Phys 231 2021

Lecture 35

Fri: 7.6

Next HW Tues:

Schrödinger Equation for Hydrogen

The TISE for the hydrogen atom in spherical co-ordinates is:

$$-\frac{\hbar^2}{2m_e}\frac{1}{r^2}\left\{\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right\} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}\psi = E\psi$$

and E = energy of the atom is a constant. We seek a solution by separation of variables

$$\psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$$

Then the process turns out to be:

$$\frac{d\Phi}{d\phi^2} = -D\Phi$$

constant D

solve + constrain D

azimuthal

Insert D into

$$\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) - (C\sin^2\theta)\Theta = D\Theta$$

constant C

solve + constrain C

polar

$$-\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}ER + \frac{2mr^2}{\hbar^2}\left(-\frac{1}{4\pi\epsilon_0 r}\right)R = CR$$

solve and find energy E!

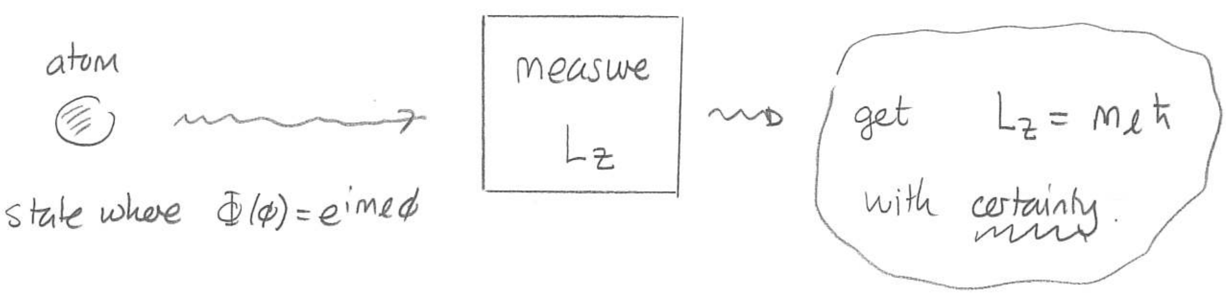
radial

Azimuthal part

We found that the only solutions which yield functions without discontinuities are:

$$\boxed{\begin{gathered}\Phi(\phi) = e^{im_\ell \phi} \\ \text{where} \\ m_\ell = 0, \pm 1, \pm 2, \pm 3, \ldots \\ D = m_\ell^2\end{gathered}}$$

We can interpret m_ℓ in terms of the z-component of angular momentum. We find that in this state a measurement of the z-component yields $m_\ell \hbar$ with certainty



Thus the z-component of angular momentum has possible values

$$L_z = 0, \pm\hbar, \pm 2\hbar, \pm 3\hbar, \ldots$$

Angular momentum is quantized.

The corresponding solution can be labeled by m_ℓ. So

$$\Phi_{m_\ell}(\phi) = e^{im_\ell \phi}$$

Polar equation

The polar equation becomes:

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{\partial \Theta}{\partial \theta}\right) - C\sin^2\theta\, \Theta = m_\ell^2\, \Theta$$

The solution to this equation is omitted but eventually yields physically reasonable solutions if:

$$\boxed{\begin{array}{l} C = -\ell(\ell+1) \quad \text{for } \ell = 0,1,2,3,\ldots \\ m_\ell = -\ell, -\ell+1, -\ell+2, \ldots, \ell-2, \ell-1, \ell. \end{array}}$$

The associated solutions are labeled by two integers: ℓ, m_ℓ

We get $\Theta_{\ell, m_\ell} \approx$ associated Legendre functions (Table 7.3)

These solutions have interpretations in terms of:

1) z-component of angular momentum L_z and m_ℓ
2) magnitude of angular momentum squared $L^2 = L_x^2 + L_y^2 + L_z^2$ and ℓ.

Specifically

> The solution Θ_{ℓ, m_ℓ} is such that measurement of the magnitude of the angular momentum yields
>
> $L = \hbar\sqrt{\ell(\ell+1)}$ $\qquad$ $\ell = 0,1,2,3\ldots$

To summarize:

Solving the angular parts of the TISE for the hydrogen atom give that

* angular momentum is quantized.
* possible values for the magnitude of angular momentum are

$$L = \hbar\sqrt{\ell(\ell+1)} \qquad \ell = 0,1,2,\ldots$$

* for any $\ell = 0,1,2,\ldots$ possible values of the z-component of angular momentum are:

$$L_z = m_\ell \hbar \qquad m_\ell = -\ell, -\ell+1, \ldots \ell-1, \ell$$

Quiz 1 90% → D

Angular wavefunctions

The angular part of the stationary state wavefunction for the hydrogen atom is

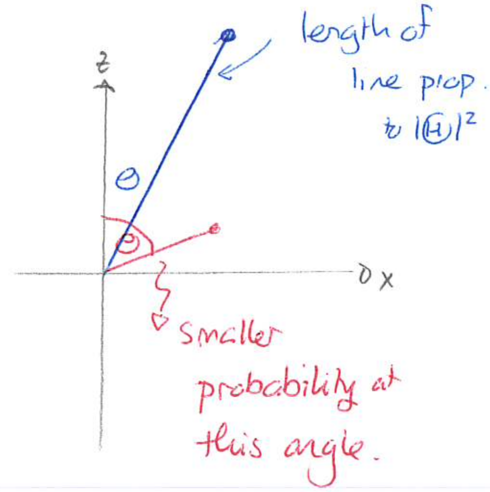
$$\Theta_{\ell,m_\ell}(\theta)\,\Phi_\ell(\phi)$$

and the probability density generated is

$$|\Theta_{\ell,m_\ell}(\theta)\,\Phi(\phi)|^2 = |\Theta_{\ell,m_\ell}(\theta)|^2\,|\Phi(\phi)|^2$$

$$= |\Theta_{\ell,m_\ell}(\theta)|^2\,\underbrace{|e^{im_\ell\phi}|^2}_{1} = |\Theta_{\ell,m_\ell}(\theta)|^2$$

Find these functions requires solving the differential equation or at least generating these solutions. We report the results and plot the resulting contribution to the probability density on an angular diagram



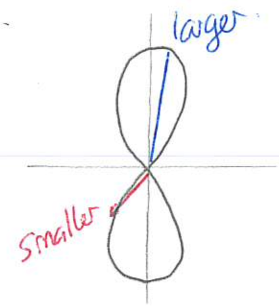
1) $l = 1, \; m_l = 0$

$$\Theta = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$|\Theta|^2 = \frac{3}{4\pi} \cos^2\theta$$

max : $\theta = 0, \pi$

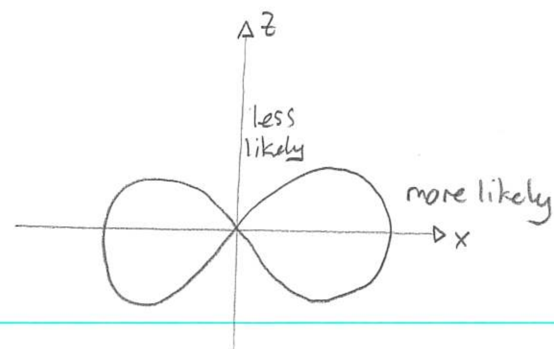
min : $\theta = \pi/2$



2) $l=1, \; m_l = 1$

$$\Theta = \sqrt{\frac{3}{8\pi}} \sin\theta$$

$$|\Theta|^2 = \frac{3}{8\pi} \sin^2\theta$$



Quiz 2