Notes on Solution of the Time Independent Schrödinger Equation (TISE) for the Simple Harmonic Oscillator

October 12, 1995

Massachusetts Institute of Technology

Department of Physics

Physics 8.04 October 12, 1995

The problem of the simple harmonic oscillator, where a particle of ass m moves in the potential

$$V(x) = \frac{1}{2}m\omega^2 x^2,$$

plays an important role in the understanding of a wide range of physical phenomena. Small oscillations of systems about their equilibrium configurations may be understood in the context of harmonic motions.

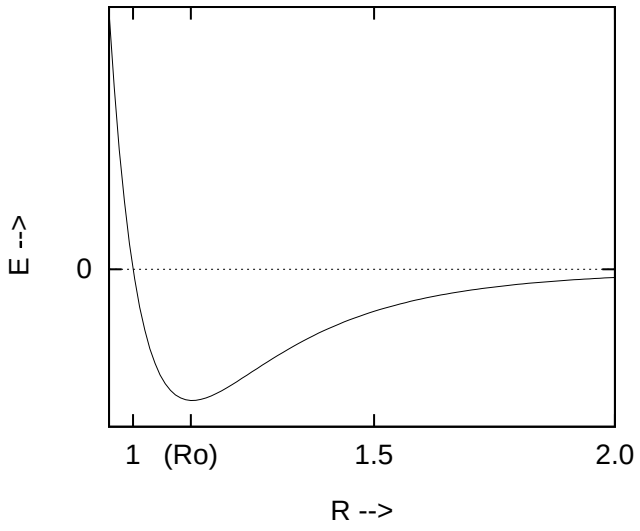
Vibrations of diatomic molecules provide perhaps the simplest example of this. The potential energy as a function of the distance R between two atoms in a diatomic molecule appears as in Figure .

For small motions about the equilibrium separation $R = R_o$ (point of minimum energy), the derivative of the potential $V'(R_o)$ is zero and the potential is harmonic to second order,

$$\begin{aligned} V(R) &\approx V(R_o) + \frac{1}{2}V''(R_o)(R - R_{min})^2 \\ &= V(R_o) + \frac{1}{2}\mu\omega^2(R - R_o)^2. \end{aligned}$$

Here we have defined ω so that $\mu\omega^2 \equiv V''(R_o)$ where μ is the *reduced* mass of the diatomic molecule, $\mu \equiv m_1 m_2/(m_1 + m_2)$. In the spectra of diatomic molecules one indeed finds the signature of a harmonic oscillator with frequency given by the above formula. The vibrations of more complex systems such as polyatomic molecules with hundreds of atoms or even solids with $\mathcal{O}(10^23)$ atoms, may be decomposed into the oscillations of collections of independent simple harmonic oscillators. The energy quanta of these mechanical vibrations are referred to as *phonons*.

The utility of the harmonic oscillator solutions goes beyond simple mechanical systems. As we learned from Planck's experience with cavity radiation, the oscillatory modes of electromagnetic radiation may be described as harmonic oscillators. We have already called the energy quanta of these oscillations *photons*. There are more esoteric examples as well. The tiny dipole moments in a magnetic solid may be set into oscillatory motions. The energy quanta of these oscillations are known as *magnons*. Finally, in particle physics, the processes by which particles are created and destroyed may be described using the same mathematics which describes the addition or removal, respectively, of energy quanta from a harmonic oscillator.



In this set of notes, we will discuss the wavefunctions and eigenenergies of the simple harmonic oscillator Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2. \tag{1}$$

This Hamiltonian gives rise to the following time independent Schrödinger equations, in the position and momentum representations respectively,

$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x) + \frac{m\omega^2}{2}x^2\psi(x) = E\psi(x) \tag{2}$$

$$\frac{\hbar^2}{2m}k^2\tilde{\psi}(k) - \frac{m\omega^2}{2}\partial_k^2\tilde{\psi}(k) = E\tilde{\psi}(k). \tag{3}$$

To find the eigenenergies and eigenstates of this system, we will proceed in three steps. First in Section 1, we will perform a *dimensional analysis* on the TISE for this problem. As we will see, dimensional analysis is a procedure by which many of the constants in an equation may be removed. This helps both to simplify the algebra and to foster insight into the deeper structure behind the equations. Next in Section 2, we will note that from the structure of the *dimensionless* TISE we can guess the solutions by *inspection*! The form of the solutions which we find in Section 2 will then lead us to a general form for the solution of the TISE for the SHO which will allow a full formal analysis of the states of the Hamiltonian (1) in Section 3.

1 Dimensional Analysis

1.1 Motivation and General Idea

In the *cgs* system of units we have been using throughout this course, there are just three fundamental *dimensions*, or types of physical quantities: *distance* L (measured in *units* of cm), *mass* M (measured in *units* of gm) and *time* T (measures in *units* of sec). *Dimension* refers to the type of physical quantity being measured (distance, mass, time) and *unit* refers to the amount of that quantity which we agree to call one one unit (1 cm, 1 gm, 1 sec). Note that the *cgs* system has no basic dimension

of charge because the cgs unit of charge is defined as the amount of charge needed to produce a unit force between two objects at a unit distance and thus requires the introduction of no additional *dimension*. The *unit* of charge in this system (the *esu*), on the other hand, does scale with the units of the fundamental dimensions; if we changed the unit of distance then the amount of charge required to produce a unit force at a unit distance would change.

