

The Harmonic Oscillator (Arfken page 822)

Introduction:

9.3.9 The one-dimensional Schrödinger wave equation for a particle in a potential field $V = \frac{1}{2}kx^2$ is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi = E\psi(x).$$

(a) Using $\xi = ax$ and a constant λ , we have

$$a = \left(\frac{mk}{\hbar^2}\right)^{1/4}, \quad \lambda = \frac{2E}{\hbar} \left(\frac{m}{k}\right)^{1/2};$$

show that

$$\frac{d^2\psi(\xi)}{d\xi^2} + (\lambda - \xi^2)\psi(\xi) = 0.$$

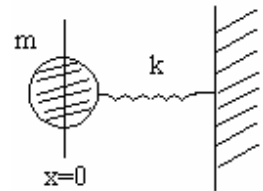
(b) Substituting

$$\psi(\xi) = y(\xi)e^{-\xi^2/2},$$

show that $y(\xi)$ satisfies the Hermite differential equation.

1. Classical description.

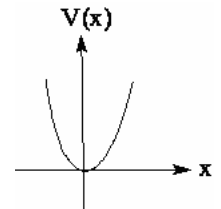
A particle of mass m is subject to a restoring force F_x , which is proportional to its displacement from the origin (Hooke's Law).



$$-\frac{dV(x)}{dx} = F_x = -kx$$

where k is the force constant. If we take the zero of the potential energy V to be at the origin $x = 0$ and integrate,

$$V(x) = \int_0^x dV = -k \int_0^x x dx = \frac{1}{2}kx^2$$



Note that this potential energy function differs from that in the particle-in-the-box problem in that the walls do not rise steeply to infinity at some particular point in space ($x = 0$ and $x = L$), but instead approach infinity much more slowly.

From Newton's second law,

$$F = ma = m \frac{d^2x}{dt^2} = -kx$$

thus,

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x = -\omega^2 x, \quad \omega = \sqrt{\frac{k}{m}}$$

This second-order differential equation is just like that for the free particle, so solutions must be of the form

$$x(t) = A \sin[\omega t] + B \cos[\omega t]$$

where A and B are constants of integration. If we assume that $x = 0$ at $t = 0$, then $B = 0$ and

$$x(t) = x_0 \sin[\omega t]$$

where $x_0 = A$ is the maximum displacement amplitude.

Since this can also be written as

$$x(t) = x_0 \sin(\omega t) = x_0 \sin(2\pi\nu t),$$

we see that the position of the particle oscillates in a sinusoidal manner with frequency

$$\nu = \frac{\omega}{2\pi} \Rightarrow k = 4\pi^2 m \nu^2.$$

The energy of the classical oscillator is

$$E = T + V = \frac{1}{2}mv^2 + \frac{1}{2}kx^2$$

$$\therefore v(t) = \frac{dx}{dt} = \omega x_0 \cos[\omega t]$$

$$\therefore E = \frac{1}{2}m\omega^2 x_0^2 \cos^2[\omega t] + \frac{1}{2}k x_0^2 \sin^2[\omega t] = \frac{1}{2}kx_0^2,$$

and is not quantized.

2. Quantum mechanical description.

Following our prescription, we begin by writing down the classical energy expression for the oscillator

$$E = T + V = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{p_x^2}{2m} + \frac{1}{2}kx^2$$

and then convert this to the quantum mechanical analog, the Hamiltonian operator \hat{H} , by replacing each of the dynamical variables (p_x and x) by their operator equivalents,

$$p_x \rightarrow \hat{p}_x = -i\hbar \frac{\partial}{\partial x}, \quad x \rightarrow \hat{x} = x$$

This yields

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2$$

We then use this form of \hat{H} in the time-independent Schrödinger equation

$$\hat{H}\psi = E\psi$$

not zero. New feature.

yielding

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + \frac{1}{2}kx^2 \psi(x) = E\psi(x). \quad (A)$$

Now, we want to solve this equation; *i.e.*, to find the set of functions $\psi(x)$ which, when operated on by the operator \hat{H} , yield a constant (E) times the function itself. The wavefunctions should also be:

- i. finite,
- ii. single-valued, and
- iii. continuous throughout the range from $x \rightarrow -\infty$ to $x \rightarrow \infty$.

As in the case of the free particle, Eq. (A) can be solved by expanding ψ in a power series, substituting this series into (A), and solving for the coefficients. In this case, it is a bit involved so we will only outline the procedure here. Details may be found in Griffith's book.

First, we transform Eq. (A) into a more useful form by introducing some new variables. To be consistent with Griffith, we choose

$$y = \sqrt{\alpha} x, \quad \alpha = \frac{4\pi^2 m v}{h} = \frac{m\omega}{\hbar}$$

Rewriting (A) as

$$\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + \left(E - \frac{1}{2} kx^2 \right) \psi(x) = 0$$

we first multiply through by $2m/\hbar^2\alpha$, yielding

$$\alpha^{-1} \frac{\partial^2}{\partial x^2} \psi(x) + \left(\frac{2mE}{\hbar^2\alpha} - \frac{mkx^2}{\hbar^2\alpha} \right) \psi(x) = 0.$$

We then define

$$\varepsilon = \frac{2mE}{\hbar^2\alpha}$$

Recognizing that $mk/\hbar^2 = \alpha^2$, we have

$$\alpha^{-1} \frac{\partial^2}{\partial x^2} \psi(x) + (\varepsilon - \alpha x^2) \psi(x) = 0$$

and, since $\alpha^{-1} \partial^2 / \partial x^2 = \partial^2 / \partial y^2$,

$$\frac{\partial^2}{\partial y^2} \psi(y) + (\varepsilon - y^2) \psi(y) = 0 \quad (\text{B})$$

We now proceed to solve this equation.

