

THE HERMITE POLYNOMIAL & QUANTIZATION OF THE HARMONIC OSCILLATOR

TIMOTHY JONES

ABSTRACT. The harmonic oscillator possesses a singular place in quantum mechanics. It is used in a wide variety of models. Here we outline the basics.

1. THE HARMONIC OSCILLATOR: A CLASSICAL OVERVIEW

Hooke first discovered the law of springs, that their force is proportional to their displacement. In reality, their force is generally a far more complicated function. In fact, many complicated forces can be approximated in a form similar to the harmonic oscillator. Consider the potential $U(x)$ describing some physical phenomenon. Close enough to the equilibrium point $x=a$, we can expand this function as a Taylor polynomial,

$$(1.1) \quad U(x) = U(a) + \overbrace{\left(\frac{\partial U(x)}{\partial x} = 0\right)}^{x=a} (x-a) + \frac{1}{2!} \overbrace{\left(\frac{\partial^2 U(x)}{\partial x^2}\right)}^{x=a} (x-a)^2 + \dots$$

Here the first derivative is zero, as we take the Taylor series around an equilibrium. How close is close enough? This would depend on the degree of accuracy one seeks, though generally it is assumed that

$$\frac{\left(\frac{\partial^3 U(x)}{\partial x^3}\right) (x-a)^3}{\left(\frac{\partial^2 U(x)}{\partial x^2}\right) (x-a)^2} \ll 1$$

We are at liberty to rescale our potential so that $U(a) = 0$, whereby we have the approximation,

$$(1.2) \quad U(x) = \frac{1}{2!} \left(\frac{\partial^2 U(x)}{\partial x^2}\right) (x-a)^2$$

It is typical to also rescale the x -axis so that $a = 0$ and, using common terminology,

$$U(x) = \frac{1}{2!} \left(\frac{\partial^2 U(x)}{\partial x^2}\right) x^2 \equiv \frac{1}{2} kx^2$$

Here k is a constant. The equation of motion for such an object becomes

$$\frac{dp}{dt} = -kx, \text{ typically } m \frac{d^2x}{dt^2} + kx = 0$$

Often it is more accurate to add a damping term, for example, a spring under water is better described by,

$$(1.3) \quad m \frac{d^2x}{dt^2} + \nu \frac{dx}{dt} + kx = 0$$

Here ν is some constant defined by the retarding force $F_r = -\nu \frac{dx}{dt}$. If a harmonic driving force is applied, Equation 1.3 becomes inhomogeneous,

$$(1.4) \quad m \frac{d^2x}{dt^2} + \nu \frac{dx}{dt} + kx = F_0 \cos(\omega t)$$

Equation 1.3 is easiest to solve. Let $\nu/m = \gamma$, $F_0/m \rightarrow A$, and $\omega_0^2 = k/m$. If we suppose the solution $x = \exp(rt)$,

$$(1.5) \quad x'' + \gamma x' + \omega_0^2 x = 0 \rightarrow r^2 + \gamma r + \omega_0^2 = 0 \ni r = \frac{-\gamma \pm \sqrt{\gamma^2 - 4\omega_0^2}}{2}$$

We seek a fundamental set of solutions to these equations. From the theory of differential equations we know that we require exactly two distinct solutions. The \pm in the solution to the characteristic equation lends us two such solutions, except in the case when $\gamma^2 = 4\omega_0^2$. In that case, our first solution is

$$(1.6) \quad x_1(t) = e^{-\gamma t/2}$$

The characteristic equation suggest no further solution. The method of reduction of order has us assume that

$$(1.7) \quad x(t) = v(t)x_1(t) = v(t)e^{-\gamma t/2}$$

Plugging Equation 1.7 into Equation 1.5, we find that $v''(t) = 0$ and so

$$v(t) = c_1 t + c_2 \ni x(t) = c_1 t e^{-\gamma t/2} + c_2 e^{-\gamma t/2}$$

The Wronskian of these two solutions is nonzero always, and so we have a fundamental set of solutions. The other cases are more easily solved and we find,

$$x(t) = \begin{cases} a_1 e^{-\gamma t/2} \exp(t\sqrt{\gamma^2 - 4\omega_0^2}/2) + a_2 e^{-\gamma t/2} \exp(-t\sqrt{\gamma^2 - 4\omega_0^2}/2) & \gamma - 4\omega_0^2 > 0 \\ b_1 t e^{-\gamma t/2} + b_2 e^{-\gamma t/2} & \gamma - 4\omega_0^2 = 0 \\ c_1 e^{-\gamma t/2} \exp(it\sqrt{-\gamma^2 + 4\omega_0^2}/2) + c_2 e^{-\gamma t/2} \exp(-it\sqrt{-\gamma^2 + 4\omega_0^2}/2) & \gamma - 4\omega_0^2 < 0 \end{cases}$$