The fundamental *cgs units* of 1 cm, 1 gm, and 1 sec were chosen for historical reasons; we can we can imagine different worlds in which all of the formulas of physics are the same but where the numerical values which we insert for the experimental constants in our equations are different. Rather than accept these historical dimensional units, we can take a more active role and make our own judicious choice of units for each problem at hand, picking our own most convenient unit distance, mass and time. For the purposed of this discussion we will name them 1 ud, 1 um and 1 ut respectively, for one "unit distance," one "unit mass," and one "unit time," respectively. These new units correspond to some amount of the standard cgs units. Calling these amounts x_0, m_0 and t_0, respectively, we have the conversions 1 $ud = x_0 \times 1\ cm$, 1 $um = m_0 \times 1\ gm$, and 1 $um = t_0 \times 1\ sec$.

Having moved to different units for the fundamental dimensions of length, mass and time, will we also have different units for all compound, or derived, dimensions such as *force* (*mass times length times time*$^{-2}$) or *energy* (*mass times length*^{2} *times time*$^{-2}$). We arrive at the units of these physical quantities through the familiar procedure of changing units. A table of examples of the conversion procedure for the basic dimensions and some dimensions of other common physical quantities is given in the table below.

TABLE I: GENERAL DIMENSIONAL ANALYSIS

Physical Quantity	New Unit & Conversion to Traditional Unit
Distance	$1\ ud = x_0 \cdot 1\ cm$
Mass	$1\ um = m_0 \cdot 1\ gm$
Time	$1\ ut = t_0 \cdot 1\ sec$
Frequency	$1\ rad\, ut^{-1} = 1\ rad\, (t_0\ sec)^{-1} = t_0^{-1} \cdot 1\ rad\, sec^{-1}$
Momentum	$1\ um\, ud\, ut^{-1} = (m_0\ gm)(x_0\ cm)(t_0\ sec)^{-1} = \frac{m_0 x_0}{t_0} \cdot 1\ gm\, cm\, sec^{-1}$
Angular Momentum	$1\ um\, ud^2\, ut^{-1} = 1\ (m_0\ gm)(x_0\ cm)^2(t_0\ sec)^{-1} = \frac{m_0 x_0^2}{t_0} \cdot 1\ gm\, cm^2\, sec^{-1}$
Energy	$1\ um\, ud^2\, ut^{-2} = 1\ (m_0\ gm)(x_0\ cm)^2(t_0\ sec)^{-2} = \frac{m_0 x_0^2}{t_0^2} \cdot 1\ gm\, cm^2\, sec^{-2}$

1.2 Application to the SHO: choice of "natural" units

Rather than working in units where mass in measured in gm, the most natural unit of mass for the problem of the SHO (2) is to take the mass of the oscillating particle to be *the* unit mass for the problem. Mathematically, 1 $um \equiv m$, or equivalently $m_0 = (m/1\ gm)$ so that m_0 is just the *numerical* value of the mass of the particle when measured in gm. Perhaps the most intuitive unit of time for the problem would be the period of the oscillator. However, this choice leads to a proliferation of factors of 2π in formulae. A more natural choice is the amount of time it takes for the oscillator to move through 1 rad of phase, this will set the value of the angular frequency within our unit system to be $\omega = 1\ rad\, ut^{-1}$. From the general conversions in TABLE I, we see that $1\ rad\ ut^{-1} = t_0^{-1} \cdot 1\ rad\ sec^{-1}$, and our choice thus sets the value $t_0^{-1} = (\omega/1 rad sec^{-1})$ so that the inverse of the natural unit of time is the numerical value of the frequency of the oscillator when measured in the traditional unit of 1 $rad\ sec^{-1}$.

Having set um and ut, there remains one basic unit to fix, the unit distance. Their also remains one final experimental constant remains in the TISE for the SHO, $\hbar$. It is a general feature of dimensional analysis that choosing units for three independent dimensions completely determines the new system of units. In our case, the most convenient choice for the unit distance is one where the numerical value of $\hbar$ is 1 $um\, ud^2\, ut^{-1}$. This fixes $1\ um\ ud^2\ ut^{-1} = \hbar = \frac{m_0 x_0^2}{t_0} 1\ gm\ cm^2\ sec^{-1}$ so that $x_0 = \left(\frac{(\hbar/1\ gm\, cm^2\, sec^{-1}) t_0}{m_0}\right)^{1/2} = \left(\frac{(\hbar/1\ gm\, cm^2\, sec^{-1})}{(m/1\ gm)(\omega/1\ rad\, sec^{-1})}\right)^{1/2} = \left(\frac{\hbar}{m\omega}\right)^{1/2}/(1\ cm)$, which sets $1\ ud = \left(\frac{\hbar}{m\omega}\right)^{1/2}$.

With the units for the basic dimensions determined, we may now generate the basic units for all physical quantities by inserting the choices we have made for the basic units, m_0, t_0 and x_0 in the table above. The results of doing this we summarize in the table below. Note that the results are always just the only combination of powers of m, ω and $\hbar$ that have the appropriate dimensions.

