

If I had spent my time learning quantum mechanics to make money, I would have my own little cafe by now.

## 1 Introduction

I, Abbas Abedini, want to take you inside the hydrogen atom.

Before learning this section, you need to know the Schrödinger equation.

Spherical coordinates and differential equations and three-dimensional modes

So let's go to the Schrödinger equation. I taught the Schrödinger equation in a book called Learning the Basics of Quantum Mechanics.

But since I didn't teach 3D, I have to explain it here. Of course, keep in mind that we have some difficult equations ahead of us, and since it's beyond my scope, I'll explain it briefly.

Here I will teach you how to get probability and I will also explain spin in hydrogen if I have the patience.

I'm trying to maintain the necessary standards here, unlike that introductory quantum book I wrote, some of which I wrote out of my own stupidity, but here I'm trying to act according to the standards.

## 2 Schrödinger in three dimensions

$$\hat{H}\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

Oh my child, but we don't need you.

But I can give you a chance to come and transform you into three dimensions or three dimensions that are in spherical coordinates.

$$h_1 = 1 \quad (for r) \quad h_2 = r \sin \phi \quad (for \theta) \quad h_3 = r \quad (for \phi)$$

Obtaining this part was also in mathematics and was obtained from geometry. Our main goal was not to obtain these values.

$$\nabla^2 f = \frac{1}{h_1 h_2 h_3} \left[ \frac{\partial}{\partial q_1} \left( \frac{h_2 h_3}{h_1} \frac{\partial f}{\partial q_1} \right) + \frac{\partial}{\partial q_2} \left( \frac{h_3 h_1}{h_2} \frac{\partial f}{\partial q_2} \right) + \frac{\partial}{\partial q_3} \left( \frac{h_1 h_2}{h_3} \frac{\partial f}{\partial q_3} \right) \right]$$

Oh, you didn't think Laplace would come??? If you don't know, go reread math or the first chapter of electromagnetism.

$$\nabla^2 f(r, \theta, \phi) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \phi} \frac{\partial}{\partial \phi} \left( \sin \phi \frac{\partial f}{\partial \phi} \right) + \frac{1}{r^2 \sin^2 \phi} \frac{\partial^2 f}{\partial \theta^2}.$$

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \phi} \frac{\partial}{\partial \phi} \left( \sin \phi \frac{\partial \psi}{\partial \phi} \right) + \frac{1}{r^2 \sin^2 \phi} \frac{\partial^2 \psi}{\partial \theta^2} \right] + V(r) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi)$$

So it went into the Schrödinger equation.

$$-\frac{\hbar^2}{2m} \left[ \frac{d}{dr} \left( r^2 \frac{d\psi}{dr} \right) + \frac{1}{\sin \phi} \frac{\partial}{\partial \phi} \left( \sin \phi \frac{\partial \psi}{\partial \phi} \right) + \frac{1}{\sin^2 \phi} \frac{\partial^2 \psi}{\partial \theta^2} \right] + r^2 V(r) \psi = r^2 E \psi$$

Multiplication :  $\cdot \hbar^2/2m$

$$\frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \left[ \frac{2m}{\hbar^2} r^2 (E - V(r)) - \ell(\ell + 1) \right] R = 0$$

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + V_{eff}(r) \cdot u(r) = E u(r)$$

$$V_{eff}(r) = V(r) + \frac{\hbar^2}{2m} \cdot \frac{\ell(\ell + 1)}{r^2}$$

Replace potential with the following phrase:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

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We begin with the angular part of the Schrödinger equation in spherical coordinates:

$$\frac{1}{\sin \phi} \frac{\partial}{\partial \phi} \left( \sin \phi \frac{\partial Y}{\partial \phi} \right) + \frac{1}{\sin^2 \phi} \frac{\partial^2 Y}{\partial \theta^2} = -\ell(\ell + 1) Y$$

Assume the separation of variables:

$$Y(\theta, \phi) = \Theta(\theta) \Phi(\phi)$$

Substituting into the equation and dividing by  $\Theta(\theta) \Phi(\phi)$ , we get:

$$\frac{1}{\Phi(\phi)} \cdot \frac{1}{\sin \phi} \frac{d}{d\phi} \left( \sin \phi \frac{d\Phi}{d\phi} \right) + \frac{1}{\Theta(\theta)} \cdot \frac{1}{\sin^2 \phi} \frac{d^2 \Theta}{d\theta^2} = -\ell(\ell + 1)$$