When y becomes very large, i.e. at $y \rightarrow \infty$ or $\varepsilon \rightarrow 0$, Eq. (B) reduces to

$$\frac{\partial^2 \psi(y)}{\partial y^2} - y^2 \psi(y) = 0.$$

In the limit as $y \rightarrow \pm \infty$, this equation has the asymptotic solution

$$\psi(y) = c e^{\pm y^2/2},$$

where c is a constant. The solution with the positive exponential does not behave properly, as $\psi(y) \rightarrow \infty$ for $y \rightarrow \pm \infty$. We want $\psi(y) \rightarrow 0$ in this limit. So we choose the solution with the negative exponential,

$$\psi(y) = c e^{-y^2/2} \quad \text{for } y \rightarrow \pm \infty.$$

But we are primarily interested in solving Eq. (B) for small, or at least finite, y . To do this, we assume a solution of the form

$$\psi(y) = c H(y) e^{-y^2/2} \quad (\text{C})$$

where $H(y)$ is a power series

$$H(y) = a_0 + a_1 y + a_2 y^2 + \dots$$

To find the values of the coefficients a_0, a_1, \dots , we substitute (C) into (B), which yields (after some algebra, worked out in Levine)

$$\frac{d^2 H(y)}{dy^2} - 2y \frac{dH(y)}{dy} + (\varepsilon - 1) H(y) = 0. \quad (\text{D})$$

This equation is very similar to a famous differential equation known as Hermite's equation

$$\frac{d^2H(y)}{dy^2} - 2y \frac{dH(y)}{dy} + 2v H(y) = 0 \quad (E)$$

In fact, (D) and (E) are identical if

$$(\varepsilon - 1) = 2v$$

The solutions $H(y)$ to Eq. (E), known as the Hermit polynomials, are of the form

$$H_v(y) = \sum_{k=0}^v \frac{(-1)^k v! (2y)^{v-2k}}{(v-2k)! k!}$$

where v is an integer ($v = 0, 1, 2, \dots$) and k is an index, running from $k = 0$ to $v/2$ if v is even, and from $k = 0$ to $k = (v-1)/2$ if v is odd. The Hermit polynomials may also be generated using the function

$$H_v(y) = (-1)^v e^{y^2} \frac{d^v}{dy^v} (e^{-y^2}).$$

At this point, we have solved the 1D harmonic oscillator problem.

2.a Eigenvalues

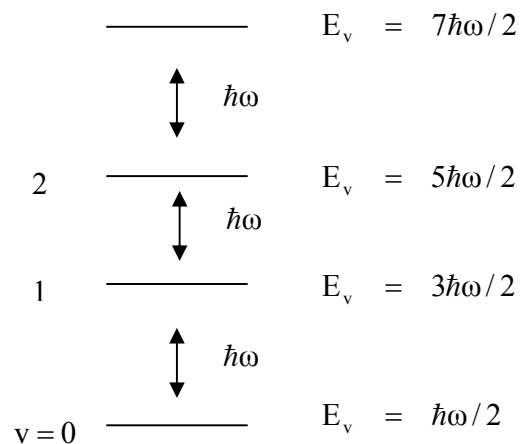
The energies (eigenvalues) of the one-dimensional harmonic oscillator may be found from the relations

$$(\varepsilon - 1) = 2v, \quad \varepsilon = \frac{2mE}{\hbar^2\alpha}, \quad \alpha = \frac{m\omega}{\hbar}$$

Combining these, we obtain

$$E_v = \left(v + \frac{1}{2}\right) \hbar\omega = \left(v + \frac{1}{2}\right) \hbar\nu, \quad v = 0, 1, 2, \dots$$

Unlike the corresponding classical result, we find that the quantum mechanical energy is quantized, in units of $\hbar\omega$, where ω is the classical frequency $\omega^2 = k/m$. v is called the vibrational quantum number. We also find that the lowest state, with $v = 0$, does not have zero energy but instead has $E = \hbar\omega/2$, the so-called zero point energy. We can summarize these results in the form of an energy level diagram



2.b Eigenfunctions.

The wavefunctions of the one-dimensional harmonic oscillator are of the form

$$\psi_v(y) = c H(y) e^{-y^2/2}$$

where c (or N_v) is a normalizing constant, $\left(\frac{\alpha}{\pi^{\frac{1}{2}} 2^v v!}\right)^{\frac{1}{2}}$. The functions $\psi_v(y)$ look complicated, but in reality they are not, at least for small v . To see this, let us examine the first few Hermite polynomials...

$$\left. \begin{aligned} H_{v=0}(y) &= 1 \\ H_{v=1}(y) &= 2y \\ H_{v=2}(y) &= 4y^2 - 2 \\ H_{v=3}(y) &= 8y^3 - 12y \end{aligned} \right\} \begin{array}{l} \text{Note that for } v \text{ even, only } \textit{even} \text{ powers} \\ \text{of } y \text{ appear whereas for } v \text{ odd, only } \textit{odd} \\ \text{powers of } y \text{ appear!} \end{array}$$

The corresponding wavefunctions are

$$\begin{aligned} \psi_{v=0}(y) &= \left(\frac{\alpha^{\frac{1}{2}}}{\pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} e^{-y^2/2}, & \psi_{v=1}(y) &= \left(\frac{\alpha^{\frac{1}{2}}}{2\pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} 2y \cdot e^{-y^2/2} \\ \psi_{v=2}(y) &= \left(\frac{\alpha^{\frac{1}{2}}}{8\pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} (4y^2 - 2) \cdot e^{-y^2/2}, \textit{ etc.} \end{aligned}$$

These are plotted on the next pages, together with their corresponding probability distributions. Note that these functions (and their magnitudes squared) are very similar to the corresponding functions for the particle-in-the-box problem, being respectively even or odd with respect to reflection about $y = 0$. There is one important difference, however, and this is that the HO functions do not go to zero at the “walls” of the potential. Thus, there is a finite probability $\sim (2v + 1)$ that the particle will be found in “classically forbidden” regions. This is the origin of the QM tunneling effect.

2. c Expectation values.