TABLE II: DIMENSIONAL ANALYSIS OF THE HARMONIC OSCILLATOR	
Physical Quantity	New Unit & Conversion to Traditional Unit
Distance	$1\ ud = \left(\frac{\hbar}{m\omega}\right)^{1/2}$
Mass	$1\ um = m$
Time	$1\ ut = \omega^{-1}$
Frequency	$1\ rad\, ut^{-1} = \omega$
Momentum	$1\ um\, ud\, ut^{-1} = (\hbar m\omega)^{1/2}$
Angular Momentum	$1\ um\, ud^2\, sec^{-1} = \hbar$
Energy	$1\ um\, ud^2\, sec^{-2} = \hbar\omega$

In our new system of units $m = 1\ um$, $\omega = 1\ ut^{-1}$ and $\hbar = 1\ um\, ud^2\, ut^{-1}$ and the TISE, in the position and momentum representations respectively, reads

$$\begin{aligned} -\frac{1}{2}\partial_X^2\Psi(X) + \frac{1}{2}X^2\Psi(X) &= \mathcal{E}\Psi(X) \\ \frac{1}{2}K^2\tilde{\Psi}(K) - \frac{1}{2}\partial_K^2\tilde{\Psi}(K) &= \mathcal{E}\tilde{\Psi}(K), \end{aligned} \tag{4}$$

Here we adopt the notation that quantities measured in our new system of units always appear as either capital or calligraphic letters.

The conversion from quantities expressed in the natural units for this problem and the standard *cgs* units is straight forward using Table II. For instance, the traditional value of energies E will just be the values we compute in our new units $\mathcal{E}$ times the new unit of energy $\hbar\omega$. Thus an energy of $\mathcal{E} = 1/2\ um\ ud^2\ ut^{-2}$ corresponds to an energy of $E = \hbar\omega/2$. It is common practice to drop writing our specialized units and write simply $\mathcal{E} = 1/2 \Rightarrow E = 1/2\hbar\omega$. Similarly, a distance or position $X = 1$ as measured in the new system corresponds to $x = \left(\frac{\hbar}{m\omega}\right)^{1/2}$ in the traditional system.

With the relation between basic quantities defined, the relationship between functions may then be determined by physical reasoning. For instance, the probability of finding the particle with a position in the range with of traditional positions $x' < x < x' + dx$ corresponds to finding the position as measured in the new system in the range $x'/x_0 < X < (x' + dx)/x_0 = (x'/x_0) + (dx/x_0)$, thus $|\psi(x')|^2 dx = |\Psi(X'/x_0)|^2 dx/x_0$. Hence, given $\Psi(X)$ in the new system we can always convert it to a traditional $\psi(x)$ through

$$\psi(x) = \frac{1}{\sqrt{x_0}}\Psi\left(\frac{x}{x_0}\right). \tag{5}$$

2 Self-trasnform property of the states of the SHO

One of the benefits of performing the dimensional analysis is removing the clutter of the constants from (2) and highlighting the striking similarity between the position and momentum representation equations. If we rewrite the two equations in (4) using U as the dummy argument,

$$\begin{aligned} -\frac{1}{2}\Psi''(U) + \frac{1}{2}U^2\Psi(U) &= \mathcal{E}\Psi(U) \\ -\frac{1}{2}\tilde{\Psi}''(U) + \frac{1}{2}U^2\tilde{\Psi}(U) &= \mathcal{E}\tilde{\Psi}(U). \end{aligned}$$

we see that Ψ and $\tilde{\Psi}$ both solve precisely the same one dimensional Schrödinger's equation with *the same eigenvalue* $\mathcal{E}$! Because there is at most one linearly independent solution for a given energy for the TISE with finite potential in one dimension, we conclude that $\tilde{\Psi}$ and Ψ must be the same

up to a proportionality constant, $\tilde{\Psi} \propto \Psi$. We know further that Ψ and $\tilde{\Psi}$ are related by the Fourier transform,

$$\Psi(X) = \mathcal{F}\{\tilde{\Psi}\} \equiv \int \frac{dK}{\sqrt{2\pi}} e^{iKX} \tilde{\Psi}(K).$$

Thus we need consider as possible solutions to the TISE for the SHO only those functions which (up to an overall normalization factor) are their own Fourier transform.

The first such function which comes to mind in the Gaussian, $f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-X^2/2\sigma^2}$. As we learned in the notes on quantum states, the Fourier transform of this function is just another Gaussian, $\tilde{f}(K) = e^{-\sigma^2 K^2/2}$. For these to be the same function, we must have $f(U) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-U^2/(2\sigma^2)} \propto \tilde{F}(U) = e^{-\sigma^2 U^2/2}$ so that $1/\sigma^2 = \sigma^2$ and hence $\sigma^2 = 1$. (If $\sigma = -1$ the functions would be unnormalizable.) Thus our first guess for a possible solution to (4) is $\Psi(X) = Ae^{-X^2/2}$. To verify this, we insert our guess, or *ansatz*, into the TISE. It is convenient to first compute the appropriate derivatives,

$$\begin{aligned} \Psi(X) &= e^{-X^2/2} \\ \Psi'(X) &= (-X)e^{-X^2/2} \\ \Psi''(X) &= (-1+X^2)e^{-X^2/2}. \end{aligned}$$

So that,

$$\begin{aligned} \mathcal{E}\Psi(X) \quad \overset{(?)}{=} \quad & -\frac{1}{2}\Psi''(X) + \frac{1}{2}X^2\Psi(X) \\ = \quad & -\frac{1}{2}(-1+X^2)e^{-X^2/2} + \frac{1}{2}X^2 e^{-X^2/2} \\ \overset{(\surd)}{=} \quad & (\frac{1}{2})e^{-X^2/2} \\ \Rightarrow \quad & \mathcal{E} = \frac{1}{2} \\ \Rightarrow \quad & E = \frac{1}{2}\hbar\omega \quad \text{(traditional units)} . \end{aligned}$$

Indeed we have found a solution by simple inspection of the dimensionless TISE! (Note that there was no need to carry the normalization factor A though our analysis because the TISE is a linear equation and all of the factors of A cancel through.)

