Quantum Harmonic Oscillator

First consider Newton's Second Law (NSL) for the classical simple harmonic oscillator (SHO):

$$F(x) = -Kx = m\frac{d^2x}{dt^2} \Rightarrow \frac{d^2x}{dt^2} + \omega_0^2 x = 0 \tag{1}$$

Here we have defined the natural oscillation frequency:

$$\omega_0 = \sqrt{\frac{K}{m}} \tag{2}$$

The solution to this second order DE is the familiar sine/cosine function:

$$x(t) = A\cos(\omega_0 t + \phi) \tag{3}$$

Furthermore, the energy is a constant of the motion which can be seen by differentiating the energy with respect to time and using NSL:

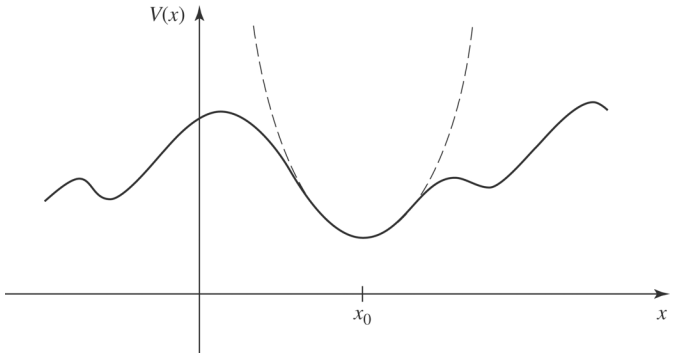
$$\begin{aligned} \frac{dE}{dt} &= \frac{d}{dt}\left[\frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2\right] \\ &= \frac{d}{dt}\left[\frac{m\dot{x}^2}{2} + \frac{1}{2}m\omega_0^2 x^2\right] \\ &= m\dot{x}\ddot{x} + m\omega_0^2 x\dot{x} \\ &= m\dot{x}\left[\ddot{x} + \omega_0^2 x\right] \\ &= 0 \end{aligned} \tag{4}$$

method but first let us consider some more aspects of the classical oscillator.

This will give us some 'hooks' to use to see where the quantum version differs from the classical version. First recall that the SHO is an idealization arising from expanding the general potential energy function in a Taylor Series:

$$V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \cdots \tag{5}$$

The first term is an arbitrary constant that can be ignored since the zero of energy is arbitrary. The second, linear term is also zero since the potential function must be at a minimum at equilibrium. So the second order term is the first one of interest and we can drop the rest for the lowest approximation of a stable potential. See the figure below from the text (Figure 2-4)



Hence to lowest order, the potential is parabolic:

$$\begin{aligned} V(x) &= \frac{1}{2}V''(x_0)(x-x_0)^2 \\ &= \frac{1}{2}m\omega_0^2 x^2 \end{aligned} \tag{6}$$

Depending on the initial conditions that begin the oscillators motion, there will be a total energy given by

$$E = \frac{1}{2}mv_0^2 + \frac{1}{2}m\omega_0^2 x_o^2 \tag{7}$$

We can see the effect of this energy by drawing a horizontal line on the potential energy curve of the figure.

We can see that such a line intercepts the potential at two points. At this points the total energy is equal to the potential energy of those points. (discuss in lecture and introduce the concept of the classical turning point and classically allowed vs quantum allowed motion.)

Quantum Harmonic Oscillator

The *quantum* harmonic oscillator problem is set up using the canonical quantization procedure in which one starts with the classical Hamiltonian function and replaces the position and momentum functions with their quantum operator equivalents.

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega_0^2 \hat{x}^2 \tag{8}$$

The time independent Schrödinger equation (TISE) is thus:

$$\begin{aligned} \hat{H}\psi(x) &= E\psi(x) \\ \left[\frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega_0^2 \hat{x}^2\right]\psi(x) &= E\psi(x) \end{aligned} \tag{9}$$

This may be converted into an ordinary differential equation by making the operator associations:

$$\hat{\mathrm{p}} \Rightarrow \frac{\hbar}{i}\frac{d}{dx} \quad \hat{x} \Rightarrow x \tag{10}$$

producing:

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega_0^2 x^2\right]\psi(x) = E\psi(x) \tag{11}$$