The latter can be written,

$$x(t) = d_1 e^{-\gamma t/2} \cos(t\sqrt{-\gamma^2 + 4\omega_0^2}/2) + d_2 e^{-\gamma t/2} \sin(t\sqrt{-\gamma^2 + 4\omega_0^2}/2)$$

The driven Equation (1.4) is slightly more complicated to solve. In Equation 1.4 one can replace $\cos(\omega t)$ with $\exp(i\omega t)$ on the condition we take the real part of the solution to be found from this ‘‘axillary equation’’ [2]. If we suppose a solution $x_d(t) = A \exp(i(\omega t + \phi))$, we find,

$$(1.8) \quad (-\omega^2 A + \gamma i \omega A + \omega_0^2 A) e^{i(\omega t + \phi)} = (F_0/m) e^{i\omega t}$$

Dividing out the exponent on the left hand side and equating real and imaginary parts of the right yields,

$$\frac{A(\omega_0^2 - \omega^2)}{F_0/m} = \cos \phi, \quad \frac{\gamma \omega A}{F_0/m} = \sin \phi \ni \begin{cases} A = \frac{F_0}{m\sqrt{(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2}} \\ \phi = \tan^{-1} \left(\frac{\gamma \omega}{\omega^2 - \omega_0^2} \right) \end{cases}$$

The full solution to the driven damped harmonic oscillator is then,

$$(1.9) \quad X(t) = x(t) + x_d(t)$$

Here $x(t)$ is the solution to the homogeneous equation we found above (one of the three variations depending on the parameters). Or, since we enjoy seeing large equations in their full forms,

$$X(t) = \left. \begin{array}{l} a_1 e^{-\gamma t/2} e^{t\sqrt{\gamma^2 - 4\omega_0^2}/2} + a_2 e^{-\gamma t/2} e^{-t\sqrt{\gamma^2 - 4\omega_0^2}/2} \\ b_1 t e^{-\gamma t/2} + b_2 e^{-\gamma t/2} \\ c_1 e^{-\gamma t/2} e^{it\sqrt{-\gamma^2 + 4\omega_0^2}/2} + c_2 e^{-\gamma t/2} e^{-it\sqrt{-\gamma^2 + 4\omega_0^2}/2} \end{array} \right\} + \frac{F_0 e^{i(\omega t + \tan^{-1}(\frac{\gamma \omega}{\omega^2 - \omega_0^2}))}}{m\sqrt{(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2}}$$

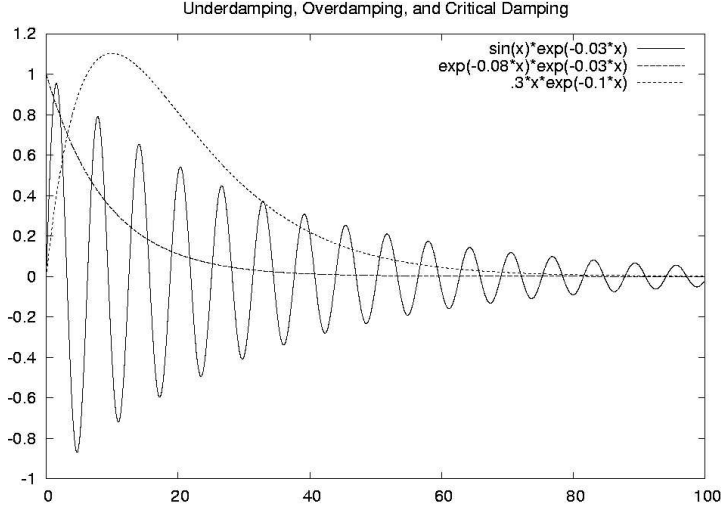


FIGURE 1.1. Examples of three possible solution types for the homogeneous damped harmonic equation.