Recall that we found in our notes on the Heisenberg uncertainty principle that the absolute lower bound which the HUP places on the ground state energy for a SHO is precisely this value of $E = \frac{1}{2}\hbar\omega$. The state we have found must therefore the ground state of the system,

$$\Psi_0(X) = \frac{1}{\pi^{1/4}} e^{-X^2/2}$$

$$\tilde{\Psi}_0(K) = \frac{1}{\pi^{1/4}} e^{-K^2/2}$$

(properly square-normalized).

This state does attain the absolute minimum energy allowed under the uncertainty principle and thus also represents the state of minimum uncertainty. From our analysis we have thus also identified the wavepacket of minimum uncertainty. It is the Gaussian wavepacket.

Having identified the ground state, we may generate other states from it using the observation that taking successive derivatives of a function generates successive factors of iK in its Fourier transform:

$$\begin{aligned} \Psi(X) &\equiv \int \frac{dK}{\sqrt{2\pi}} \tilde{\Psi}(K) e^{iKX} \\ \Rightarrow \Psi'(X) &\equiv \int \frac{dK}{\sqrt{2\pi}} (iK)\tilde{\Psi}(K) e^{iKX}. \end{aligned}$$

If $f(X) \equiv \Psi_0'(X)$, then $f(X) = -X\frac{1}{\pi^{1/4}}e^{-X^2/2}$ *but also* $\tilde{f}(K) = iK\frac{1}{\pi^{1/4}}e^{-K^2/2}$! Once again, $f(U) \propto \tilde{f}(U)$, and may have found yet another state,

$$\Psi_1(X) = Xe^{-X^2/2}.$$

To verify that we have indeed found another state, we first compute the derivatives of $\Psi_1(X)$,

$$\begin{aligned}
\Psi(X) &= Xe^{-X^2/2} \\
\Psi'(X) &= (1-X^2)e^{-X^2/2} \\
\Psi''(X) &= (-3X+X^3)e^{-X^2/2}.
\end{aligned}$$

Inserting into the TISE,

$$\begin{aligned}
\mathcal{E}\Psi(X) \quad \overset{(?)}{=} \quad & -\frac{1}{2}\Psi''(X) + \frac{1}{2}X^2\Psi(X) \\
= \quad & -\frac{1}{2}(-3X+X^3)e^{-X^2/2} + \frac{1}{2}X^2(Xe^{-X^2/2}) \\
\overset{(\surd)}{=} \quad & (\frac{3}{2})Xe^{-X^2/2} \\
\Rightarrow \quad & \mathcal{E} = \frac{3}{2} \\
\Rightarrow \quad & E = \frac{3}{2}\hbar\omega \quad \text{(traditional units)} .
\end{aligned}$$

When properly normalized, this state is

$$\Psi_1(X) = \frac{\sqrt{2}}{\pi^{1/4}}Xe^{-X^2/2}.$$

Unfortunately, simply taking yet another derivative will not work. The basic properties of the fourier transform tell us that if $f(U) \equiv \Psi_0''(U)$ then $\tilde{f}(U) = -U^2\tilde{\Psi}(U)$, but we found above that $\Psi''(U) = (-1+U^2)\Psi(U)$. This is not proportional to $U^2\tilde{\Psi}(U)$ but has an additional term proportional to $1\cdot\tilde{\Psi}(U)$. One may develop a procedure to deal with this issue and find a method for finding an algebraic solution for the TISE for the SHO which does not require the direct solution of any differential equations.

For now, we will take as our main lesson , the strong suspicion that the eigenfunctions of the SHO are of the form of polynomials times $e^{-X^2/2}$, $\Psi_n(X) = \left(\sum_{n=0}^{N} a_n X^n\right) e^{-X^2/2}$. As we shall see in the next section, this *ansatz* is correct. The polynomials which multiply the Gaussian factor $e^{-X^2/2}$ are given a special name, the Hermite polynomials, and the symbol $\mathcal{H}_n(X)$. The solutions to the Harmonic oscillator will turn out to be

$$\Psi_n(X) = A_n\mathcal{H}_n(X)e^{-X^2/2}, \tag{6}$$

where A_n is an appropriate normalization factor.

3 Series solution for the states of the SHO

One way to derive the form for the Hermite polynomials $\mathcal{H}_n(x)$ is to solve Schrödinger's equation using a power series method. Although this is not the most elegant method, it serves to illustrate important features of the TISE. It is also important to understand this method because it may often may be applied when a more clever solution is not so apparent.

