rho$ ,  $\theta$  and  $\phi$  are independent of each other we can argue that each individual portion should be independently Hermitian so that the sum is Hermitian. Hence the special functions noted above are all eigenstates of Hermitian operators!!
3. Hence the Legendre polynomials, the Laguerre polynomials, the Hermite polynomials and the Fourier functions all form complete sets, using which *any* function can be expanded as a linear combination. We already know this is true for the Fourier series

since any function  $f(x)$  can be written as:

$$f(x) = \sum_n a_n \cos nx + b_n \sin nx \quad (21.1)$$

where the coefficients  $a_n$  and  $b_n$  are given by the Fourier transform of the function  $f(x)$ .

4. But now we see that there are other complete sets that the function  $f(x)$  can be expanded about, and the Fourier series and Fourier transform is just a special case.
5. In fact special functions and complete sets of functions form an important part of quantum chemistry. In practical calculations the wavefunction is expanded about some assumed to be complete set of basis functions and the coefficients are determined by solving the Schrödinger Equation.