2. ELEMENTARY QUANTIZATION OF THE HARMONIC OSCILLATOR IN ONE AND THREE DIMENSIONS IN COORDINATE REPRESENTATION

The one dimensional case can be extended easily to the three dimensional case; one might not be satisfied with such a solution. We will also demonstrate the solution in spherical coordinates. With a harmonic oscillator potential, Schrödinger's equation in one dimension becomes,

$$(2.1) \quad -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 = E\psi, \quad \eta = \sqrt{\frac{m\omega}{\hbar}}x, \quad K = \frac{2E}{\hbar\omega} \rightarrow \frac{d^2\psi}{d\eta^2} = (\eta^2 - K)\psi$$

A solution to this equation can be found with the traditional approach.

2.1. Asymptotic behavior and the Hermite Polynomial.

$$(2.2) \quad \begin{aligned} \eta \gg K : \quad \psi_{as}(\eta) = Ae^{-\eta^2/2} &\Rightarrow \psi(\eta) = Af(\eta)e^{-\eta^2/2} \\ \frac{d^2\psi}{d\eta^2} = \left(\frac{d^2f(\eta)}{d\eta^2} - 2\eta \frac{df(\eta)}{d\eta} + (\eta^2 - 1)f(\eta) \right) e^{-\eta^2/2} \\ \frac{d^2f(\eta)}{d\eta^2} - 2\eta \frac{df(\eta)}{d\eta} + (K - 1)f(\eta) &= 0 \end{aligned}$$

We introduce the ansatz, based on the middle term and the overall structure of Equation 2.2, that $f(\eta)$ will have a derivative-cyclic solution (such as the Legendre and Laguerre functions) with the kernel $\exp(-\eta^2)$. Indeed the first two derivatives suggest a correct direction,

$$(2.3) \quad \frac{d}{d\eta}e^{-\eta^2} = -2\eta e^{-\eta^2}, \quad \frac{d^2}{d\eta^2}e^{-\eta^2} = -2e^{-\eta^2} + 4\eta^2 e^{-\eta^2}$$

In accordance with the Laguerre polynomial solution (specifically the Rodriguez formulation), we would try the following solution:

$$(2.4) \quad f(\eta) = (-1)^n \alpha e^{\eta^2} \frac{d^n}{d\eta^n} e^{-\eta^2}$$

We sample the $n = 2$ case,

$$f_2(\eta) = \alpha(-2+4\eta^2), \quad f_2'(\eta) = \alpha 8\eta, \quad f_2''(\eta) = 8\alpha \rightarrow 8-2\eta(8\eta) + (K-1)(4\eta^2-2) = 0$$

This equation is satisfied when $K - 1 = 4$ or generally $K = 2n + 1$. This is the **quantization condition**. The reader might not be satisfied with our methodology, and so we wish to re-demonstrate this condition with another approach. Here we suppose a series solution to $f(\eta)$.

$$f(\eta) = \sum_{j=0}^{\infty} a_j \eta^j \longrightarrow \sum_{j=0}^{\infty} ((j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j) \eta^j = 0$$

$$(2.5) \quad a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)} a_j$$

As $j \rightarrow \infty$ the series will approach zero at a rate of $1/j$ which is a condition for divergence. We thus need the series to terminate for some $j = n \ni K = 2n + 1$ so that $a_{n+1} = 0$. From our definition of K , we have found the energy levels to be

$$(2.6) \quad E = (2n+1) \frac{\hbar\omega}{2}$$

2.2. Normalization of wave function. The solution we demonstrated is called a Hermite polynomial,

$$(2.7) \quad H(\eta) = (-1)^n e^{\eta^2} \frac{d^n}{d\eta^n} e^{-\eta^2}$$

Properties of this function can be found with repeated activation of the derivatives,

$$\begin{aligned} H_n(\eta) &= (-1)^n e^{\eta^2} \frac{d^{n-1}}{d\eta^{n-1}} (-2\eta e^{-\eta^2}) \\ &= (-1)^n e^{\eta^2} \frac{d^{n-2}}{d\eta^{n-2}} \left(-2e^{-\eta^2} - 2\eta \frac{d}{d\eta} e^{-\eta^2} \right) \\ (2.8) \quad &= (-1)^n e^{\eta^2} \frac{d^{n-3}}{d\eta^{n-3}} \left(-2 \frac{d}{d\eta} e^{-\eta^2} - 2 \frac{d}{d\eta} e^{-\eta^2} - 2\eta \frac{d^2}{d\eta^2} e^{-\eta^2} \right) \end{aligned}$$