3.1 The eigenvalue equation for the $\mathcal{H}_n(X)$

Although from our discussion in section (2) we would strongly suspect that the solutions for the SHO are of the form (6), the considerations of that section alone did not rule out the possibility of other solutions. One way to keep our search for solutions completely general but take advantage of our insights from the previous section is to write the wavefunction in the form of the product of a Gaussian and an unknown function $f(X)$, which we then expand in a Taylor series,

$$\begin{aligned}\Psi(X) &= f(X)e^{-X^2/2} \\ &\equiv \left(\sum_{n=0}^{\infty} a_n X^n\right) e^{-X^2/2}. \end{aligned} \tag{7}$$

We may then derive an alternate equation for the $f(X)$. Because we expect the solutions for this alternate equation to just be polynomials, the hope is that this new equation will be easier to solve than the original Schrödinger equation (4.

It is important that when writing the form (7), we have *not* limited our search for solutions to the TISE in any way. We see that this is so through the following argument. Given any wavefunction $\Psi(X)$ which is a solution to the TISE, we may always write it in the form (7) by simply defining $f(X) \equiv \Psi(X)/e^{-X^2/2}$. Written this way we see that $f(X)$ may indeed be expanded in a power series because it is the ratio (with non-zero denominator) of two well-behaved analytic functions, $\Psi(X)$ and $e^{-X^2/2}$. (We know that $\Psi(X)$ is well-behaved and analytic because it is the solution to the TISE with a potential which is finite with all derivatives continuous.)

To derive the equation for $f(X)$, we first take the appropriate derivatives of $\Psi(X)$,

$$\begin{aligned}\Psi(X) &= f(X)e^{-X^2/2} \\ \Psi'(X) &= \left(f'(X) - Xf(X)\right) e^{-X^2/2} \\ \Psi''(X) &= \left(f''(X) - 2Xf'(X) - f(X) + X^2 f(X)\right) e^{-X^2/2}.\end{aligned}$$

Inserting the result into the TISE (4) then gives

$$\begin{aligned}-\frac{1}{2}\left(f''(X) - 2Xf'(X) - f(X) + X^2 f(X)\right) e^{-X^2/2} & \\ +\frac{1}{2}X^2 f(X)e^{-X^2/2} &= \mathcal{E} f(X)e^{-X^2/2} \\ -\frac{1}{2}f''(X) + Xf'(X) + \frac{1}{2}f(X) &= \mathcal{E} f(X) \\ -\frac{1}{2}f''(X) + Xf'(X) &= (\mathcal{E} - \frac{1}{2})\eta f(X); \quad \eta \equiv \mathcal{E} - \tfrac{1}{2} \\ f''(X) - 2Xf'(X) &= -2\eta f(X)\end{aligned} \tag{8}$$

Equation (8) is now our equation for the function $f(X)$, where we have defined a new parameter describing the energy $\eta \equiv (\mathcal{E} - \frac{1}{2})$ so that $\mathcal{E} = \eta + \frac{1}{2}$. In terms of traditional units the eigenenergies are

$$E = \hbar\omega\mathcal{E} = (\eta + \frac{1}{2})\hbar\omega.$$

Note that Eq. (8) is a new eigenvalue equation, one which determines the allowed $f(X)$ which will turn out to be the Hermite polynomials $\mathcal{H}_n(X)$.

To illustrate the use of this equation, we now use it to verify the results that we have already. To see that that $\Psi(X) \propto e^{-X^2/2}$ is indeed a solution to the TISE and that the corresponding energy is $E = \frac{1}{2}\hbar\omega$, we first identify that $f(X) = 1$ and then insert *this* into (8),

$$\begin{aligned}f''(X) - 2Xf'(X) + 2\eta f(X) &= 0 \\ (0) - 2X(0) + 2\eta(1) &= 0 \\ \Rightarrow \quad \eta &= 0 \\ \Rightarrow \quad E &= (\eta + \frac{1}{2})\hbar\omega = \frac{1}{2}\hbar\omega \ (\surd)\end{aligned}$$

For the first excited state we have $f(X) = X$, which we may also verify as a solution with energy $E = \frac{3}{2}\hbar\omega$ by direct substitution,

$$\begin{aligned} f''(X) - 2Xf'(X) + 2\eta f(X) &= 0 \\ (0) - 2X(1) + 2\eta(X) &= 0 \\ \Rightarrow \qquad \eta &= 1 \\ \Rightarrow \qquad E &= (\eta + \frac{1}{2})\hbar\omega = \frac{3}{2}\hbar\omega \ (\surd). \end{aligned}$$

Finally, we might 'guess' at the solution for a new case and consider the next state which must involve a quadratic term *and* a constant term to make up for the error in taking a pure quadratic term. The correct form turns out to be $f(X) = 2X^2 - 1$, for then

$$\begin{aligned} f''(X) - 2Xf'(X) + 2\eta f(X) &= 0 \\ (4) - 2X(4X) + 2\eta(2X^2 - 1) &= 0 \\ \Rightarrow \qquad \eta &= 2 \\ \Rightarrow \qquad E &= (\eta + \frac{1}{2})\hbar\omega = \frac{5}{2}\hbar\omega, \end{aligned}$$

which we will find to represent the second excited state, $\Psi_2(X) = \frac{1}{\sqrt{2}\pi^{1/4}}(2X^2 - 1)e^{-X^2/2}$ (properly normalized).

3.2 The eigenvalue equation for the a_n.

We now proceed to search for the general solution of the eigenvalue equation (8) in the form of power series,

$$f(X) = \sum_{n=0}^{\infty} a_n X^n. \tag{9}$$

After inserting this form into the eigenvalue equation for $f(X)$, we will generate, not surprisingly, an eigenvalue equation, for the a_n. This equation at last will be one which we may solve easily by recursion.

