

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 : : $\hbar^2/2m$

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

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

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

Replace potential with the following phrase:

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

article amsmath

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 θ and one only on ϕ , we can set both equal to a constant, m^2 , and write:

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

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

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

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

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 θ, ϕ) 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

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

article amsmath,amssymb

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.
article amsmath amssymb

Ground State Wavefunction of 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

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