Review—10-14-09

1. Discussed Quantum systems from postulates
   a. State—wave function, observable – operator
   b. Measurement – eigenvalue or expectation value
   c. Interpretation – $\psi^*\psi d\tau$ – probability in $d\tau$
      i. Integrate over all space = 1 – exists in space
      ii. Intergrate over region, probability in region
2. model problems exemplify behavior (e.g. free & pib)
3. harmonic oscillator, more physical, vibrations molec.

4. Talked about the H-atom problem – see Web page

   a. 2-particle problem, 3-D total 6-dimensions
   b. Separation of C of M from relative coord.

   $\rightarrow$ interested in relative position e vs. p

   c. Separation into spherical coordinates

   $\rightarrow$ idea $V = -Ze^2/r$; 1 coord. Spher., 3 – Cartes.

   d. Method – get all of one variable on one side
      i. must be equal to constant
      ii. use product wavefct.: $\psi = R(r)\,\Theta(\theta)\,\Phi(\phi)$

internal: $\boldsymbol{H(r)}\,\psi(r,\theta,\phi) = [(-\hbar^2/2\mu)\nabla_r^{\,2} - Ze^2/r]\,\psi(r,\theta,\phi) = E_{int}\psi$

$$\boldsymbol{H(r)}\psi(r) = [(-\hbar^2/2\mu r^2)\{\partial/\partial r(r^2\partial/\partial r)+[1/\sin\theta]\partial/\partial\theta(\sin\theta\ \partial/\partial\theta) + [1/\sin^2\theta]\partial^2/\partial\phi^2\} - Ze^2/r]\psi(r) = E_{int}\psi(r)$$

separation:

$$(-\hbar^2/2\mu)\{\sin^2\theta\ \partial/\partial r(r^2\partial/\partial r)+\sin\theta\partial/\partial\theta(\sin\theta\partial/\partial\theta) - r^2\sin^2\theta(E_{int}+Ze^2/r)\}\psi(r,\theta,\phi) = -\partial^2/\partial\phi^2\ \psi(r,\theta,\phi) = m^2$$

Use $\psi(r, \theta, \phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$ divide through as before

$$-[\Phi(\phi)]^{-1}\,\partial^2/\partial\phi^2\,\Phi(\phi) = \text{const.}$$

ϕ problem separates easily

1-D problem: $\partial^2/\partial\phi^2\,\Phi(\phi) = -m^2\,\Phi(\phi)$

Solutions: $\Phi(\phi) = e^{im\phi}$ $\quad m = 0, \pm1, \pm2, \ldots$

θ problem also easily separates, solution trickier

$$(-\hbar^2/2\mu)\{(\sin\theta)^{-1}\partial/\partial\theta(\sin\theta\,\partial/\partial\theta) - \mathbf{m^2}/\sin^2\theta\}\Theta(\theta) = l(l+1)\,\Theta(\theta)$$

Solution: LeGendre polynomial:

$\Theta(\theta) = P_\ell^{|m|}(\cos\theta)$ $\quad \ell = 0, 1, 2, \ldots;\ \ell \geq |m|$

Radial problem is left, already separated:

$$(-\hbar^2/2\mu)\{\partial/\partial r(r^2\partial/\partial r)\,r^2 - (E_{int} + Ze^2/r - l(l+1))\}\,\mathbf{R(r) = 0}$$

Solution: LaGuerre Polynomial $n = 1, 2, \ldots$ and $\ell \leq n-1$

$R_{n\ell}(r) = (\text{constant})(2Zr/na_0)\,L_{n+\ell}^{2\ell+1}(2Zr/na_0)e^{-Zr/na_0}$ $\quad \sigma = Zr/a_0$

(only r dependent equation has energy in it)

$E_n = -Z^2e^2\mu/2h^2n^2$ – same as Bohr

energy levels vary as $1/n^2$ collapse with increasing n