As before, it is useful to take the appropriate derivatives before inserting the general form (9) into the equation (8),

$$f(X) = \sum_{n=0}^{\infty} a_n X^n \tag{10}$$

$$f'(X) = \sum_{n=0}^{\infty} n a_n X^{n-1} \tag{11}$$

$$f''(X) = \sum_{n=0}^{\infty} n(n-1) a_n X^{n-2}. \tag{12}$$

The form we now have for the first derivative is particularly convenient because in (8) f' appears with a factor of X which will combine with the factor of X^{n-1} in the series in (11 to produce a net factor of X^n allowing us to combine terms in (8) easily. Unfortunately, the same is not true of the above series for the second derivative. To put the second derivative term on the same footing with the other terms in (8), we should shift the indexing of the sum by 2 so that the terms can combine. This procedure is analogous to a change of variables when integrating,

$$f''(X) = \sum_{m=0}^{\infty} m(m-1) a_m X^{m-2} \quad ; \text{change dummy summation index}$$

$$f''(X) = \sum_{m=2}^{\infty} m(m-1) a_m X^{m-2} \quad ; m = 0 \text{ and } m = 1 \text{ terms are zero}$$

$$f''(X) \quad = \quad \sum_{n=0}^{\infty}(n+2)(n+1)a_{n+2}X^n \quad ; \text{let } m = 2+n \tag{13}$$

We are ready to substitute the series expansion for $f(X)$ into (8). Inserting (10,11,13) into (8), we find

$$\begin{aligned}\sum_{n=0}^{\infty}(n+2)(n+1)a_{n+2}X^n - 2X\sum_{n=0}^{\infty}na_nX^{n-1} + 2\eta\sum_{n=0}^{\infty}a_nX^n &= 0 \\ \sum_{n=0}^{\infty}\big((n+2)(n+1)a_{n+2} - 2na_n + 2\eta a_n\big)X^n &= 0 \end{aligned} \tag{14}$$

For the series to be identically zero, *all* of its terms must be zero separately and therefore we must have

$$(n+2)(n+1)a_{n+2} - 2na_n \quad = \quad -2\eta a_n. \tag{15}$$

This is the eigenvalue equation we expected for the a_n. Because this equation describes a discrete sequences of numbers (a_n) rather that a continuous function (such as $f(X)$), it is known as a *finite difference* eigenvalue equation.

3.3 Putting the pieces together

We now complete the series solution for the eigenvalue equation by solving (15) for the a_n, reconstructing the $f(X) \equiv \sum_n a_nX^n$ and, finally, producing the wavefunctions $\Psi(X) \equiv f(X)e^{-X^2/2}$.

Equation (15) is solved by rewriting it as a linear recursion relation,

$$a_{n+2} = \frac{2(n-\eta)}{(n+2)(n+1)}a_n \quad \text{(for all } n) \tag{16}$$

Applying (16) recursively for $n = 0, 1, 2, \ldots$ in sequence, we find

$$\begin{aligned} a_2 &= \frac{-2\eta}{2\cdot 1}a_0 \\ a_3 &= \frac{(2(1-\eta))}{3\cdot 2}a_1 \\ a_4 = \frac{2(2-\eta)}{4\cdot 3}a_2 &= \frac{2^2(2-\eta)(-\eta)}{4!}a_0 \\ a_5 = \frac{2(3-\eta)}{5\cdot 4}a_3 &= \frac{2^2(3-\eta)(1-\eta)}{5!}a_1 \\ a_6 = \frac{2(4-\eta)}{6\cdot 5}a_4 &= \frac{2^3(4-\eta)(2-\eta)(-\eta)}{6!}a_0 \\ &\vdots \\ a_{2m} &= \frac{2^m(2m-2-\eta)(2m-4-\eta)\ldots(-\eta)}{m!}a_0 \\ a_{2m+1} &= \frac{2^m(2m-1-\eta)(2m-3-\eta)\ldots(1-\eta)}{m!}a_1 \\ &\vdots \end{aligned}$$

Note that in this case, the even and odd terms form *independent* sequences so that we may write $f(X)$ as the sum of an even part $a_0f_e(X)$ and an odd part $a_1f_o(X)$,

$$f(X) \quad \equiv \quad \sum_n a_nX^n$$

$$
\begin{aligned}
&= \sum_{n \text{ even}} a_n X^n + \sum_{n \text{ odd}} a_n X^n \\
&= \sum_{m=0}^{\infty} a_{2m} X^{2m} + \sum_{m=0}^{\infty} a_{2m+1} X^{2m+1} \\
&= a_0 \left(1 + \frac{-2\eta}{2 \cdot 1} X^2 + \frac{2^2(2-\eta)(-\eta)}{4!} X^4 + \ldots + \frac{2^m(2m-2-\eta)(2m-4-\eta)\ldots(-\eta)}{(2m)!} X^{2m} + \ldots\right) \\
&\quad + a_1 \left(X + \frac{(2(1-\eta))}{3 \cdot 2} X^3 + \ldots + \frac{2^m(2m-1-\eta)(2m-3-\eta)\ldots(1-\eta)}{(2m+1)!} X^{2m+1} + \ldots\right) \\
&\equiv a_0 f_e(X) + a_1 f_o(X),
\end{aligned}
$$

where $f_e(X)$ and $f_o(X)$ are even and odd functions of X respectively. Note that the functions $f_e(X)$ and $f_o(X)$ may be generated according to the above formulas for any value of η, the parameter describing the energy.