A continuation of this activation would thus find,

$$(2.9) \quad H_n(\eta) = -2(n-1)H_{n-2} + 2\eta H_{n-1} \rightarrow H_{n+1} = -2nH_{n-1} + 2\eta H_n$$

This implies that,

$$\begin{aligned} \frac{d}{d\eta} H_n(\eta) &= 2\eta(-1)^n e^{\eta^2} \frac{d^n}{d\eta^n} e^{-\eta^2} + (-1)^n e^{\eta^2} \frac{d^{n+1}}{d\eta^{n+1}} e^{-\eta^2} \\ (2.10) \quad &= 2\eta H_n(\eta) - H_{n+1}(\eta) = 2nH_{n-1}(\eta) \end{aligned}$$

The normalization equation is, via integration by parts,

$$(2.11) \quad \int \psi_n^*(\eta) \cdot \psi_n(\eta) dx = A^2 \sqrt{\frac{\hbar}{m\omega}} \int \left(\frac{d^{n-1}}{d\eta^{n-1}} e^{-\eta^2} \right) \cdot H'_n(\eta) d\eta = 1$$

Use of Equation 2.10 and repeated integration by parts will diminish the stand-alone derivative and the Hermite polynomial until we have,

$$(2.12) \quad A^2 \sqrt{\frac{\hbar}{m\omega}} 2^n n! \int e^{-\eta^2} = A^2 \sqrt{\frac{\hbar}{m\omega}} 2^n n! \sqrt{\pi} = 1$$

Thus we have

$$(2.13) \quad \psi_n(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{e^{-\eta^2/2}}{\sqrt{2^n n!}} \left((-1)^n e^{\eta^2} \frac{d^n}{d\eta^n} e^{-\eta^2} \right)$$

Where a most general solution is

$$\Psi = \sum_{n=0}^{\infty} C_n \psi_n$$

Here C_n are coefficients which can only be determined when the specific physical situation is given.

3. THE SPHERICAL HARMONIC OSCILLATOR

Next we consider the solution for the three dimensional harmonic oscillator in spherical coordinates.

It is obvious that our solution in Cartesian coordinates is simply,

$$(3.1) \quad E = \hbar\omega \left(n_x + n_y + n_z + \frac{3}{2} \right)$$

Less simple, but more edifying is the case in spherical coordinates. With the conversions,

$$(3.2) \quad \begin{aligned} x &= r \sin \theta \cos \phi \\ y &= r \sin \theta \sin \phi \\ z &= r \cos \theta \end{aligned}$$

we have,

$$(3.3) \quad \begin{pmatrix} dx \\ dy \\ dz \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \phi & r \cos \theta \cos \phi & -r \sin \theta \sin \phi \\ \sin \theta \sin \phi & r \cos \theta \sin \phi & r \sin \theta \cos \phi \\ \cos \theta & -r \sin \theta & 0 \end{pmatrix} \begin{pmatrix} dr \\ d\theta \\ d\phi \end{pmatrix}$$

We invert the matrix,

$$(3.4) \quad \begin{vmatrix} \sin \theta \cos \phi & r \cos \theta \cos \phi & -r \sin \theta \sin \phi \\ \sin \theta \sin \phi & r \cos \theta \sin \phi & r \sin \theta \cos \phi \\ \cos \theta & -r \sin \theta & 0 \end{vmatrix} \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \\ \begin{vmatrix} 1 & 0 & 0 \\ 0 & 0 & r \sin \theta \\ 0 & r & 0 \end{vmatrix} \begin{vmatrix} \sin \theta \cos \phi & \sin \phi \sin \theta & \cos \theta \\ -\sin \phi & \cos \phi & 0 \\ \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \end{vmatrix}$$

Thus,

$$(3.5) \quad \begin{pmatrix} dr \\ d\theta \\ d\phi \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \phi & \sin \phi \sin \theta & \cos \theta \\ \frac{1}{r} \cos \theta \cos \phi & \frac{1}{r} \cos \theta \sin \phi & -\frac{1}{r} \sin \theta \\ -\frac{\sin \phi}{r \sin \theta} & \frac{\cos \phi}{r \sin \theta} & 0 \end{pmatrix} \begin{pmatrix} dx \\ dy \\ dz \end{pmatrix}$$