We will develop solutions to this equation using the so-called operator. To see this, we first introduce a notational convenience:

$$\frac{d^2\psi}{dx^2} = \psi_{xx} \quad \text{and similarly for other derivatives.} \tag{12}$$

The we can re-write the TISE to bring out the transition from classically allowed to classically forbidden motion:

$$\psi_{xx} = -\left[\frac{2m}{\hbar^2}\right]\left(E - \frac{m\omega_0^2}{2}x^2\right)\psi$$
$$= -k^2\psi \text{ where } k^2 = \left[\frac{2m}{\hbar^2}\right]\left(E - \frac{m\omega_0^2}{2}x^2\right) \quad (13)$$

The parameter k^2 is positive as long as x is less than the turning point. In that case, the TISE has the structure of an oscillator (in space), i.e. the second derivative of the wave function is a negative number times the wave function itself. Of course, the solution is not just a simple sinusoid because k^2 depends on x. But the wave function can oscillate from positive to negative values just like an ordinary wave.

On the other hand, when x goes beyond the point where E is less than the potential energy, k^2 becomes negative and we should rewrite the TISE. First let:

$$\kappa^2 = \left[\frac{2m}{\hbar^2}\right]\left(\frac{m\omega_0^2}{2}x^2 - E\right) \quad (14)$$

Then we have

$$\psi_{xx} = \kappa^2\psi \quad (15)$$

This is the DE for a decaying (or growing) function that does not oscillate (remember that an exponential function has a positive second derivative regardless of the sign of the exponent). Again, the solution is not just a simple exponential as κ^2 depends on x, but the behavior will be similar.

To explore this a little further, consider the region well beyond the turning point. It will be convenient to define the dimensionalizing parameter β:

$$\beta^2 = \frac{m\omega_0}{\hbar} \quad (16)$$

As an exercise, show that the dimension of β is 1/length.

We can use β to non-dimensionalize the position variable x as follows:

$$\xi=\beta x \Rightarrow \frac{d}{dx}=\frac{d\xi}{dx}\frac{d}{d\xi}=\beta\frac{d}{d\xi} \tag{17}$$

Then we can write the TISE in the limit $\frac{m\omega_0^2 x^2}{2} \gg E$.

$$\psi_{\xi\xi}=\xi^2\psi \tag{18}$$

(show this as an exercise)

We can use a trial solution

$$\psi(\xi)=\text{Aexp}(-\xi^2/2) \tag{19}$$

and obtain:

$$\begin{aligned}\frac{d^2}{d\xi^2}\left(\text{Aexp}(-\xi^2/2)\right)&=\left(\xi^2-1\right)\text{Aexp}(-\xi^2/2)\\ &\approx \xi^2\text{Aexp}(-\xi^2/2) \quad \xi^2 \gg 1\end{aligned} \tag{20}$$

This tells us that the wave function must have the asymptotic form $\exp(-\xi^2/2)$.

We will now obtain the general solution using the operator method.

The Creation and Annihilation Operator Method

Note: These notes differ somewhat from the section in Griffiths on the quantum harmonic oscillator, but they are equivalent. You may find it helpful to compare the two to see that this is the case.

First, we need to introduce the concept of the commutator. Consider two operators, $\hat{A}$ and $\hat{B}$ acting on a function f . If $\hat{A}$ operates first followed by $\hat{B}$ we would write the result as

$$\hat{B}\hat{A}f \tag{21}$$

In other words the sequence of operations is written right to left when operating from the left. Consequently, with the order of $\hat{A}$ and $\hat{B}$ reversed we would write

$$\hat{A}\hat{B}f \tag{22}$$

We can ask the question: Are these two expressions equivalent? If they are then we should able to write:

$$\hat{B}\hat{A}f = \hat{A}\hat{B}f \tag{23}$$

If the two expressions are not equal then Eq. 23 is not valid and we say that $\hat{A}$ and $\hat{B}$ are non-commuting operators. This concept can be made quantitative by taking the difference between the two sides of Eq. 23:

$$\begin{aligned} \hat{A}\hat{B}f - \hat{B}\hat{A}f &= \left[\hat{A}\hat{B} - \hat{B}\hat{A}\right]f \\ &= \left[\hat{A},\hat{B}\right]f \end{aligned} \tag{24}$$