At last our solution is $\Psi(X) = f(X)e^{-X^2/2} = \big(a_0 f_e(X) + a_1 f_o(X)\big)e^{-X^2/2} \equiv a_0\Psi_e(X) + a_1\Psi_o(X)$. At this point is seems we have identified *two* linearly independent solutions, $\Psi_e(X)$ (even) and $\Psi_o(X)$ (odd) for every (continuous) value of the energy parameter η. We know that all of these solutions which we have found cannot represent pure energy states of the SHO. First, all SHO states are bound ($V(\pm\infty) \to \infty$) and bound states exhibit a discrete, not continuous, spectrum. Second, we expect (in one dimension) only a *single* physical state for each allowed energy, but here we appear to have found two. There must therefore be a physical reason for rejecting many of the solutions we have found.

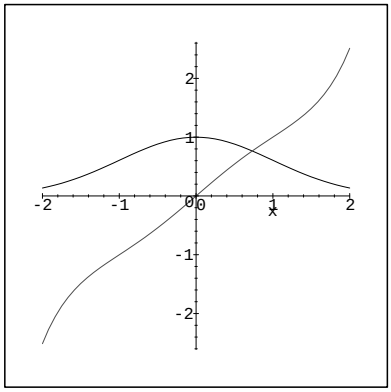
The physical reason for rejecting some of these solutions is clearly illustrated when we look at the two solutions corresponding to the ground state of the harmonic oscillator, $E = \frac{1}{2}\hbar\omega$, or $\eta = 0$. From the series solution we have

$$
\begin{aligned}
\Psi_e(X) = f_e(X)e^{-X^2/2} &= a_0 e^{-X^2/2} \\
\Psi_o(X) = f_o(X)e^{-X^2/2} &= a_1\big(X + \frac{(2(1))}{3 \cdot 2} X^3 + \frac{2^2(3)(1)}{5!} X^5 + \ldots \\
&\quad \ldots + \frac{2^m(2m-1)(2m-3)\ldots(1)}{(2m+1)!} X^{2m+1} + \ldots\big)e^{-X^2/2} \\
&= a_1 \left(X + \frac{1}{3}X^3 + \frac{1}{5 \cdot 2!}X^5 + \ldots + \frac{1}{(2m+1)m!} X^{2m+1} + \ldots\right) e^{-X^2/2}.
\end{aligned}
$$

A plot of these two functions is provided in Figure 3.3. While the even solution, $\Psi_e(X)$, is well behaved and decays into the forbidden regions at $|X| > 1$ while curving away from the x-axis, the odd solution enters the forbidden region with too great of a slope and thus begins to grow exponentially as $X \to \pm\infty$. As in the case of the square well, because this function is not be normalizable, we reject it as unphysical.

We could have anticipated this behavior analytically with out resorting to a plot. The key observation is that *only* when the series for $f(X)$ "terminates" and the coefficients became zero after some point leaving only a polynomial, then the wave function $\Psi(X) = f(X)e^{-X^2/2}$ drops sufficiently rapidly for large X that it is normalizable. If the series does not terminate, the function $f(X)$ grows so rapidly with X that even after multiplication by $e^{-X^2/2}$ the wavefunction cannot be normalized. In the next subsection we will proof that this is so. For now, we will take this intuitively reasonable result as given.

The form of the recursion (16) is such that the series terminates only for $\eta = n$ where n is a nonnegative integer. If η is not an integer, then neither $f_e(X)$ nor $f_o(X)$ will terminate, and neither the even or odd solution is normalizable or physical. Thus we see that η must be an integer. Moreover, if η is an even (odd) integer, the series for $f_e(X)$ ($f_o(X)$) will terminate at the point where $n = \eta$ but the series for $f_o(X)$ ($f_e(X)$) will not terminate because $f_o(X)$ ($f_e(X)$) contains terms only for odd (even) n. If η is even (odd), the only allowable solution will be the finite polynomial $f_e(X)$ ($f_o(X)$). Up to an overall normalization constant, the *Hermite* polynomials are defined as



these terminated $f_e(X)$ and $f_o(X)$. Because (8) is a linear equation, it does not determine the overall normalization of the Hermite polynomials. By convention, this normalization is set so that the highest order term in $\mathcal{H}_n(X)$ is $2^n X^n$. Using this definition and the recursion (16), we find the following for the first few Hermite polynomials,

$$\begin{aligned} C_0 1 = \quad & \mathcal{H}_0(X) && = 1 \\ C_1 X = \quad & \mathcal{H}_1(X) && = 2X \\ C_2(1-2X^2) = \quad & \mathcal{H}_2(X) && = 4X^2 - 2 \\ C_3(X - \frac{2}{3}X^3) = \quad & \mathcal{H}_3(X) && = (8X^3 - 12X) \\ C_4(1 - 4X^2 + \frac{4}{3}X^4) = \quad & \mathcal{H}_4(X) && = (16X^4 - 48X^2 + 12) \end{aligned}$$

To sum up, we thus have,

$$E_n(X) = (n + \frac{1}{2})\hbar\omega \quad ; n = 0, 1, \ldots \tag{17}$$

$$\Psi_n(X) = A_n \mathcal{H}_n(X) e^{-X^2/2}, \tag{18}$$

where, the A_n are normalization constants defined so that $\int |\Psi(X)|^2 \, dX = 1$, which can be show to leave them with the values,

$$A_n = (2^n n! \sqrt{\pi})^{-1/2}.$$

Note that these solutions also obey the rule that the n^{th} excited state is even or odd according to the value of n and has n nodes.