Of course,

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi}$$

So we also have,

$$(3.6) \quad \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \phi & \frac{1}{r} \cos \theta \cos \phi & -\frac{\sin \phi}{r \sin \theta} \\ \sin \theta \sin \phi & \frac{1}{r} \cos \theta \sin \phi & \frac{\cos \phi}{r \sin \theta} \\ \cos \theta & \frac{1}{r} \sin \theta & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \phi} \end{pmatrix}$$

Here we begin an aside on the angular momentum operators. This will be useful because it will bring us half the solution. We have,

$$(3.7) \quad \begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} = \begin{pmatrix} 0 & -z & y \\ z & 0 & -x \\ -y & x & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix}$$

We convert this,

$$r \begin{pmatrix} 0 & -\cos \theta & \sin \theta \sin \phi \\ \cos \theta & 0 & -\sin \theta \cos \phi \\ -\sin \theta \sin \phi & \sin \theta \cos \phi & 0 \end{pmatrix} \begin{pmatrix} \sin \theta \cos \phi & \frac{1}{r} \cos \theta \cos \phi & -\frac{\sin \phi}{r \sin \theta} \\ \sin \theta \sin \phi & \frac{1}{r} \cos \theta \sin \phi & \frac{\cos \phi}{r \sin \theta} \\ \cos \theta & \frac{1}{r} \sin \theta & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \phi} \end{pmatrix}$$

We let

$$u = \begin{pmatrix} \cos \phi \\ \sin \phi \end{pmatrix}, \quad u' = \frac{du}{d\phi}, \quad A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

We quickly note that $Au = u'$ and u and u' are orthogonal, so we have:

$$(3.8) \quad \begin{pmatrix} L_{xy} \\ L_z \end{pmatrix} = \begin{pmatrix} rA \cos \theta & -r \sin \theta Au \\ r \sin \theta u'^T & 0 \end{pmatrix} \begin{pmatrix} \sin \theta u & \frac{\cos \theta}{r} u & \frac{u'}{r \sin \theta} \\ \cos \theta & -\frac{\sin \theta}{r} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \phi} \end{pmatrix}$$

$$(3.9) \quad \begin{pmatrix} L_{xy} \\ L_z \end{pmatrix} = \begin{pmatrix} 0 & Au & Au' \cot \theta \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \phi} \end{pmatrix}$$

Properly, none of the terms involves ∂r . Throwing in the proper $\frac{\hbar}{i}$ we find,

$$(3.10) \quad \begin{pmatrix} L_x \\ L_y \end{pmatrix} = \frac{\hbar}{i} \begin{pmatrix} -\sin \phi \\ \cos \phi \end{pmatrix} \frac{\partial}{\partial \theta} - \cot \theta \begin{pmatrix} \cos \phi \\ \sin \phi \end{pmatrix} \frac{\partial}{\partial \phi}, \quad L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$$

With some algebra we can show that

$$(3.11) \quad L^2 = L_x^2 + L_y^2 + L_z^2 = -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$

We know that $L^2 Y(\theta, \phi) = \hbar^2 l(l+1) Y(\theta, \phi)$. We also have that the Laplacian in spherical coordinates is,

$$\begin{aligned} \nabla^2 &= \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \\ \nabla^2 &= \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{L^2}{\hbar^2 r^2} \end{aligned}$$

(3.13)

Thus, in three dimensions and spherical coordinates, the Schrödinger equation is,

$$(3.14) \quad -\frac{\hbar}{2m} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) \psi + \frac{L^2}{2mr^2} \psi + V\psi = E\psi$$

By separation of variables, the radial term and the angular term can be divorced. The solution to the angular equation are hydrogeometrics. The reader is referred to the supplement on the basic hydrogen atom for a detailed and self-contained derivation of these solutions. Our resulting radial equation is, with the Harmonic potential specified,

$$(3.15) \quad \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) R + \frac{2m}{\hbar^2} \left(E - \frac{m}{2} \omega^2 r^2 - \frac{l(l+1)\hbar^2}{2mr^2} \right) R = 0$$

We can quickly solve this equation by applying the SAP method (Simplify, Asymptote, Power Series). We set the stage by first rewriting the above equation in a form which will later simplify our process,

$$(3.16) \quad \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) R + \left(-\frac{m^2 \omega^2}{\hbar^2} \quad \frac{2mE}{\hbar^2} \quad -l(l+1) \right) \begin{pmatrix} r^2 \\ 1 \\ \frac{1}{r^2} \end{pmatrix} R = 0$$