Here we have introduced the commutator operation $\left[\hat{A},\hat{B}\right]$ between the operators $\hat{A}$ and $\hat{B}$. If the commutator is zero, we say the operators commute, and if it is non-zero we say they have a commutator

$$\begin{aligned} \hat{C} &= \left[\hat{A},\hat{B}\right] \\ &= \left[\hat{A}\hat{B} - \hat{B}\hat{A}\right] \end{aligned} \tag{25}$$

The archetypal example of non-commuting operators are the position and momentum operators. Let us explore why. First recall their definitions from Eq. 10

$$\hat{\mathrm{p}} \Rightarrow \frac{\hbar}{i}\frac{d}{dx} \quad \hat{x} \Rightarrow x \tag{26}$$

To test their commutativity, we have to operate on a 'test' function, call this function $f(x)$. Now operate on x with the two operators in order. We will use a breakout room to figure this out.

In the breakout room you should have been able to show that:

$$\left[\hat{x}, \hat{p}\right] = i\hbar \tag{27}$$

Thus, the position and momentum operators do not commute, and we say they are canonically conjugate. To see how this helps solve the quantum harmonic oscillator we introduce two new operators derived from the position and momentum operators. These are called annihilation and creation operators for reasons that will become apparent.

$$\hat{\mathrm{a}} = \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) \tag{28}$$

$$\hat{\mathrm{a}}^{\dagger} = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right) \tag{29}$$

Recall that for the position and momentum operator are connected through their commutator,

$$\left[\hat{x}, \hat{p}\right] = i\hbar. \tag{30}$$

Armed with this result we can now show that the annihilation and creation operators have a similar property:

$$\left[\hat{a}, \hat{a}^{\dagger}\right] = 1 \tag{31}$$

This allows us to substitute as needed using the following:

$$\begin{aligned}&\left[\hat{a},\hat{a}^{\dagger}\right]=1\Rightarrow \hat{a}\hat{a}^{\dagger}-\hat{a}^{\dagger}\hat{a}=1\\&\Rightarrow \hat{a}\hat{a}^{\dagger}=1+\hat{a}^{\dagger}\hat{a}\\&\text{and}\\&\hat{a}^{\dagger}\hat{a}=\hat{a}\hat{a}^{\dagger}-1\end{aligned} \tag{32}$$

The operators $\hat{a}$ and $\hat{a}^{\dagger}$ are called annihilation and creation operators or lowering and raising operators for reasons that will become apparent below.

Their defining expressions can be inverted and used to write the TISE in a particularly simple form:

$$\hat{x}=\frac{\hat{a}+\hat{a}^{\dagger}}{\sqrt{2}\beta} \tag{33}$$

$$\hat{p}=\frac{m\omega_0}{i}\frac{\hat{a}-\hat{a}^{\dagger}}{\sqrt{2}\beta} \tag{34}$$

Recall the TISE for the QHO:

$$\left[\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega_0^2\hat{x}^2\right]\psi(x)=E\psi(x) \tag{35}$$

The next block of equations should be followed carefully:

$$\left[\frac{1}{2m}\left(\frac{m\omega_0}{i}\frac{\hat{a}-\hat{a}^{\dagger}}{\sqrt{2}\beta}\right)^2+\frac{1}{2}m\omega_0^2\left(\frac{\hat{a}+\hat{a}^{\dagger}}{\sqrt{2}\beta}\right)^2\right]\psi(x)=E\psi s(x) \tag{36}$$

$$\frac{m\omega_0^2}{2\cdot 2\cdot\beta^2}\left[-\left(\hat{a}-\hat{a}^{\dagger}\right)^2+\left(\hat{a}+\hat{a}^{\dagger}\right)^2\right]\psi(x)=E\psi(x) \tag{37}$$

$$\frac{\hbar\omega_0}{4}\left[-\hat{a}^2-\hat{a}^{\dagger 2}+\hat{a}\hat{a}^{\dagger}+\hat{a}^{\dagger}\hat{a}+\hat{a}^2+\hat{a}^{\dagger 2}+\hat{a}\hat{a}^{\dagger}+\hat{a}^{\dagger}\hat{a}\right]\psi(x)=E\psi(x) \tag{38}$$