Using these functions, we can calculate the expectation value of any dynamical variable we wish, according to the recipe

$$a = \langle A \rangle = \frac{\int \psi^* \hat{A} \psi \, d\Gamma}{\int \psi^* \psi \, d\Gamma}$$

Suppose, for example, that we wish to calculate the average position, $\langle x \rangle$, in some particular state. (Clearly, it is zero, but can we prove it?). We have (since the ψ 's are normalized)

$$\langle x \rangle = \frac{1}{\sqrt{\alpha}} \langle y \rangle = \frac{1}{\sqrt{\alpha}} \left(\frac{\alpha^{\frac{1}{2}}}{\pi^{\frac{1}{2}} 2^v v!} \right) \int_{-\infty}^{\infty} H_v(y) \hat{y} H_v(y) e^{-y^2} dy$$

Now, you may substitute in the explicit expressions for $H_v(y)$ if you wish, and integrate, but it is easier in the present case to make use of the following useful relation (**called the three term recursion relation**)

$$\hat{y} H_v(y) = v H_{v-1}(y) + \frac{1}{2} H_{v+1}(y)$$

Then, the integral becomes

$$\int_{-\infty}^{\infty} \dots = \int_{-\infty}^{\infty} H_v(y) \left\{ v H_{v-1}(y) + \frac{1}{2} H_{v+1}(y) \right\} e^{-y^2} dy$$

Separating the pieces, we have

$$\begin{aligned} \int_{-\infty}^{\infty} \dots &= \int_{-\infty}^{\infty} H_v(y) \nu H_{v-1}(y) e^{-y^2/2} dy + \int_{-\infty}^{\infty} H_v(y) \frac{1}{2} H_{v+1}(y) e^{-y^2/2} dy \\ &= \nu \int_{-\infty}^{\infty} H_v(y) \cdot e^{-y^2/2} \cdot H_{v-1}(y) e^{-y^2/2} dy \\ &\quad + \frac{1}{2} \int_{-\infty}^{\infty} H_v(y) e^{-y^2/2} \cdot H_{v+1}(y) e^{-y^2/2} dy \end{aligned}$$

But $H_v(y)$ and $H_{v\pm 1}(y)$ are, respectively, either even and odd or odd and even functions of y . Since the limits on the integral are $\pm \infty$, the integrals are zero.

Therefore,

$$\langle x \rangle = 0.$$

One can proceed in a similar fashion when calculating $\langle x^2 \rangle$, $\langle x^3 \rangle$, ...etc. Also, one can make use of another relation

$$\frac{d H_v(y)}{dy} = 2v H_{v-1}$$

when calculating expectation values of other dynamical variables that involve, in their operator form, derivatives with respect to displacements (e.g., the momentum operator).

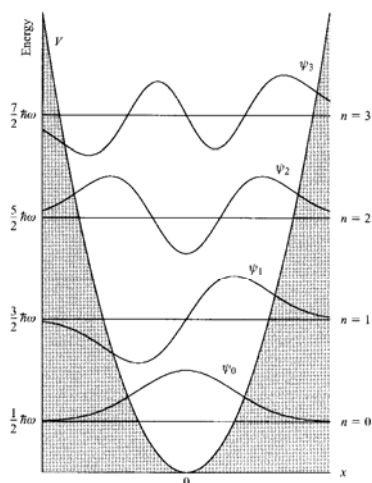


Figure 4.2 Wave functions and energy levels for a particle in a harmonic potential well. The outline of the potential energy is indicated by shading.

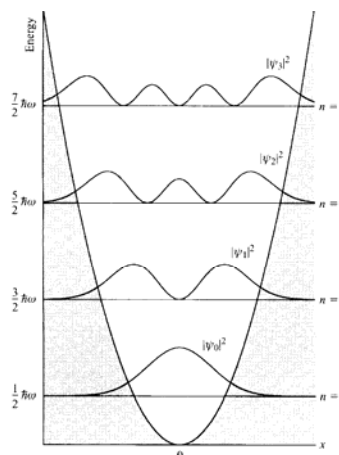
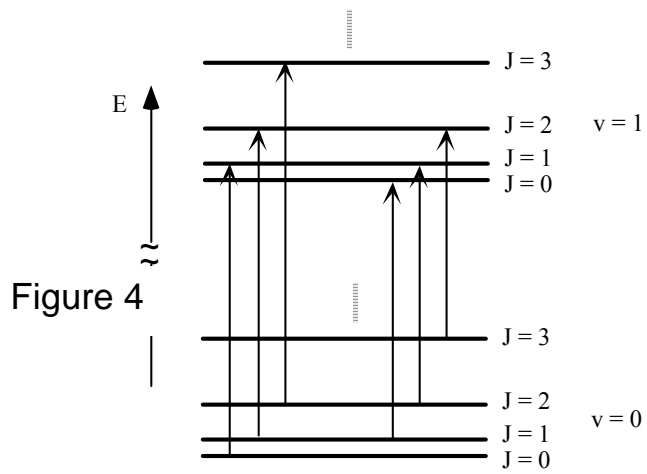


Figure 4.3 Probability densities and energy levels for a particle in a harmonic potential well. The outline of the potential energy is indicated by shading.

When we consider both rotations and vibrations simultaneously, we take advantage of the fact that these transitions occur on different timescales. Typically, a molecular vibration takes on the order of 10^{-14} s. A molecular rotation is normally much slower, taking on the order of 10^{-9} s or 10^{-10} s. Hence, as a molecule rotates one revolution, it vibrates many, many times. Since the vibrational energies are large compared with the rotational energies, the appropriate energy level diagram is:



Operator theory (Arfken page 822)

We have already discussed the solution of the quantum mechanical simple harmonic oscillator (s.h.o.) in class by direct substitution of the potential energy

$$V(x) = \frac{1}{2}kx^2 \quad (3.1)$$

into the one-dimensional, time-independent Schrödinger equation. Recall that k is the spring constant of the spring attached to a mass m . The spring is assumed to obey Hooke's Law so that the force on the mass is

$$F(x) = -kx \quad (3.2)$$

The resulting differential equation is solved by a series solution to find the quantized energies and the energy eigenfunctions. Recall that the allowed energies are given by

$$E_n = (n + 1/2)\hbar\omega \quad (3.3)$$

where
$$\omega = \sqrt{k/m} \quad (3.4)$$

In order to have a physical solution, we had to truncate our series. The series solution is quite involved and a bit "messy". We are going to solve the problem again using an operator theory approach. There is one interesting difference in the two approaches that we will observe. Using the operator theory approach,

we will find the energies and will be able to evaluate the averages of quantities like position and momentum *without knowing the specific forms of the eigenfunctions!*

This is remarkable since we have said before that you must know the wavefunction of the particle in order to solve for physical quantities of its motion. In the differential equation approach that we originally used, we had to make some guesses about the nature of the wavefunctions in order to find the energies, and to find the averages of position or momentum, we had to know the wavefunctions exactly.