3.4 The growth of $f(X)$ when the series does not terminate

In considering the physical admissibility of the solutions $\Psi(X) = f(X)e^{-X^2/2}$ we first noted that if $f(X)$ is a finite polynomial that $\Psi(X)$ is normalizable because of the extremely rapid fall of the Gaussian factor. We then *assumed* that if the series for $f(X)$ did not terminate, that the resulting $f(X)$ would grow so rapidly that even the Gaussian decay of the factor $e^{-X^2/2}$ could not make $\Psi(X)$ normalizable. In this subsection, we shall investigate why this should be the case.

The key observation which we shall exploit is that for large n the coefficients a_n in the sequence defining $f(X)$ behave much like the terms in the expansion for $g(X) \equiv e^{X^2}$ so that, for large X, $f(X)$ grows at least like e^{X^2}, so that not even multiplication by the Gaussian decay factor $e^{-X^2/2}$

will render the wave function normalizable. The basic similarity of the two expansions comes from the behavior of the ratio of the $(n+1)^{th}$ to the n^{th} terms in the sequence successive terms. For $f_e(X)$ the ratio is

$$\frac{a_{2n}X^{2n}}{a_{2n-2}X^{2n-2}} = \frac{a_{2n}}{a_{2n-2}}X^2 = \frac{2(2n-2-\eta)}{2n(2n-1)}X^2 \longrightarrow \frac{X^2}{n}.$$

For $f_o(X)$ the ratio approaches the same limit,

$$\frac{a_{2n+1}X^{2n+1}}{a_{2n-1}X^{(2n-1)}} = \frac{a_{2n+1}}{a_{2n-1}}X^2 = \frac{2(2n-1-\eta)}{2n(2n+1)}X^2 \longrightarrow \frac{X^2}{n}.$$

We find precisely the same limit in the case of our auxiliary function, $g(Y)$. For

$$g(Y) = e^{Y^2} = \sum_{n=0}^{\infty} \frac{1}{n!}Y^{2n},$$

the ratio is

$$\frac{\frac{Y^{2n}}{n)!}}{\frac{Y^{2(n-1)}}{(n-1)!}} = \frac{Y^2}{n} \longrightarrow \frac{Y^2}{n}.$$

Note that the ratio of successive terms may be negative for small values of n so that the terms in the series for the $f(X)$ may alternate in sign. Because the ratio approaches a positive limit, However, we are assured that for sufficiently large n, all terms will be of the same sign. Moreover, because $F_n^{e,o}(X) \longrightarrow \frac{X^2}{n}$, we may find an N so that for all $n > N$ the ratio of successive terms in $f_{e,o}(X)$ will exceed $\nu^2\frac{X^2}{n}$ where $0 < \nu < 1$ is any number between zero and one. This is important because this is just the quantity $(G_n^{e,o}(\nu X)$, which is the ratio of successive terms in $g(\nu X)$. If we now multiply $g(\nu X)$ by a constant α_N so that the N^{th} term of $\alpha_N g(\nu X)$ is equal in magnitude to the N^{th} term of $f_{e,o}(X)$, this implies that all successive terms in $f_{e,o}(X)$ will exceed their counterparts in $\alpha_N g(\nu X)$. Because all of the terms in question are of the same sign, the absolute value of the sum of all remaining terms in $f_{e,o}(X)$ exceeds that of the associated terms in $\alpha_N g(\nu X)$, which is important because we know that g grows too fast to yield a normalizable function. To complete the argument, let $f_N(X)$ be the sum of the first N terms in $f(X)$ and $g_N(X)$ be the sum of the first N terms in $g(\nu X)$. Note that both $f_N(X)$ and $g_N(X)$ are finite polynomials. We have just shown that for every $0 < \nu < 1$ there exist a constant $\alpha_N > 0$ and integer N such that for all X,

$$\begin{aligned} |f(X) - f_N(X)| &> \alpha_N |g(\nu X) - g_N(\nu X)| \\ \Rightarrow |f(X)| &> \alpha_N g(\nu X) - \alpha_N(|g_N(\nu X)| + |f_N(X)|) \\ &> \alpha_N e^{\nu^2 X^2} - P_N(X), \end{aligned}$$

where $P_N(X)$ is a function which grows at most as quickly as an N^{th} order polynomial. If we now consider the behavior of the wave function at large values of X, $|\Psi(X)| = |f(X)|\,|e^{-X^2/2}| > \left(\alpha_N e^{\nu^2 X^2} - P_N(X)\right)e^{-X^2/2} \longrightarrow e^{-(\frac{1}{2}-\nu^2)X^2}$. (The limit of any polynomial times a Gaussian factor is zero.) This statement is true of any $0 < \nu < 1$. For this to be true for $\nu > \sqrt{\frac{1}{2}}$, we see that, as long as the series for $f(X)$ does not terminate, we must have $\Psi(X) \longrightarrow \infty$ as $X \longrightarrow \infty$. This completes the proof of our claim that we must reject all solutions of $f(X)$ for which the series do not terminate and culminates our power series analysis of the quantum states of the SHO.