$$\frac{\hbar\omega_0}{4}\left[2\hat{a}^\dagger\hat{a}+2\hat{a}\hat{a}^\dagger\right]\psi(x)=E\psi(x) \text{ (In the above, substituted } \beta=\frac{m\omega_0}{\hbar}) \quad (39)$$

$$\frac{\hbar\omega_0}{4}\left[2\hat{a}^\dagger\hat{a}+2\left(1+\hat{a}^\dagger\hat{a}\right)\right]\psi(x)=E\psi(x) \quad (40)$$

$$\hbar\omega_0\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\psi(x)=E\psi(x) \quad (41)$$

We now introduce the number operator

$$\hat{N}=\hat{a}^\dagger\hat{a} \quad (42)$$

Then the TISE is written

$$\hbar\omega_0\left(\hat{N}+\frac{1}{2}\right)\psi(x)=E\psi(x) \quad (43)$$

We really only need to solve the number operator eigenvalue equation

$$\hat{N}\psi_n=n\psi_n \quad (44)$$

The eigenvalue n will turn out to be an integer but for now it should be considered just any number.

The solution to this eigenvalue equation is connected to the commutator of the raising and lowering operators. Consider the state arising from operating on a solution to the number operator eigenvalue equation.

$$\psi'=\hat{a}\psi_n \quad (45)$$

This turns out to be an eigenfunction of the number operator too. Watch and follow:

$$\hat{N}\hat{a}\psi_n=\hat{a}^\dagger\hat{a}\hat{a}\psi_n=\left(\hat{a}\hat{a}^\dagger-1\right)\hat{a}\psi_n \quad (46)$$

(we use one of the commutator forms to do this)

$$\begin{aligned}\hat{N}\hat{a}\psi_n &= \hat{a}\left(\hat{a}^\dagger\hat{a}-1\right)\psi_n \\ &= \hat{a}\left(\hat{N}-1\right)\psi_n \\ &= (n-1)\hat{a}\psi_n\end{aligned} \tag{47}$$

So apart from a normalization constant we still have to derive, the function $\hat{a}\phi_n$ is also an eigenfunction with an eigenvalue reduced by 1 unit. It should be obvious we could repeat this process any number of times, each time reducing the eigenvalue by 1.

As an exercise, show that the raising operator 'raises' the eigenfunction to one having an eigenvalue *increased* by 1 unit.

$$\hat{N}\hat{a}^\dagger\psi_n = (n+1)\hat{a}^\dagger\psi_n$$

To see that there is actually a lower limit to the lowering process we use a theorem that shows the expectation value of the square of an Hermitian operator must be positive definite. A brief proof of this is as follows. (sorry we have not really defined Hermitian operators yet so just take this step on faith. In Griffiths this step is done in a problem.)

$$\begin{aligned}\left\langle \hat{A}^2 \right\rangle &= \int \psi^* \hat{A}^2 \psi dx \\ &= \int \hat{A}^\dagger\psi^* \hat{A}\psi dx \text{ (from definition of adjoint)} \\ &= \int \hat{A}\psi^* \hat{A}\psi dx \ (\hat{A} \text{ is assumed to be self adjoint}) \\ &= \int \left|\left|\hat{A}\psi\right|\right|^2 dx \ \geq 0 \text{ since this is the integral of a positive function.}\end{aligned} \tag{48}$$

Now we can apply this theorem to the Hamiltonian of the QHO since

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 \tag{49}$$

From this we conclude that

$$n \geq -\frac{1}{2} \tag{50}$$

The way to guarantee this to be the case is to force there to be a lowest eigenstate. Label that state with the eigenvalue 0 and you get:

$$\hat{a}\psi_0 = 0 \tag{51}$$

Clearly any further operations with $\hat{a}$ will yield zero also.