Let's begin by writing the Hamiltonian for the s.h.o. (Using Eq. 3.1):

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 \quad (3.5)$$

Note that we have written the potential energy operator in terms of the position operator for x .

We now will find the energy eigenvalues E_n for this Hamiltonian that satisfy Schrödinger's equation:

$$\begin{aligned} \hat{H} |n\rangle &= E_n |n\rangle, \\ E_n &= \hbar\omega(n + \frac{1}{2}), \quad n = 0, 1, 2, \dots \end{aligned} \quad (3.6)$$

With the orthonormality relation:

$$\langle m | n \rangle = \delta_{m,n} = \begin{cases} 1 & \text{for } m = n \\ 0 & \text{for } m \neq n \end{cases} \quad (3.7)$$

To do this, let's **define** two new operators:

$$\begin{aligned} \hat{a} &\equiv \frac{1}{\sqrt{2m\hbar\omega}}(i\hat{p} + m\omega\hat{x}) \\ \hat{a}^+ &\equiv \frac{1}{\sqrt{2m\hbar\omega}}(-i\hat{p} + m\omega\hat{x}) \end{aligned} \quad (3.8)$$

Note that the operators are defined in terms of two observable operators (position & momentum) and are adjoints (complex conjugates) of one another, i.e. $(\hat{a}^\dagger)^\dagger = \hat{a}$. They are concocted. Why make them? The usual answer....wait and see.

H.W. Prove that $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)$, $\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a})$

With these new operators, one can show that the Hamiltonian can be written as

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2) \quad (3.9)$$

or
$$\hat{H} = \hbar\omega(\hat{a}\hat{a}^\dagger - 1/2) \quad (3.10)$$

If these two equations are solved for $\hat{a}^\dagger\hat{a}$ and $\hat{a}\hat{a}^\dagger$ then one can also show, using the commutation relation $[\hat{x}, \hat{p}] = i\hbar$, that the commutator of the two operators is one,

$$[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1 \quad (3.11)$$

☞ **Comment:**

$$\begin{aligned} \hat{x}^2 &= \left[\sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \right]^2 = \left(\frac{\hbar}{2m\omega} \right) \{ (\hat{a} + \hat{a}^\dagger)(\hat{a} + \hat{a}^\dagger) \} = \left(\frac{\hbar}{2m\omega} \right) \{ \hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \}, \\ \hat{p}^2 &= \left[i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a}) \right]^2 = -\left(\frac{m\hbar\omega}{2} \right) \{ (\hat{a}^\dagger - \hat{a})(\hat{a}^\dagger - \hat{a}) \} = -\left(\frac{m\hbar\omega}{2} \right) \{ \hat{a}^2 + \hat{a}^{\dagger 2} - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} \} \\ \hat{H} &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = -\frac{1}{2m}\left(\frac{m\hbar\omega}{2} \right) \{ \hat{a}^2 + \hat{a}^{\dagger 2} - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} \} + \frac{1}{2}m\omega^2\left(\frac{\hbar}{2m\omega} \right) \{ \hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \} \\ &= \frac{\hbar\omega}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger) = \frac{\hbar\omega}{2}(\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a} + 1) = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \end{aligned}$$

Now consider what happens if we operate on an energy eigenfunction $|n\rangle$ with \hat{a} . We get a new vector. What happens if we then operate on this new vector with the Hamiltonian \hat{H} ? Let's see:

$$\hat{H}(\hat{a}|n\rangle) = \left\{ \hbar\omega\left(\hat{a}\hat{a}^\dagger - \frac{1}{2}\right) \right\}(\hat{a}|n\rangle) \quad (3.12)$$

Note that (3.10) was used for the Hamiltonian. Distributing the two terms in the Hamiltonian gives:

$$\hat{H}(\hat{a}|n\rangle) = \hbar\omega(\hat{a}\hat{a}^\dagger\hat{a})|n\rangle - \frac{1}{2}\hbar\omega\hat{a}|n\rangle \quad (3.13)$$

Examination of (3.9) shows that the operators in curly brackets can be replaced by $\hat{H} - \frac{1}{2}\hbar\omega$ so that

$$\begin{aligned} \hat{H}(\hat{a}|n\rangle) &= \hat{a}\left\{ \hat{H} - \frac{1}{2}\hbar\omega \right\}|n\rangle - \frac{1}{2}\hbar\omega\hat{a}|n\rangle \\ &= \hat{a}\hat{H}|n\rangle - \frac{1}{2}\hbar\omega\hat{a}|n\rangle - \frac{1}{2}\hbar\omega\hat{a}|n\rangle \\ \hat{H}(\hat{a}|n\rangle) &= \hat{a}\hat{H}|n\rangle - \hbar\omega\hat{a}|n\rangle \end{aligned} \quad (3.14)$$

Look at the first term in the above expression. It has the Hamiltonian operating on an energy eigenfunction. We know the result of this operation: it is the energy eigenvalue E_n ($\hat{H}|n\rangle = E_n|n\rangle$).

Thus, we can write the equation as

$$\hat{H}(\hat{a}|n\rangle) = (E_n - \hbar\omega)(\hat{a}|n\rangle) \quad (3.15)$$

A similar sequence of steps can be performed to show that

$$\hat{H}(\hat{a}^+|n\rangle) = (E_n + \hbar\omega)(\hat{a}^+|n\rangle) \quad (3.16)$$

What can we conclude from these two expressions? Look at (3.15). Note that it is an *eigenvalue equation*! The operator \hat{a} creates a new vector when it operates on $|n\rangle$ and this vector is an eigenvector of the Hamiltonian with an energy eigenvalue of $E_n - \hbar\omega$. The operator \hat{a} has taken the original eigenvector $|n\rangle$ with eigenvalue E_n and has created a new eigenvector with a new eigenvalue of $E_n - \hbar\omega$. Since the new energy eigenvalue is less than the original energy, the operator \hat{a} is called the **annihilation operator**.