Write $\mathcal{U}^2 = \frac{m^2 \omega^2}{\hbar^2}$, then our first asymptote is towards infinity where the r^2 terms dominate; our second is towards zero where $1/r^2$ dominates and we find that

$$(3.17) \quad \frac{d^2 R}{dr^2} \propto \mathcal{U}^2 r^2 R \implies R \propto e^{\mathcal{U} r^2 / 2}$$

The next term is,

$$(3.18) \quad \frac{d^2 R}{dr^2} \propto \frac{2}{r} \frac{dR}{dr} \text{ @ } r \ll 1 \implies \frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} \propto \frac{l(l+1)}{r^2} R$$

To solve such equations, we suppose there exist a function $z(r)$ which will bring this equation into a more conventionally solvable form. We will determine what z is by the consequences of this demand. With

$$\begin{aligned} \frac{dR}{dr} &= \frac{dR}{dz} \frac{dz}{dr} \equiv R' \frac{dz}{dr} \\ \frac{d^2 R}{dr^2} &= R'' \left(\frac{dz}{dr} \right)^2 + R' \left(\frac{d^2 z}{dr^2} \right) \end{aligned}$$

We now solve

$$(3.19) \quad R'' \left(\frac{dz}{dr} \right)^2 + R' \left(\frac{d^2 z}{dr^2} + \frac{2}{r} \frac{dz}{dr} \right) - \frac{l(l+1)}{r^2} R = 0$$

This equation is solvable if the coefficients are proportional, or even better, equal:

$$(3.20) \quad \frac{dz}{dr} = \frac{\sqrt{l(l+1)}}{r} \implies R'' \sqrt{l(l+1)} + R' - \sqrt{l(l+1)} R = 0$$

This equation has solutions easily found as,

$$(3.21) \quad R = A \exp \left(-\frac{l+1}{\sqrt{l(l+1)}} z(r) \right) + B \exp \left(\frac{l}{\sqrt{l(l+1)}} z(r) \right)$$

But we can solve for z and find that $z = \sqrt{l(l+1)} \ln(r)$, whereby,

$$R = A r^{-(l+1)} + B r^l$$

We dismiss A since we are considering the infinitesimally near zero asymptote. Next we suppose our complete solution is a power series via,

$$(3.22) \quad R = r^l e^{-\mathfrak{U}r^2/2} \sum_k a_k r^k = \sum_k a_k r^{(k+l)} e^{-\mathfrak{U}r^2/2}$$

Our first derivative is,

$$\begin{aligned} \frac{dR}{dr} &= \sum_k a_k \left((k+l) r^{k+l-1} e^{-\mathfrak{U}r^2/2} - \mathfrak{U} r^{k+l+1} e^{-\mathfrak{U}r^2/2} \right) \\ &= \sum_k a_k r^{(k+l)} e^{-\mathfrak{U}r^2/2} \left(-\mathfrak{U} \quad k+l \right) \begin{pmatrix} r \\ \frac{1}{r} \end{pmatrix} \\ (3.23) \quad \frac{2}{r} \frac{dR}{dr} &= \sum_k a_k r^{(k+l)} e^{-\mathfrak{U}r^2/2} \left(-2\mathfrak{U} \quad 2(k+l) \right) \begin{pmatrix} 1 \\ r^{-2} \end{pmatrix} \end{aligned}$$

Our second derivative is,

$$\begin{aligned} &\sum_k a_k \left((k+l)(k+l-1) r^{k+l-2} e^{-\mathfrak{U}r^2/2} - \mathfrak{U}(2k+2l+1) r^{k+l} e^{-\mathfrak{U}r^2/2} + \mathfrak{U}^2 r^{k+l+2} e^{-\mathfrak{U}r^2/2} \right) \\ &= \sum_k a_k r^{k+l} e^{-\mathfrak{U}r^2/2} \left(\mathfrak{U}^2 \quad -\mathfrak{U}(2k+2l+1) \quad (k+l)(k+l-1) \right) \begin{pmatrix} r^2 \\ 1 \\ r^{-2} \end{pmatrix} \end{aligned}$$