To see that the eigenvalue n must itself be an integer, use the number operator to operate on the lowest state and on the first excited state:

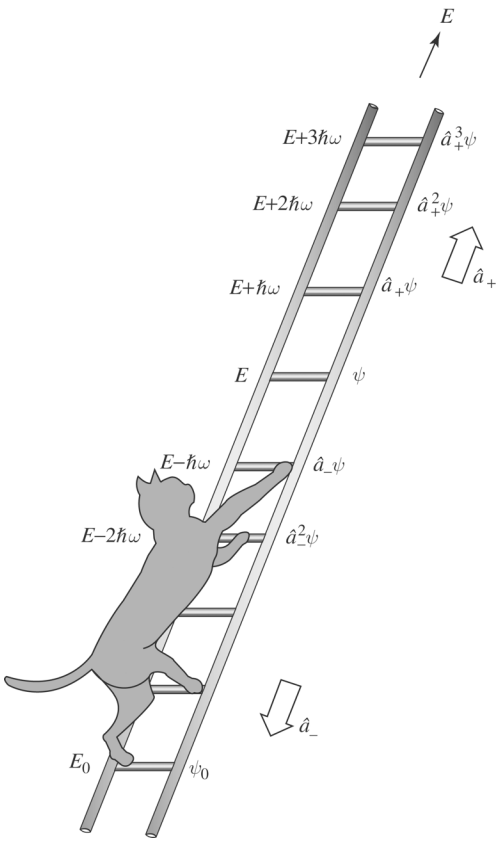
$$\begin{aligned} \hat{N}\psi_0 &= \hat{a}^\dagger\hat{a}\psi_0 = 0 \\ \hat{N}\hat{a}^\dagger\psi_0 &= \hat{a}^\dagger\hat{a}\hat{a}^\dagger\psi_0 = \hat{a}^\dagger\left(\hat{a}^\dagger\hat{a}+1\right)\psi_0 = \hat{a}^\dagger\psi_0 \end{aligned} \tag{52}$$

The last step shows that the state $\hat{a}^\dagger\psi_0$ must have the eigenvalue 1 for the number operator. Hence the eigenvalue for the first excited state must be the integer one and since you can create up and down from there in units of 1 all the eigenvalues must be integers.

Putting this altogether we have the complete form for the TISE as follows:

$$\begin{aligned} \hat{H}\psi_n &= \hbar\omega_0\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\psi_n \\ &= \hbar\omega_0\left(\hat{N}+\frac{1}{2}\right)\psi_n \\ &= \hbar\omega_0\left(n+\frac{1}{2}\right)\psi_n \\ &= E_n\psi_n \\ \Rightarrow E_n &= \hbar\omega_0\left(n+\frac{1}{2}\right) \quad n = 0,1,2,... \end{aligned} \tag{53}$$

This is the central result of the eigenvalue problem for the quantum harmonic oscillator. The energy levels are evenly spaced. The lowest energy level is not equal to zero energy and is called the zero-point energy. It originates in the fact that the lowest energy eigenfunction has position and momentum uncertainty and hence a non-zero kinetic energy. Griffiths has a nice cartoon to show this, Figure 2-5:



Griffiths Figure 2.5 illustrating concept of the evenly spaced harmonic oscillator states.

There are many applications of the quantized harmonic oscillator in physics. We will look at some of these next semester and you can also find them in courses on molecular physics, solid state physics and quantum optics.

The final step in solving the full problem is to find the actual functions $\phi_n(x)$. To do that we will go back to the definition of the creation/annihilation operators to develop a derivative method to generate the functions.

Construction of Harmonic Oscillator Eigenfunctions

The first step is to rewrite the operators and the TISE using the dimensionless position variable $\xi=\beta x$. The annihilation operator takes the form:

$$\begin{aligned}\hat{a}&=\frac{\beta}{\sqrt{2}}\left(\hat{x}+\frac{i\hat{p}}{m\omega_0}\right)\\&=\frac{\beta}{\sqrt{2}}\left(x+\frac{\hbar}{m\omega_0}\frac{d}{dx}\right)\\&=\frac{1}{\sqrt{2}}\left(\xi+\frac{d}{d\xi}\right)\end{aligned} \tag{54}$$

Likewise for the creation operator:

$$\hat{a}^{\dagger}=\frac{1}{\sqrt{2}}\left(\xi-\frac{d}{d\xi}\right) \tag{55}$$

As an exercise show that the number operator $\hat{a}^{\dagger}\hat{a}$ takes the form:

$$\hat{a}^{\dagger}\hat{a}=\frac{1}{2}\left[\xi^2-1-\frac{d^2}{d\xi^2}\right] \tag{56}$$