A similar analysis applies to (3.16). Here, though, we see that operator \hat{a}^+ creates a new eigenvector of the Hamiltonian with an energy eigenvalue that is greater than the original energy E_n . Thus, we call operator \hat{a}^+ the **creation operator**.

Let us examine the annihilation operator and (3.15) a bit closer. The total energy of the s.h.o. can't be negative. But if we operate on the state with the lowest energy (the ground state where $n = 0$) with \hat{a} , then we might get a negative energy resulting when $\hbar\omega$ is subtracted from E_0 . So we *require* that

$$\hat{a}|0\rangle = 0 \quad (3.17)$$

This condition allows us to find the ground state energy. Let's operate on the ground state with the Hamiltonian to see what we obtain. We will make use of (3.9) to express the Hamiltonian.

$$\hat{H}|0\rangle = \hbar\omega(\hat{a}^+\hat{a} + 1/2)|0\rangle = \hbar\omega\hat{a}^+\hat{a}|0\rangle + \frac{1}{2}\hbar\omega|0\rangle$$

Note that invoking the requirement for the ground state expressed in (3.17) makes the first term in the above equation become zero. Thus, we have

$$\hat{H}|0\rangle = \frac{1}{2}\hbar\omega|0\rangle \quad (3.18)$$

so the ground state energy is

$$E_0 = \frac{1}{2}\hbar\omega \quad (3.19)$$

How do we find the other energies? Let's start with the ground state and operate on it with the creation operator, \hat{a}^+ . Then let's operate on that new eigenfunction with the Hamiltonian and see what we get. This is equivalent to taking the expression in (3.16) with $n=0$.

$$\hat{H}(\hat{a}^+|0\rangle) = (E_0 + \hbar\omega)(\hat{a}^+|0\rangle) = \frac{3}{2}\hbar\omega(\hat{a}^+|0\rangle) \quad (3.20)$$

We get a new eigenfunction that has an eigenvalue of $3\hbar\omega/2$. If we operate on this eigenfunction with \hat{a}^+ and then \hat{H} again, we would get another eigenfunction with an eigenvalue of $5\hbar\omega/2$. Successive operations by the creation operator and Hamiltonian lead us to conclude that the possible energy eigenvalues of states created in this manner are

$$\boxed{E_n = (n + 1/2)\hbar\omega} \quad \text{where } n = 0, 1, 2, \dots \quad (3.21)$$

But are these the energies of the eigenfunctions $|n\rangle$? That is, are these the actual energies of the s.h.o.? The answer is *yes!* How can we show this?

It appears that the creation operator, \hat{a}^+ , operates on $|n\rangle$ and gives as a result the eigenstate $|n+1\rangle$ since the energy eigenvalue increases by one increment of $\hbar\omega/2$. Let us postulate then that

$$\hat{a}^+ |n\rangle = c_{n+1} |n+1\rangle \quad (3.22)$$

If we can find the constant c_{n+1} then our assumption is correct. This would mean that these new eigenfunctions that we obtain by operating on the $|n\rangle$ vectors with \hat{a}^+ are just other old eigenfunctions! Thus, the energy eigenvalues of the “new” eigenfunctions are really just the energy eigenvalues of the original eigenfunctions and these are the actual energies of the s.h.o. To find the constant, let’s evaluate the following scalar product:

$$\begin{aligned} \langle n | \hat{a} \hat{a}^+ | n \rangle &= (\langle n | \hat{a}) (\hat{a}^+ | n \rangle) = (c_{n+1}^*) (c_{n+1}) \langle n+1 | n+1 \rangle \\ &\Rightarrow \langle n | \hat{a} \hat{a}^+ | n \rangle = |c_{n+1}|^2 \end{aligned} \quad (3.23)$$

We have assumed that the $|n\rangle$ eigenfunctions are normalized. Recall that eigenfunctions with different eigenvalues are orthogonal, thus the ψ eigenfunctions form an orthonormal set. Using the commutation relation in (3.11), we can replace $\hat{a} \hat{a}^+$ by $\hat{a}^+ \hat{a} + 1$ to find

$$|c_{n+1}|^2 = \langle n | \hat{a}^+ \hat{a} + 1 | n \rangle = \langle n | \hat{a}^+ \hat{a} | n \rangle + \langle n | n \rangle = \langle n | \hat{a}^+ \hat{a} | n \rangle + 1 \quad (3.24)$$

Now what? Look at the product of the creation and annihilation operator. It operates on $|n\rangle$. Do we know what this operation does? Yes! We can use (3.9) to write

$$\hat{a}^+ \hat{a} = \frac{1}{\hbar\omega} \hat{H} - \frac{1}{2} \quad (3.25)$$

Let’s see what this operator does when it operates on a ψ eigenfunction:

$$\begin{aligned} \hat{a}^+ \hat{a} | n \rangle &= \left\{ \frac{1}{\hbar\omega} \hat{H} - \frac{1}{2} \right\} | n \rangle = \frac{1}{\hbar\omega} \hat{H} | n \rangle - \frac{1}{2} | n \rangle = \frac{1}{\hbar\omega} E_n | n \rangle - \frac{1}{2} | n \rangle \\ &\Rightarrow \hat{a}^+ \hat{a} | n \rangle = \left(\frac{E_n}{\hbar\omega} - 1/2 \right) | n \rangle \end{aligned} \quad (3.26)$$

Using (3.21) for the energy E_n gives

$$\begin{aligned} \hat{a}^+ \hat{a} | n \rangle &= \left(\frac{(n+1/2)\hbar\omega}{\hbar\omega} - 1/2 \right) | n \rangle \\ &\Rightarrow \hat{a}^+ \hat{a} | n \rangle = n | n \rangle \end{aligned} \quad (3.27)$$