Recalling that,

$$(3.24) \quad \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) R + \left(-\mathfrak{U}^2 \quad \frac{2mE}{\hbar^2} \quad -l(l+1) \right) \begin{pmatrix} r^2 \\ 1 \\ \frac{1}{r^2} \end{pmatrix} = 0$$

our net equation thus requires that

$$a_k r^{k+l} e^{-\mathcal{U}r^2/2} \left(\frac{2mE}{\hbar^2} - \mathcal{U}(2k+2l+3) \quad (k+l)(k+l+1) - l(l+1) \right) \left(\frac{1}{r^{-2}} \right) = 0$$

Or more simply,

$$(3.25) \quad r^{k+l} e^{-\mathcal{U}r^2/2} \left(\frac{2mE}{\hbar^2} - \mathcal{U}(2k+2l+3) \quad k(k+2l+1) \right) \left(\frac{a_k}{a_k r^{-2}} \right) = 0$$

We seek to match the coefficients of r , since they must vanish independently, whereby,

$$(3.26) \quad r^{k+l} e^{-\mathcal{U}r^2/2} \left(\frac{2mE}{\hbar^2} - \mathcal{U}(2k+2l+3) \quad (k+2)(k+2l+3) \right) \left(\frac{a_k}{a_{k+2}} \right) = 0$$

This gives us the recursion relation,

$$(3.27) \quad a_{k+2} = \frac{-\frac{2mE}{\hbar^2} + \mathcal{U}(2k+2l+3)}{(k+2)(k+2l+3)} a_k$$

Requiring this series to terminate to prevent non-physical behavior is our quantization condition, whereby we must have,

$$(3.28) \quad \exists k_f \ni \frac{2mE}{\hbar^2} - \mathcal{U}(2k_f+2l+3) = 0 \implies E = \hbar\omega \left(k_f + l + \frac{3}{2} \right)$$

This recursion relationship and eigenvalue formula thus define a three dimensional harmonic oscillator.

4. ALGEBRAIC SOLUTION

The time independent Schrödinger equation for this first order potential approximation is:

$$(4.1) \quad \begin{aligned} & -\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi \\ & \frac{1}{2m} \left(\left(\frac{\hbar}{i} \frac{d}{dx} \right)^2 + (m\omega x)^2 \right) \psi = E\psi \\ & \frac{1}{2m} \left(\left(\frac{\hbar}{i} \frac{d}{dx} - im\omega x \right) \left(\frac{\hbar}{i} \frac{d}{dx} + im\omega x \right) - \frac{\hbar\omega}{2} \right) \psi = E\psi \\ & \left(a_- a_+ - \frac{\hbar\omega}{2} \right) \psi = E\psi \end{aligned}$$

Here we have:

$$(4.2) \quad a_{\pm} = \frac{1}{\sqrt{2m}} \left(\frac{\hbar}{i} \frac{d}{dx} \pm im\omega x \right)$$

It is easy to show that $a_- a_+ - a_+ a_- = \hbar\omega$, and as well, we have:

$$(4.3) \quad \left(a_+ a_- + \frac{\hbar\omega}{2} \right) \psi = E\psi$$

We now introduce the following chain of logic:

$$\begin{aligned}
& \left(a_+ a_- + \frac{\hbar\omega}{2} \right) (a_+ \psi) = \left(a_+ a_- a_+ + \frac{\hbar\omega a_+}{2} \right) \psi \\
& = a_+ \left(\left(a_- a_+ - \frac{\hbar\omega}{2} \right) \psi + \hbar\omega \psi \right) = (E + \hbar\omega) (a_+ \psi) \\
& \left(a_+ a_- + \frac{\hbar\omega}{2} \right) (a_+ \psi) = (E + \hbar\omega) (a_+ \psi) \\
(4.4) \quad \text{As well, } & \left(a_- a_+ - \frac{\hbar\omega}{2} \right) (a_- \psi) = (E - \hbar\omega) (a_- \psi)
\end{aligned}$$

It is now obvious to see why a_+ is called the raising operator and a_- is called the lowering operator. We do of course require a minimum lowering, a ground level. This requirement puts upon us that $\exists \psi_o \ni a_- \psi_o = 0 \implies \psi_o(x) = A_o e^{-\frac{m\omega}{2\hbar} x^2}$. We finally conclude that $E_o = \hbar\omega/2$, and

$$(4.5) \quad \psi_n(x) = A_n (a_+)^n e^{-\frac{m\omega}{2\hbar} x^2}, \quad E_n = (n + 1/2)\hbar\omega$$