Hence the TISE in dimensionless form becomes:

$$\hbar\omega_0\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\psi(\xi)=E\psi(\xi)$$

$$\hbar\omega_0\left(\frac{1}{2}\left[\xi^2-1-\frac{d^2}{d\xi^2}\right]+\frac{1}{2}\right)\psi(\xi)=E\psi(\xi)$$

$$\left(\left[\xi^2-1-\frac{d^2}{d\xi^2}\right]+1\right)\psi(\xi)=\frac{2}{\hbar\omega_0}E\psi(\xi) \qquad (57)$$

$$\left[\xi^2-\frac{d^2}{d\xi^2}-\frac{2}{\hbar\omega_0}E\right]\psi(\xi)=0$$

$$\phi_{\xi\xi}(\xi)+\left(\frac{2}{\hbar\omega_0}E-\xi^2\right)\psi(\xi)=0$$

So, you can see that we still have the same DE, just a different variable. This DE can be solved using a series solution method like many other 2nd order ordinary differential equations but here we can take advantage of the operator method to 'generate' solutions. To see this, consider:

$$\hat{a}\psi_0(\xi)=\frac{1}{\sqrt{2}}\left(\xi+\frac{d}{d\xi}\right)\psi_0(\xi)=0 \qquad (58)$$

This is a first order DE that can be integrated directly to obtain

$$\psi_0(\xi)=A\exp\left(-\frac{\xi^2}{2}\right) \qquad (59)$$

(As an exercise, confirm this solves DE above)

This function must be normalized to unity. Since we are eventually going to want the dimensionalized version, let's convert back and then normalize the dimensionalized function.

$$\psi_0(\xi)=A\exp\left(-\frac{\xi^2}{2}\right)\Rightarrow\psi_0(x)=B\exp\left(-\frac{(\beta x)^2}{2}\right) \qquad (60)$$

$$1=\int_{-\infty}^{\infty}\psi_0^*(x)\psi_0(x)dx=|B|^2\int_{-\infty}^{\infty}\exp\left(-(\beta x)^2\right)dx \qquad (61)$$

To complete the integral, we must again make the variable change

$$\xi = \beta x \Rightarrow d\xi = \beta dx \Rightarrow dx = \frac{d\xi}{\beta} \tag{62}$$

Then we have

$$\begin{aligned} 1 &= |\mathrm{B}|^2 \int_{-\infty}^{\infty} \exp\left(-(\beta x)^2\right) dx = \frac{|\mathrm{B}|^2}{\beta} \int_{-\infty}^{\infty} \exp\left(-\xi^2\right) d\xi = \frac{|\mathrm{B}|^2}{\beta} \sqrt{\pi} \\ \Rightarrow \mathrm{B} &= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \end{aligned} \tag{63}$$

So, this gives us the first normalized wave function

$$\psi_0(x) = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{(\beta x)^2}{2}\right) \tag{64}$$

The remaining eigenfunctions are built up using the creation operator.

$$\begin{aligned} \hat{a}^{\dagger} \psi_0(\xi) &= \frac{1}{\sqrt{2}} \left(\xi - \frac{d}{d\xi}\right) A \exp\left(-\frac{\xi^2}{2}\right) \\ &= \frac{1}{\sqrt{2}} (\xi + \xi) A \exp\left(-\frac{\xi^2}{2}\right) \\ &= A' \xi \exp\left(-\frac{\xi^2}{2}\right) \end{aligned} \tag{65}$$

As before the constant A' must be chosen to normalize. This process can be repeated indefinitely, each time generating an eigenfunction of one higher unit in eigenvalue. Each time of course the exponential factor will appear, multiplied by a polynomial of successively higher order. The polynomials are called Hermite Polynomials. In compact form, we have

$$\psi_n(\xi) = A_n \mathrm{H}_n(\xi) \exp\left(-\frac{\xi^2}{2}\right)$$

$$\mathrm{H}_n(\xi) = \exp\left(\frac{\xi^2}{2}\right)\left(\xi - \frac{d}{d\xi}\right)^n \exp\left(-\frac{\xi^2}{2}\right) \qquad (66)$$