Aha! This operator gives back the eigenfunction times an integer n . In other words, the $|n\rangle$ functions are eigenfunctions not only of the Hamiltonian, but also of this creation-annihilation product operator. (You should recognize (3.27) as an eigenvalue equation.) This operator is a handy one to remember so let’s give it its own name and symbol. We define this operator to be the **number operator**

$$\hat{n} \equiv \hat{a}^+ \hat{a} \quad (3.28)$$

The functions $|n\rangle$ are eigenfunctions of the number operator with corresponding eigenvalues that are the integers that label the eigenfunctions:

$$\hat{n} | n \rangle = n | n \rangle \quad (3.29)$$

The Hamiltonian can be written using this number operator as

$$\hat{H} = (\hat{n} + 1/2)\hbar\omega \quad (3.30)$$

This is all very interesting but how does this find the constant c_{n+1} ? Recall that is the task at hand. Look back at (3.24). We can rewrite this as

$$\begin{aligned} |c_{n+1}|^2 &= \langle n | \hat{n} | n \rangle + 1 = \langle n | n | n \rangle + 1 = n \langle n | n \rangle + 1 = n + 1 \\ \Rightarrow c_{n+1} &= \sqrt{n+1} \end{aligned} \quad (3.31)$$

We have done it! We have found the constant and can write

$$\boxed{\hat{a}^+ | n \rangle = \sqrt{n+1} | n+1 \rangle} \quad (3.32)$$

We have shown that the creation operator does give back one of the original energy eigenfunctions. In fact, it gives back the eigenfunction with the next highest energy. The energies expressed in (3.21) are the energies of the s.h.o.

It will also be useful to us to find out what the annihilation operator does when it operates on a ψ eigenfunction. In analogy to the creation operator, we are led to postulate that

$$\hat{a} | n \rangle = c_{n-1} | n-1 \rangle \quad (3.33)$$

Can we find the constant c_{n-1} to verify this statement? Knowing what the creation operator does via (3.32), we can write that

$$\hat{a}^+ | n-1 \rangle = \sqrt{n} | n \rangle \quad (3.34)$$

Solving this for $| n \rangle$ gives

$$| n \rangle = \frac{1}{\sqrt{n}} \hat{a}^+ | n-1 \rangle \quad (3.35)$$

Substituting this into (3.33) gives

$$\frac{1}{\sqrt{n}} \hat{a} \hat{a}^+ | n-1 \rangle = c_{n-1} | n-1 \rangle \quad (3.36)$$

Once again, we use the commutation relation in (3.11) to replace $\hat{a} \hat{a}^+$ by $\hat{a}^+ \hat{a} + 1$ to obtain

$$\begin{aligned} c_{n-1} | n-1 \rangle &= \frac{1}{\sqrt{n}} (\hat{a}^+ \hat{a} + 1) | n-1 \rangle = \frac{1}{\sqrt{n}} (\hat{n} + 1) | n-1 \rangle = \frac{1}{\sqrt{n}} (n-1+1) | n-1 \rangle \\ c_{n-1} | n-1 \rangle &= \sqrt{n} | n-1 \rangle \end{aligned} \quad (3.37)$$

Thus, we can finally write that

$$\boxed{\hat{a} | n \rangle = \sqrt{n} | n-1 \rangle} \quad (3.38)$$

Let us briefly summarize what we have found. First, we have found the quantized energies of the s.h.o. which are given by (3.21). Second, we have found how the creation and annihilation operators operate on the energy eigenfunctions. These results are given in (3.32) and (3.38). This information is valuable since it allows us to find the average values of quantities such as position and momentum as you will see in the homework problems. It should be stressed that we are able to find all of these physical quantities without knowing the actual functional form of the eigenfunctions themselves! As mentioned before, this is a very attractive benefit for using this creation/annihilation operator approach to analyze the simple harmonic oscillator.

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2$$

$$\hat{a} \equiv \frac{1}{\sqrt{2m\hbar\omega}} (m\omega\hat{x} + i\hat{p}), \quad \hat{a}^\dagger \equiv \frac{1}{\sqrt{2m\hbar\omega}} (m\omega\hat{x} - i\hat{p})$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger), \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}} (\hat{a}^\dagger - \hat{a})$$

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2), \quad \hat{H} = \hbar\omega(\hat{a}\hat{a}^\dagger - 1/2)$$

$$\hat{N} \equiv \hat{a}^\dagger\hat{a} \quad [\hat{a}, \hat{a}^\dagger] = 1$$

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad \hat{a} |n\rangle = \sqrt{n} |n-1\rangle$$

Problems

$$\begin{aligned} \hat{a}^\dagger |m\rangle = \sqrt{m+1} |m+1\rangle &\Rightarrow \langle n | \hat{a}^\dagger |m\rangle = \sqrt{m+1} \langle n | m+1\rangle = \sqrt{m+1} \delta_{n,m+1}; \\ \hat{a} |m\rangle = \sqrt{m} |m-1\rangle &\Rightarrow \langle n | \hat{a} |m\rangle = \sqrt{m} \langle n | m-1\rangle = \sqrt{m} \delta_{n,m-1}; \end{aligned}$$

1- Use the definition $\langle \hat{A} \rangle = \langle n | \hat{A} | n \rangle$, check the following:

| | | | |
|--|-------|-----------------------------|---|
| $\langle \hat{a} \rangle$ | 0 | $\langle \hat{x} \rangle$ | 0 |
| $\langle \hat{a}^\dagger \rangle$ | 0 | $\langle \hat{p} \rangle$ | 0 |
| $\langle \hat{a}\hat{a}^\dagger \rangle$ | $n+1$ | $\langle \hat{x}^2 \rangle$ | $\frac{\hbar}{m\omega} (n + \frac{1}{2})$ |
| $\langle \hat{a}^\dagger\hat{a} \rangle$ | n | $\langle \hat{p}^2 \rangle$ | $m\hbar\omega (n + \frac{1}{2})$ |

