8 The Harmonic Oscillator

We want to solve the Schroedinger equation with a quadratic potential

$$-\frac{h^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\Psi \quad = \quad E\Psi.$$

You've done this before with ladder operators. Now we do the brute-force approach as a practice for the Hydrogen Atom. By introducing the constants

$$\begin{aligned}\xi &\equiv \sqrt{\frac{m\omega}{\hbar}}x \\ K &\equiv \frac{2E}{\hbar\omega}\end{aligned}$$

the Schroedinger equation simplifies to

$$\frac{d^2\psi}{d\xi^2} \quad = \quad \left(\xi^2-K\right)\psi.$$

The problem now is to look for allowed value of K. Let's begin by looking at the limit $\xi \gg K$. Then, the equation simplifies to

$$\frac{d^2\psi}{d\xi^2} \quad = \quad \xi^2\psi.$$

This equation is approximately solved by

$$\psi(x) \quad = \quad Ae^{-\xi^2/2}+Be^{\xi^2/2}.$$

The second term blows up as $\xi \to \infty$, thus is not normalizable and not physical. The first term looks physical. That motivates us to try the following ansatz:

$$\xi(x) \quad = \quad h(\xi)e^{-\xi^2/2}$$

First, let's calculate the derivatives

$$\begin{aligned}\frac{d\psi}{d\xi} &= \left(\frac{dh}{d\xi}-\xi h\right)e^{-\xi^2/2} \\ \frac{d^2\xi}{d^2\xi} &= \left(\frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(\xi^2-1)h\right)e^{-\xi^2/2}\end{aligned}$$

So the Schroedinger equation from above becomes

$$\frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(K-1)h \quad = \quad 0$$

Let us use yet another ansatz, this time in the form of a power series:

$$h(\xi)=\sum_{j=0}^{\infty}a_j\xi^j$$

The derivatives are:

$$\begin{aligned}\frac{dh}{d\xi} &= \sum_{j=1}^{\infty}ja_j\xi^{j-1} \\ \frac{d^2h}{d\xi^2} &= \sum_{j=2}^{\infty}j(j-1)a_j\xi^{j-2}\end{aligned}$$

Note that there is a typo in Griffiths. Putting everything back into the Schroedinger equation gives us

$$\sum_{j=0}^{\infty}\left[(j+1)(j+2)a_{j+2}-2ja_j+(K-1)a_j\right]\xi^j=0$$

Because of the uniquness of the power series expansion, we can get rid of the sum an look at each term individually

$$(j+1)(j+2)a_{j+2}-2ja_j+(K-1)a_j=0$$

or equivalently

$$a_{j+2}=\frac{2j+1-K}{(j+1)(j+2)}a_j$$

This is still the Schroedinger equation! Once we specify a_0 all the even coefficients are determined. Once we specify a_1 all the odd coefficients are determined. Thus, lets write

$$\begin{aligned} h(\xi) &= h_{even}(\xi)+h_{odd}(\xi), \qquad \text{where} \\ h_{even}(\xi) &= a_0+a_2\xi^2+\ldots \\ h_{odd}(\xi) &= a_1\xi+a_3\xi^3+\ldots \end{aligned}$$

Remember, solutions have to be normalizable. So let's look at the limit for large j. We have $a_{j+2}\approx\frac{2}{j}a_j$, or up to some constant $a_j\approx\frac{C}{(j/2)!}$. Thus:

$$\begin{aligned} h(\xi) &\approx C\sum\frac{j}{(j/2)!}\xi^j \\ &\approx C\sum\frac{1}{j!}\xi^{2j}\approx Ce^{\xi^2} \end{aligned}$$

Note that that would make the function ψ not normalizable. So something else has to be going on. We need to make sure the series of a's will terminate. Thus, there is an $a_n=0$. This ends the series of either the odd or the even part of h. The other one has to be 0 from the beginning ($a_1=0$ or $a_0=0$ depending on wether n is even or ordd). Thus:

$$K=2n+1$$

Remember what K is to get

$$E_n=\left(n+\frac{1}{2}\right)\hbar\omega \quad \text{for} \quad n=0,1,\ldots.$$

Using the allowed values for K, the recursion formula reads

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)}a_j$$

Suppose $n=0$, then there is only on term in the series (we have to set $a_1=0$ to kill h_{odd}). Thus:

$$h_0(\xi)=a_0$$

and hence

$$\psi_0(\xi)=a_0e^{-\xi^2/2}$$

Similarly for $n = 1$, we take $a_0 = 0$, giving us

$$h_1(\xi) = a_1\xi$$

and hence

$$\psi_1(\xi) = a_1\xi e^{-\xi^2/2}$$

Now let's look at $n = 2$. This yields

$$\begin{aligned} a_2 &= -2a_0 \\ a_4 &= 0 \end{aligned}$$

hence

$$h_2(\xi) = a_0(1 - 2\xi^2)$$

and

$$\psi_2(\xi) = a_0(1 - 2\xi^2)e^{-\xi^2/2}$$

And so on. Probably time to stop with the algebra. Apart from the overall normalization, the solutions are involve Hermite polynomials $H_n(\xi)$. The wavefunction has the general form of

$$\Phi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)e^{-\xi^2/2}$$

where

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} = \left(2x - \frac{d}{dx}\right)^n \cdot 1$$

The first part is called Rodrigues formula.