Since the left-hand side is a sum of two terms, one depending only on  $\theta$  and one only on  $\phi$ , we can set both equal to a constant,  $m^2$ , and write:

$$\frac{d^2 \Theta(\theta)}{d\theta^2} + m^2 \Theta(\theta) = 0$$

$$\frac{1}{\sin \phi} \frac{d}{d\phi} \left( \sin \phi \frac{d\Phi(\phi)}{d\phi} \right) + \left[ \ell(\ell + 1) - \frac{m^2}{\sin^2 \phi} \right] \Phi(\phi) = 0$$

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

$$P_\ell^m(x) = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} P_\ell(x)$$

Notice here we added a constant to it.

This constant was also added for the radial and angular parts.

This is essentially angular momentum. Angular momentum can be used to describe the shape of our wave function.

I'll add the angular momentum, how it changes with the u's.

Angular momentum in a hydrogen atom is because the hydrogen atom is in an s orbital. We don't have angular momentum and it's spherically distributed equally everywhere. I'll add the shape of it.

Here, due to the uncertainty principle, we cannot obtain the angular momentum z and the angular momentum y simultaneously, and we always consider the momentum of the z component.

You don't need to add this in the angular wave function because this property is in the Legendre equation.

## Probability Wave Function

In problems with spherical symmetry, the wavefunction separates as:

$$\Psi(r, \theta, \phi) = R(r) \times Y_\ell^m(\theta, \phi)$$

where  $Y_\ell^m(\theta, \phi)$  are the **spherical harmonics** describing the angular dependence.

The angular probability density (probability to find the particle at angles  $\theta, \phi$ ) is

$$P(\theta, \phi) = |Y_\ell^m(\theta, \phi)|^2$$

The spherical harmonics have the form:

$$Y_\ell^m(\theta, \phi) = N_{\ell m} P_\ell^m(\cos \theta) e^{im\phi}$$

$$N_{\ell m} = (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \cdot \frac{(\ell-m)!}{(\ell+m)!}}$$

$$P(\theta, \phi) = |Y_\ell^m(\theta, \phi)|^2 = |N_{\ell m}|^2 |P_\ell^m(\cos \theta)|^2$$

Well, my beauty, we were able to obtain the probability of an angle, we need to go to Lagor.

$$R_{n\ell}(r) = N_{n\ell} \left( \frac{2r}{na_0} \right)^\ell e^{-r/(na_0)} L_{n-\ell-1}^{2\ell+1} \left( \frac{2r}{na_0} \right),$$

where  $a_0$  is the Bohr radius,  $L_k^\alpha(x)$  is the associated Laguerre polynomial of degree  $k = n - \ell - 1$  and parameter  $\alpha = 2\ell + 1$ , and the normalization constant is

$$N_{n\ell} = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}}.$$

Thus the full radial part reads

$$R_{n\ell}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}} \left(\frac{2r}{na_0}\right)^\ell e^{-r/(na_0)} L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right).$$

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The full hydrogenic wavefunction in spherical coordinates is

$$\Psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_\ell^m(\theta, \phi)$$

where

$$R_{n\ell}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}} \left(\frac{2r}{na_0}\right)^\ell e^{-r/(na_0)} L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right)$$

and

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

Putting it all together:

$$\begin{aligned} \Psi_{n\ell m}(r, \theta, \phi) &= \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}} \left(\frac{2r}{na_0}\right)^\ell e^{-r/(na_0)} L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right) \\ &\quad (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} P_\ell^m(\cos \theta) e^{im\phi}. \end{aligned}$$

This is the general wave function for radial and for angular we get  
The Lagord equation, which gives a radius, the spherical Schrödinger equation,  
which we solved radially, had many equations, we just put them in.  
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## Hydrogen ( $n = 1$ , $\ell = 0$ , $m = 0$ )

The angular part is

$$Y_0^0(\theta, \phi) = \frac{1}{\sqrt{4\pi}}.$$

The radial part is

$$R_{10}(r) = 2 a_0^{-3/2} e^{-r/a_0},$$

where  $a_0$  is the Bohr radius.

Hence the full normalized wavefunction is

$$\Psi_{100}(r, \theta, \phi) = R_{10}(r) Y_0^0(\theta, \phi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}.$$

The probability density reads

$$|\Psi_{100}(r, \theta, \phi)|^2 = \frac{1}{\pi a_0^3} e^{-2r/a_0}.$$