2- Calculate the expressions $\Delta\hat{p} = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2}$ and $\Delta\hat{x} = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2}$ then prove that:

$$\Delta\hat{x}\Delta\hat{p} = (n + \frac{1}{2})\hbar.$$

3- Prove that $|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle$

4- Prove the following:

$$\hat{H} = \frac{\hbar\omega}{2} (\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger);$$

$$[\hat{a}, H] = \hbar\omega\hat{a};$$

$$[\hat{a}^\dagger, H] = -\hbar\omega\hat{a}^\dagger$$

4- Check the following:

$$\langle l | \hat{x}^3 | n \rangle = \left(\frac{\hbar}{2m\omega} \right)^{3/2} \times \begin{cases} \sqrt{(n+1)(n+2)(n+3)} & \text{for } l = n+3 \\ 3(n+1)\sqrt{n+1} & \text{for } l = n+1 \\ 3n\sqrt{n} & \text{for } l = n-1 \\ \sqrt{n(n-1)(n-2)} & \text{for } l = n-3 \\ 0 & \text{otherwise} \end{cases}$$

$$(\hat{a}) = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}; \quad (\hat{a}^\dagger \hat{a}) = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 2 & 0 & \dots \\ 0 & 0 & 0 & 3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix};$$

$$(\hat{a} \hat{a}^\dagger) = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 2 & 0 & 0 & \dots \\ 0 & 0 & 3 & 0 & \dots \\ 0 & 0 & 0 & 4 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}; \quad (\hat{a} \hat{a}^\dagger - \hat{a}^\dagger \hat{a}) = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

To calculate the ground state wavefunction, we have to use $\hat{a}|\psi_0\rangle = 0$, where

$$\hat{a} = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} + i\hat{p}) \text{ and } \hat{p} = -i\hbar\frac{\partial}{\partial x}. \text{ This gives}$$

$$\left(i(-i\hbar\frac{d}{dx}) + m\omega x \right) \psi_0(x) = 0 \Rightarrow \left(\hbar\frac{d}{dx} + m\omega x \right) \psi_0(x) = 0$$

With arrangement, one gets: $\frac{d\psi_0(x)}{\psi_0} = -\frac{m\omega}{\hbar} x dx$. After integration, we have

$$\psi_0(x) = N e^{-\alpha x^2}, \quad \alpha = \frac{m\omega}{2\hbar}, \quad N^2 = \sqrt{\frac{m\omega}{\pi\hbar}}$$

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

[3.1]

(a) Using the definitions of \hat{a} and \hat{a}^\dagger in (3.8) and the fact that $[\hat{p}, \hat{x}] = -i\hbar$, show that you can write the Hamiltonian as expressed in (3.9), i.e. $\hat{H} = \hbar\omega(\hat{a}^\dagger \hat{a} + 1/2)$.

(b) In a similar fashion, show that you can also write the Hamiltonian as expressed in (3.10), i.e. $\hat{H} = \hbar\omega(\hat{a} \hat{a}^\dagger - 1/2)$.

[3.2]

(a) Show that you can write the position and momentum operators as

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^+) \quad \hat{p} = -i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a} - \hat{a}^+)$$

(b) Using these results and the knowledge of how the creation and annihilation operators operate on the energy eigenfunctions (Equations (3.32) & (3.38)), show that the average position and average momentum of the s.h.o. in the n th state (which means any state) are identically zero. Recall that the energy eigenfunctions form an orthonormal set.

[3.3]

(a) Show for a s.h.o. in the n th state (any state) that the average values of the squares of position and momentum are

$$\langle x^2 \rangle = \frac{\hbar}{m\omega}(n + 1/2) \quad \langle p^2 \rangle = m\hbar\omega(n + 1/2)$$

Hint: Use the commutator result in (3.11) to replace $\hat{a}\hat{a}^+$. Recall that $\hat{a}^+\hat{a} = \hat{n}$ and we know what the number operator does when it operates on an eigenfunction as expressed in (3.29).

(b) Combine your results from [3.2] and part (a) to show for a s.h.o. in the n th state that the uncertainty product is

$$\Delta x \Delta p = (n + 1/2)\hbar$$

(c) What is the uncertainty product in the ground state? Note that this is the smallest possible uncertainty product that exists in nature as stated by the Heisenberg Uncertainty Principle.

Prove that

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^+), \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^+ - \hat{a})$$

Simple Harmonic Motion Hermit Polynomial

The combination of Newton and Hook laws implies:

$$F_x = ma_x = -k x$$

$$\Rightarrow \frac{d^2x}{dt^2} = -\frac{k}{m}x = -\omega^2 x, \quad k = m\omega^2$$

The solution will be: $x = A \sin(\omega t + \theta)$

Where A and θ are constants, and $\omega = 2\pi\nu = \frac{2\pi}{T}$

Potential is related to the work by the equation: $V = -W = -\int_0^x F_x dx = \frac{1}{2}kx^2,$

And the K.E. will be:

$$K = \frac{1}{2}m v^2 = \frac{1}{2}m \left(\frac{dx}{dt}\right)^2 = \frac{1}{2}mA^2\omega^2 \cos^2(\omega t + \theta)$$

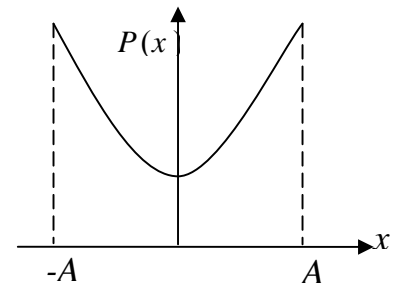
$$= \frac{1}{2}mA^2\omega^2 [1 - \sin^2(\omega t + \theta)]$$

$$= \frac{1}{2}m\omega^2 (A^2 - x^2)$$

And the total energy

$$E = K + V = \frac{1}{2}m\omega^2 (A^2 - x^2) + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2 A^2$$

$$P(x)dx = \frac{dt}{T/2} = \frac{2 \frac{dx}{v}}{T} = \frac{2}{T v} dx = \frac{2}{T \sqrt{\omega^2 (A^2 - x^2)}} dx = \frac{1}{\pi \sqrt{A^2 - x^2}} dx$$