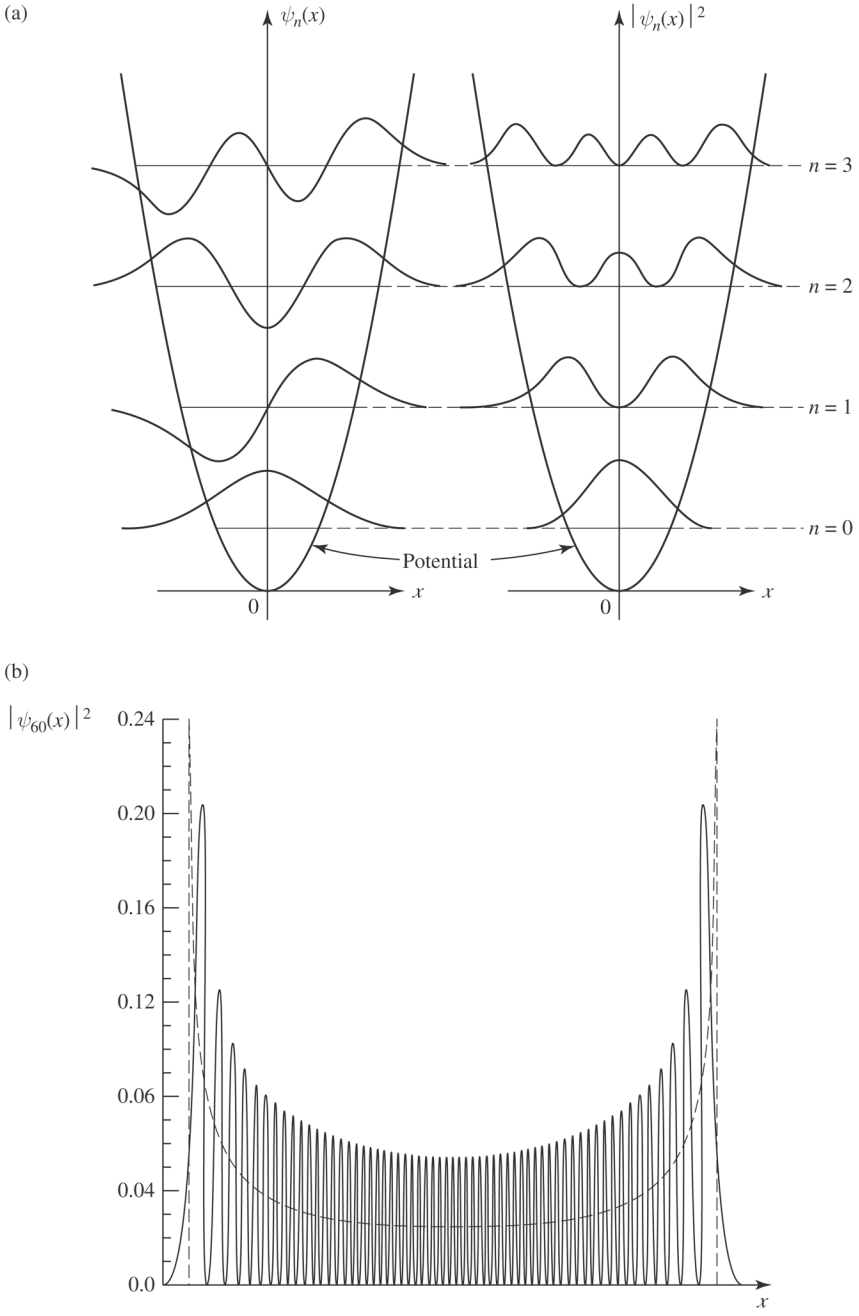
$$A_n = \sqrt{\frac{1}{\left(2^n n!\sqrt{\pi}\right)}}$$

$$E_n = \hbar\omega_0\left(n + \frac{1}{2}\right)$$

Table 2.1 in Griffiths tabulates the first five solutions. The normalization constant A_n must be multiplied by $\sqrt{\beta}$ if you need the dimensionalized functions.

$$H_0 = 1,$$
$$H_1 = 2\xi,$$
$$H_2 = 4\xi^2 - 2,$$
$$H_3 = 8\xi^3 - 12\xi,$$
$$H_4 = 16\xi^4 - 48\xi^2 + 12,$$
$$H_5 = 32\xi^5 - 160\xi^3 + 120\xi.$$

Figure 2.7 graphs the actual functions.