9 Quantum Mechanics in Three dimensions

9.1 Schroedinger Equation in Three dimensions

The time dependent Schroedinger equation is

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

Written in this way, this equation can already be interpreted as the three dimensional Schroedinger equation. We write the Hamiltonian as

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V(x, y, z)$$

Using the standard definitions for the momentum operators we get

$$\begin{aligned} H &= \frac{-\hbar^2}{2m}\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right) + V(x, y, z) \\ &= \frac{-\hbar^2}{2m}\nabla^2 + V(x, y, z). \end{aligned}$$

The operator ∇ is called the Laplacian, or `nabla` in LaTeX. We again normalize the wave function for physical states. The integral is now a three dimensional integral:

$$\int |\Phi| d^3r = 1.$$

If the Hamiltonian is independent of time, we can factor of the time dependent exponential just as in the one dimensional case to get the three dimensional time independent Schroedinger Equation

$$\begin{aligned} H\psi &= E\psi \\ -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi &= E\psi \end{aligned}$$

The time dependent solution is then

$$\Phi(x, y, z, t) = \sum c_n \Psi_n(x, y, z) e^{-iE_n t/\hbar}$$

9.2 Separation of variables

In most cases the potential is just a function of the radius

$$V(x, y, z) = V(r)$$

This motivates the introduction of spherical coordinates (r, θ, ϕ). In spherical coordinates the Laplacian takes the following form

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

So let's look for solutions to the Schroedinger Equation in the form of

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

Let's put this Ansatz in the Schroedinger Equation

$$-\frac{\hbar^2}{2m}\left(\frac{Y}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} R\right) + \frac{R}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta} Y\right) + \frac{R}{r^2 \sin^2\theta}\left(\frac{\partial^2}{\partial \phi^2} Y\right)\right) + VRY = ERY$$

Multiplying with $-2mr^2/(\hbar^2 RY)$ gives:

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} R\right) + \frac{1}{Y\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta} Y\right) + \frac{1}{Y \sin^2\theta}\left(\frac{\partial^2}{\partial \phi^2} Y\right) - \frac{2mr^2}{\hbar^2}(V - E) \quad = \quad 0$$

Our Ansatz worked! Note that only the first and last term depend on R. Only the middle two terms depend on ϕ and θ. Therefore, the two terms have to be constats to cancel each other. The constant can be any complex number. W.l.o.g. let us call this constant $l(l+1)$ for reasons that will become obvious in a second. We now have two equations

$$\begin{aligned} \frac{1}{R}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} R\right) - \frac{2mr^2}{\hbar^2}(V - E) &= l(l+1) \\ \frac{1}{Y\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta} Y\right) + \frac{1}{Y \sin^2\theta}\left(\frac{\partial^2}{\partial \phi^2} Y\right) &= -l(l+1) \end{aligned}$$

Let's look at both of those equations individually.

9.3 The Angular Equation

The equation we are trying to solve is

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

or equivalently

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

Let's try an Ansatz as follow

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

This gives (after dividing by $\Theta\Phi$)

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

In the same way we defined the constant $l(l+1)$ in the radial equation, we can agan see that this equation is only satisfied if we have a constant m^2 (arbitrary name) such that

$$\begin{aligned} \frac{1}{\Theta}\sin\theta \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\Theta\right) + l(l+1)\sin^2\Theta &= m^2 \\ \frac{1}{\Phi}\left(\frac{\partial^2}{\partial\phi^2}\Phi\right) &= -m^2 \end{aligned}$$

The last equation (the one for Φ) is easy to solve:

$$\Phi(\phi) = e^{im\phi}$$

Because of symmetry, we must have

$$\Phi(\phi + 2\pi) = \Phi(\phi)$$

It follows that only certain values of m are allowed

$$m = 0, \pm 1, \pm 2, \ldots$$

Let's look at the other equation

$$\sin\theta \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\Theta\right) + \Theta\left(l(l+1)\sin^2\Theta - m^2\right) = 0$$

This is harder to solve, so I'm giving you the answer:

$$\Theta(\theta) = A P_l^m(\cos\theta)$$

The P_l^m's are the associated Legendre functions, defined by

$$P_l^m(x) \equiv (1-x^2)^{|m|/2}\left(\frac{\partial}{\partial x}\right)^{|m|} P_l(x)$$

where P_l are the Lengendre polynomials

$$P_l(x) \equiv \frac{1}{2^l l!}\left(\frac{\partial}{\partial x}\right)^l (x^2-1)^l$$

The first few examples are

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= x \\ P_3(x) &= \frac{3}{2}x^2 - \frac{1}{2} \end{aligned}$$

The associated Legendre polynomials are in general not a polynomial. Here are a few examples:

$$\begin{aligned} P_0^0 &= 1 \\ P_1^0 &= x \\ P_1^1 &= -\sqrt{1-x^2} \\ P_1^{-1} &= \tfrac{1}{2}\sqrt{1-x^2} \end{aligned}$$

Lecture 6 Ends