Quantum Mechanics — April 20th, 2015

Lect 34

I Last time

$\rightsquigarrow$ All things H

II More than one quantum object: herding cats

I • completed the derivation of the hydrogen atom wavefunctions

Let's reassemble all the pieces!

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$$

with $\Psi = \Psi(\vec{r}, t)$

$$\rightsquigarrow \Psi_n = \psi_n(r,\theta,\phi)\, e^{-iE_n t/\hbar}$$

Then

$$\psi(r,\theta,\phi) = R(r)\, Y(\theta,\phi)$$

leads to

$$Y_\ell^m(\theta,\phi) = \epsilon \sqrt{\frac{(2\ell+1)(\ell-|m|)!}{4\pi\,(\ell+|m|)!}}\, e^{im\phi} P_\ell^m(\cos\theta)$$

with

$$P_\ell^m(x) \equiv (1-x^2)^{|m|/2} \left(\frac{d}{dx}\right)^{|m|} P_\ell(x)$$

and

$$P_\ell(x) \equiv \frac{1}{2^\ell \ell!} \left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$

For the radial piece we have found

$$R(r) = \frac{1}{r} \rho^{\ell+1} e^{-\rho} v(\rho)$$

with $\rho \equiv \kappa r$, $\kappa = \frac{\sqrt{-2mE}}{\hbar}$ and

$$v(\rho) = \sum_{j=0}^{j_{max}} c_j \rho^j$$

here $$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)} c_j$$

and $j_{max} = n - l - 1$.

Note then that the radial wave functions are labelled by two quantum numbers n, the principle quant #, and l, the azimuthal quant. #:

$$R(r) = R_{nl}(r)$$

In fact the series (*) with coeff.s is a well known named function set

$$v(\rho) = L_{n-l-1}^{2l+1}(2\rho)$$

with

$$L_{q-p}^{p}(x) \equiv (-1)^p \left(\frac{d}{dx}\right)^p L_q(x) \quad \begin{Bmatrix} p = 2l+1 \\ q = n+l \end{Bmatrix}$$

and

$$L_q(x) \equiv e^x \left(\frac{d}{dx}\right)^q (e^{-x} x^q)$$

the associated and Laguerre polynomials.

Then, the energies are

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2}$$

$n = 1, 2, 3, 4, \ldots$

the Bohr radius is

$$a = \frac{\hbar^2}{m} \frac{4\pi\epsilon_0}{e^2} = 0.529 \times 10^{-10}\, m$$

and

$$E_n = -\left[\frac{\hbar^2}{2m} \frac{1}{a^2}\right]\frac{1}{n^2}$$

The wave functions are

$$\psi_{n\ell m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}}\; e^{-r/na} \left(\frac{2r}{na}\right)^{\ell} \left[L^{2\ell+1}_{n-\ell-1}\left(\frac{2r}{na}\right)\right] Y_\ell^m(\theta,\phi)$$

Pretty glorious!

II Say you want to combine one spin, say that of an electron, with a second one, e.g. the proton spin. These two states come from different Hilbert spaces, call 'em $\mathcal{H}_1$ and $\mathcal{H}_2$. The combined system has four possibilities

$\uparrow\uparrow$, $\uparrow\downarrow$, $\downarrow\uparrow$, $\downarrow\downarrow$

Here we denote the combined system state by juxtaposition. The space of all such states is denoted

$$\mathcal{H}_1 \otimes \mathcal{H}_2$$

What is the total angular momentum of the atom (say the e is in the ground state)?

We can check this using the combined operators

$$S_x \equiv \underbrace{S_x^{(1)}}_{\text{acts on } \mathcal{H}_1} + \underbrace{S_x^{(2)}}_{\text{acts on } \mathcal{H}_2}$$

$\vdots$

$$S_z \equiv S_z^{(1)} + S_z^{(2)}$$

or

$$\vec{S} = \vec{S}^{(1)} + \vec{S}^{(2)}$$

So, if the combined state is $\chi = \chi_1 \chi_2$ then

$$S_z \chi_1 \chi_2 = \left(S_z^{(1)} + S_z^{(2)}\right) \chi_1 \chi_2$$

$$= \left(S_z^{(1)} \chi_1\right) \chi_2 + \chi_1 \left(S_z^{(2)} \chi_2\right)$$

$$= \hbar m_1 \chi_1 \chi_2 + \hbar m_2 \chi_1 \chi_2$$

$$= \hbar \underbrace{(m_1 + m_2)}_{\text{call it } m} \chi_1 \chi_2$$

Then

$\uparrow\uparrow$: $m = 1$

$\uparrow\downarrow$: $m = 0$

$\downarrow\uparrow$: $m = 0$

$\downarrow\downarrow$: $m = -1$

Why are there two $m=0$ states? Cool surprise,

Let $S_- = S_-^{(1)} + S_-^{(2)}$,

$$S_- \uparrow\uparrow = \left(S_-^{(1)} \uparrow\right)\uparrow + \uparrow\left(S_-^{(2)} \uparrow\right)$$

$$= \hbar \downarrow\uparrow + \hbar \uparrow\downarrow$$

$$= \hbar (\downarrow\uparrow + \uparrow\downarrow)$$

So, it is this state that we should think of as $s=1$, $m=0$!

This leads us to collect

$$\left.\begin{cases} |1\,1\rangle = \uparrow\uparrow \\ |1\,0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ |1\,{-1}\rangle = \downarrow\downarrow \end{cases}\right\} \begin{array}{c} s=1 \\ \text{(triplet)} \end{array}$$

and

$$\left\{ |0\,0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) \right\} \begin{array}{c} s=0 \\ \text{(singlet)} \end{array}$$