The Quantum Harmonic Oscillator in Dirac Notation

While the spatially dependent functions are necessary when plotting the actual shape of the wave functions, many quantum calculations may be done using just the operator properties. Here is a summary of useful things, expressed using Dirac notation.

Let

$$|\psi_n\rangle = |n\rangle \tag{67}$$

Then it is a simple matter to show that the following relationships hold:

$$\begin{aligned} \hat{a}|n\rangle &= \sqrt{n}|n-1\rangle \\ \hat{a}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \end{aligned} \tag{68}$$

The factors $\sqrt{n}$ and $\sqrt{n+1}$ are necessary for normalization.

It is then easy to show that the number state eigenvalue equation follows directly:

$$\begin{aligned} \hat{a}^\dagger\hat{a}|n\rangle &= \hat{a}^\dagger\sqrt{n}|n-1\rangle \\ &= \sqrt{n}\hat{a}^\dagger|n-1\rangle \\ &= \sqrt{n}\sqrt{n-1+1}|n-1+1\rangle \\ &= n|n\rangle \end{aligned} \tag{69}$$

The kets $|n\rangle$ are also orthonormal

$$\langle n|m\rangle = \delta_{nm} \tag{70}$$

It is very easy to show from these relationships that for instance the expectation value for the position operator is zero for any QHO state:

$$\begin{aligned}\langle n|\hat{x}|n\rangle &= \langle n|\left(\frac{\hat{a}+\hat{a}^{\dagger}}{\sqrt{2}\beta}\right)|n\rangle \\ &= \frac{1}{\sqrt{2}\beta}\left[\langle n|\hat{a}|n\rangle + \langle n|\hat{a}^{\dagger}|n\rangle\right] \\ &= \frac{1}{\sqrt{2}\beta}\left[\sqrt{n}\langle n|n-1\rangle + \sqrt{n+1}\langle n|n+1\rangle\right] \\ &= 0\end{aligned} \tag{71}$$

The average position is always the center of the potential, due to the fact that the wave functions are even or odd about the center and the probability distribution is hence even and symmetric about the center.

A valuable technique in this analysis has been the use of a dimensionalizing parameter, in this case $\beta = \frac{m\omega_0}{\hbar}$. Let see what this evaluates to for a typical case, say the CO molecule with vibrational level given by $2170\,cm^{-1}$:

$$\begin{aligned} & m_{CO} = 28\,amu \\ & \frac{1}{\lambda_{CO}} = 2170 cm^{-1} \\ & \hbar\omega_{CO} = \frac{hc}{\lambda_{CO}} \Rightarrow \omega_{CO} = \frac{2\pi c}{\lambda_{CO}} = 4.1x10^{14}\ \text{sec}^{-1} \\ & \beta = \sqrt{\frac{m\omega_0}{\hbar}} = 4.24\times 10^{11} m^{-1}\end{aligned} \tag{72}$$

Let's use this to find the classical turning point for the lowest energy state of the CO vibration. We need to equate the harmonic potential to the lowest energy state and solve for the x coordinate.

The potential energy and lowest energy state are given by:

$$\begin{aligned} V(x) &= \frac{m\omega_0^2}{2}x^2 \\ E_0 &= \frac{\hbar\omega_{CO}}{2}\end{aligned} \tag{73}$$

Equating these two quantities and solving for x yields the classical turning point.

$$\frac{m\omega_{CO}^2}{2}x^2 = \frac{\hbar\omega_{CO}}{2} \Rightarrow x_{turning} = \sqrt{\frac{\hbar}{m\omega_{CO}}} = \frac{1}{\beta} \tag{74}$$

So, the classical turning point is none other than the inverse of β. This is characteristic of many physics problems. The dimensional parameter is typically a characteristic length, energy, momentum, etc. of the problem.