4.1. Fock states and a more mature development of the algebraic solution. A more canonical approach to the previous section is as follows. We write the Hamiltonian as

$$(4.6) \quad H = \frac{1}{2m} P^2 + \frac{m\omega^2}{2} Q^2$$

This can be written dimensionlessly with the introduction of substitute operators,

$$(4.7) \quad q = \sqrt{\frac{m\omega}{\hbar}} Q$$

$$(4.8) \quad p = \sqrt{\frac{1}{m\hbar\omega}} P$$

$$(4.9) \quad H = \frac{\hbar\omega}{2} (p^2 + q^2)$$

In parallel with the previous section, we consider the operators,

$$(4.10) \quad a = \frac{q + ip}{\sqrt{2}}$$

$$(4.11) \quad a^\dagger = \frac{q - ip}{\sqrt{2}}$$

$$(4.12) \quad H = \frac{\hbar\omega}{2} (aa^\dagger + a^\dagger a)$$

From basic quantum mechanics we know that $[Q, P] = i\hbar$, thus $[q, p] = i$, and so $[a, a^\dagger] = 1$, whereby

$$(4.13) \quad H = \frac{1}{2} \hbar\omega (aa^\dagger + a^\dagger a) = \hbar\omega (aa^\dagger - \frac{1}{2}) = \hbar\omega (a^\dagger a + \frac{1}{2})$$

The Hamiltonian thus shares its eigenvalue spectrum with $N = a^\dagger a$, and

$$(4.14) \quad [N, a] = a^\dagger a a - a a^\dagger a = [a^\dagger, a] a = -a$$

$$(4.15) \quad [N, a^\dagger] = a^\dagger a a^\dagger - a^\dagger a^\dagger a = a^\dagger [a, a^\dagger] = a^\dagger$$

Thus we find,

$$(4.16) \quad N|n\rangle = n|n\rangle \implies Na|n\rangle = a(N-1)|n\rangle = (n-1)a|n\rangle$$

$$(4.17) \quad Na^b|n\rangle = (n-b)a^b|n\rangle$$

Thus $a^b|n\rangle$ is an eigenvector of N with eigenvalues $n - b$. We require these eigenvalues be positive for the following reason. An operator is required to have a real expectation value since the expectation value is what we would measure, i.e. we require that for an operator R ,

$$\langle\psi|R|\psi\rangle = \langle\psi|R|\psi\rangle^*$$

This implies R is Hermitian, and given $R|\psi\rangle = r|\psi\rangle$ then we have,

$$\langle\psi|R|\psi\rangle = r\langle\psi|\psi\rangle = \langle\psi|R|\psi\rangle^* = r^*\langle\psi|\psi\rangle$$

Since the eigenvalues are real, then the squared norm of these eigenvectors follow the form:

$$(4.18) \quad (\langle n|a^\dagger)(a|n\rangle) = \langle n|N|n\rangle = n\langle n|n\rangle \geq 0$$

and so we conclude that there must be a $n - b = 0$ cutoff

As well,

$$(4.19) \quad Na^\dagger|n\rangle = a^\dagger(N+1)|n\rangle = (n+1)a^\dagger|n\rangle$$

$$(4.20) \quad (\langle n|a)(a^\dagger|n\rangle) = (n+1)\langle n|n\rangle$$

We compare equation 22 with the fact that $N|n+1\rangle = (n+1)|n+1\rangle$ and conclude that

$$(4.21) \quad a^\dagger|n\rangle = |n+1\rangle \implies |C_n|^2 = (\langle n|a)(a^\dagger|n\rangle) = (n+1) \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

A similar argument yields $a|n\rangle = \sqrt{n}|n-1\rangle$. It follows that

$$(4.22) \quad |n\rangle = \frac{a^{\dagger n}|0\rangle}{\sqrt{n!}}$$

These are the so-called Fock states.

REFERENCES

- [1] W. E. Boyce, R. C. DiPrima, *Elementary Differential Equations and Boundary Value Problems*, (John Wiley & Sons, Inc., 1996)
- [2] Wikipedia contributors, "Harmonic oscillator," *Wikipedia, The Free Encyclopedia*, http://en.wikipedia.org/w/index.php?title=Harmonic_oscillator&oldid=40874822 (accessed March 1, 2006).