$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0,$$

$$\Rightarrow \boxed{\frac{d^2\psi}{dx^2} + (\beta - \alpha^2 x^2)\psi = 0} \quad (1)$$

Where $\alpha = m\omega/\hbar$, $\beta = 2mE/\hbar^2$. Equation (1) could be simplified using the substitution:

$$q = \sqrt{\alpha} x$$

H.W. Check these derivatives:

$$\frac{d\psi}{dx} = \frac{d\psi}{dq} \frac{dq}{dx} = \sqrt{\alpha} \frac{d\psi}{dq}$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dq} \left(\frac{d\psi}{dx} \right) \frac{dq}{dx} = \alpha \frac{d^2\psi}{dq^2}$$

$$\frac{d^2\psi}{dq^2} + (\lambda - q^2)\psi = 0 \quad (2)$$

with

$$\lambda = \frac{\beta}{\alpha} = \frac{2E}{\hbar\omega} \quad (3)$$

Equation (2) has a physical solution at:

$$\lambda = \frac{2E}{\hbar\omega} = 2n + 1,$$

$$\Rightarrow E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, \dots \quad (4)$$

what is the asymptotic solution? i.e. when $q \rightarrow \pm \infty$. In that case we can neglect λ comparing to q^2 .

$$\frac{d^2\psi_\infty}{dq^2} - q^2\psi_\infty = 0 \Rightarrow \psi_\infty = e^{aq^2} \quad (5)$$

H.W. find the values of a, by differentiating eq (5) twice and substitute in (2),

$$\frac{d^2\psi_\infty}{dq^2} = (4a^2q^2 + 2a)e^{aq^2} \approx 4a^2q^2e^{aq^2} \quad a^2 = \frac{1}{4} \Rightarrow a = \pm \frac{1}{2}$$

So, solution of (5) will be:

$$\psi_\infty = ce^{-q^2/2} + de^{+q^2/2}$$

Where c and d are constants. Due to the condition $\lim_{q \rightarrow \infty} e^{+q^2/2} = \infty$ the solution $e^{+q^2/2}$ will be rejected, i.e. d=0.

So, equation (2) will take the form:

$$\psi = \psi_{\infty} H(q) = e^{-q^2/2} H(q) \quad (6)$$

Where H(q) is the power series in the variable q (will call it Hermit polynomial).

H.W. Using the function $\psi = e^{-q^2/2} H(q)$, prove the following equation.

$$\frac{d^2\psi}{dq^2} = \left[\frac{d^2H(q)}{dq^2} - 2q \frac{dH(q)}{dq} + (q^2 - 1)H(q) \right] e^{-q^2/2}$$

Then (2) will take the form:

$$\frac{d^2H(q)}{dq^2} - 2q \frac{dH(q)}{dq} + (\lambda - 1)H(q) = 0 \quad (7)$$

This is similat to Hermit equation

$$\frac{d^2H_n(q)}{dq^2} - 2q \frac{dH_n(q)}{dq} + 2n H_n(q) = 0, \quad n = 0, 1, 2, \dots \quad (8)$$

By putting $H(q) = H_n(q)$ and using the condition

$$\lambda = \frac{2E}{\hbar\omega} = 2n + 1, \quad (9)$$

$$E = (n + \frac{1}{2})\hbar\omega = (n + \frac{1}{2})\hbar\nu, \quad n = 0, 1, 2, \dots$$

H.W. Using power series solve equation 7.

Start with the equation:

$$\frac{d^2H(q)}{dq^2} - 2q \frac{dH(q)}{dq} + (\lambda - 1)H(q) = 0 \quad (10)$$

And use the power series:

$$H(q) = \sum_{k=0}^{\infty} e_k q^k = e_0 + e_1 q + e_2 q^2 + e_3 q^3 + \dots$$

Differentiate once and twice,

$$\frac{dH(q)}{dq} = \sum_{k=0}^{\infty} k e_k q^{k-1} = e_1 + 2e_2 q + 3e_3 q^2 + \dots;$$

$$\frac{d^2H(q)}{dq^2} = \sum_{k=0}^{\infty} k(k-1)e_k q^{k-2} = 2e_2 + 2 \cdot 3e_3 q + 3 \cdot 4e_4 q^2 + \dots$$

Equating the coefficient of q^m to zero, we have the following relations:

$$2e_2 + (\lambda - 1)e_0 = 0$$

$$2 \cdot 3e_3 + (\lambda - 1 - 2)e_1 = 0$$

$$3 \cdot 4e_4 + (\lambda - 1 - 2 \cdot 2)e_2 = 0$$

.....

To the power k , we have:

$$(k+1)(k+2)e_{k+2} + (\lambda - 1 - 2k)e_k = 0$$

And Recursion relation will be:

$$e_{k+2} = \frac{\lambda - 1 - 2k}{(k+1)(k+2)} e_k \quad (11)$$

Where e_0 and e_1 are arbitrary constants. We reach the solution:

$$H(q) = e_0 \underbrace{\left(1 + \frac{e_2}{e_0} q^2 + \frac{e_4 e_2}{e_2 e_0} q^4 + \frac{e_6 e_4 e_2}{e_4 e_2 e_0} q^6 + \dots \right)}_{\text{even}} + e_1 \underbrace{\left(q + \frac{e_3}{e_1} q^3 + \frac{e_5 e_3}{e_3 e_1} q^5 + \frac{e_7 e_5 e_3}{e_5 e_3 e_1} q^7 + \dots \right)}_{\text{odd}} \quad (12.)$$

H.W. Discuss the behavior of the above series at $k \gg 1$ and compare it with the diverging series: $e^{q^2} = 1 + q^2 + \frac{q^4}{2} + \dots + \frac{q^{2k}}{k!} + \dots$ to prove that $H(q) \propto e^{q^2}$.

So, our wave function will take the form:

$$\psi \propto e^{-q^2/2} e^{q^2} \propto e^{q^2/2}$$

And this is a diverging series when $q \rightarrow \pm\infty$. This enforces us to terminate our series when $k = n$ in which $\lambda = 2n + 1$.