Chapter 8 The Simple Harmonic Oscillator

A winter rose. How can a rose bloom in December? Amazing but true, there it is, a yellow winter rose. The rain and the cold have worn at the petals but the beauty is eternal regardless of season. Bright, like a moon beam on a clear night in June. Inviting, like a fire in the hearth of an otherwise dark room. Warm, like a…wait! Wait just a MINUTE! What is this...Emily Dickinson? Mickey Spillane would NEVER… Misery Street…that's more like it…a beautiful secretary named Rose…back at it now…the mark turned yellow…yeah, yeah, all right…the elegance of the transcendance of Euler's number on a Parisian morning in 1873…what?…

The infinite square well is useful to illustrate many concepts including energy quantization but the infinite square well is an unrealistic potential. The simple harmonic oscillator (SHO), in contrast, is a realistic and commonly encountered potential. It is one of the most important problems in quantum mechanics and physics in general. It is often used as a first approximation to more complex phenomena or as a limiting case. It is dominantly popular in modeling a multitude of cooperative phenomena. The electrical bonds between the atoms or molecules in a crystal lattice are often modeled as "little springs," so group phenomena is modeled by a system of coupled SHO's. If your studies include solid state physics you will encounter phonons, and the description of multiple coupled phonons relies on multiple simple harmonic oscillators. The quantum mechanical description of electromagnetic fields in free space uses multiple coupled photons modeled by simple harmonic oscillators. The rudiments are the same as classical mechanics…small oscillations in a smooth potential are modeled well by the SHO.

If a particle is confined in any potential, it demonstrates the same qualitative behavior as a particle confined to a square well. Energy is quantized. The energy levels of the SHO will be different than an infinite square well because the "geometry" of the potential is different. You should look for other similarities in these two systems. For instance, compare the shapes of the eigenfunctions between the infinite square well and the SHO.

Part 1 outlines the basic concepts and focuses on the arguments of linear algebra using **raising and lowering operators** and matrix operators. This approach is more modern and elegant than brute force solutions of differential equations in position space, and uses and reinforces Dirac notation, which depends upon the arguments of linear algebra. The raising and lowering operators, or **ladder operators**, are the predecessors of the creation and annihilation operators used in the quantum mechanical description of interacting photons. The arguments of linear algebra provide a variety of raising and lowering equations that yield the eigenvalues of the SHO,

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

and their eigenfunctions. The eigenfunctions of the SHO can be described using **Hermite polynomials** (pronounced "her meet"), which is a complete and orthogonal set of functions.

Part 2 will explain why the Hermite polynomials are applicable and reinforce the results of part 1. Part 2 emphasizes the method of **power series solutions** of a differential equation. Chapter 5 introduced the separation of variables, which is usually the first method applied in an attempt to solve a partial differential equation. Power series solutions apply to ordinary differential equations. In the case the partial differential equation is separable, it may be appropriate to solve one or more of the resulting ordinary differential equations using a power series method. We will encounter this circumstance when we address the hydrogen atom. You should leave this chapter understanding how an ordinary differential equation is solved using a power series solution.

We do not reach the coupled harmonic oscillator in this text. Of course, the SHO is an important building block in reaching the coupled harmonic oscillator. There are numerous physical systems described by a single harmonic oscillator. The SHO approximates any individual bond, such as the bond encountered in a diatomic molecule like O_2 or N_2. The SHO applies to any system that demonstrates small amplitude vibration.

The Simple Harmonic Oscillator, Part 1

Business suit, briefcase, she's been in four stores and hasn't bought a thing...so this mall has got to be the meet! Now a video store. She's as interested in videos as a cow is in eating meat. But, right in the middle of the drama section, suddenly face to face... "Sir, do you have a cigarette?" and walks off more briskly than Lipton ice tea. Blown. Gone. Done. Just to tell me she knows me...no meet for me. I've got to hang up my hat, but only my hat... She doesn't know Charlie's face, and maybe the meet will happen in Part 2...

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1. Justify the use of a simple harmonic oscillator potential, $V(x) = kx^2/2$, for a particle confined to any smooth potential well. Write the time–independent Schrodinger equation for a system described as a simple harmonic oscillator.

The sketches may be most illustrative. You have already written the time–independent Schrodinger equation for a SHO in chapter 2.

The functional form of a simple harmonic oscillator from classical mechanics is $V(x) = \frac{1}{2}kx^2$. Its graph is a parabola as seen in the figure on the left. Any relative minimum in a smooth potential energy curve can be approximated by a simple harmonic oscillator if the energy is small compared to the height of the well meaning that oscillations have small amplitudes.

Figure 8 − 1. Simple Harmonic Oscillator. Figure 8 − 2. Relative Potential Energy Minima.

Expanding an arbitrary potential energy function in a Taylor series, where x_0 is the minimum,

$$V(x) = V(x_0) + \frac{dV}{dx}\Big|_{x_0}(x - x_0) + \frac{1}{2!}\frac{d^2V}{dx^2}\Big|_{x_0}(x - x_0)^2 + \frac{1}{3!}\frac{d^3V}{dx^3}\Big|_{x_0}(x - x_0)^3 + \cdots$$

defining $V(x_0) = 0$, $\frac{dV}{dx}\Big|_{x_0} = 0$ because the slope is zero at the bottom of a minimum, and if $E \ll$ the height of the potential well, then $x \approx x_0$ so terms where the difference $(x - x_0)$ has a power of 3 or greater are negligible. The Taylor series expansion reduces to

$$V(x) = \frac{1}{2}\frac{d^2V}{dx^2}\Big|_{x_0}(x-x_0)^2 \qquad \text{where} \qquad \frac{d^2V}{dx^2}\Big|_{x_0} = k\,.$$

Define $x_0 = 0 \;\Rightarrow\; V(x) = \dfrac{1}{2}kx^2$. Since $k = m\omega^2$, this means $V(x) = \dfrac{1}{2}m\omega^2x^2$. Using this potential to form a Hamiltonian operator, the time–independent Schrodinger equation is

$$\mathcal{H}\,|\,\psi> = E_n\,|\,\psi> \quad\Rightarrow\quad \left[\frac{\mathcal{P}^2}{2m} + \frac{1}{2}\,m\omega^2\mathcal{X}^2\right]|\,\psi> = E_n\,|\,\psi>\ .$$

Postscript: Notice that this Schrodinger equation is basis independent. The momentum and position operators are represented only in abstract Hilbert space.

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2. Show that the time-independent Schrodinger Equation for the SHO can be written

$$\hbar\omega\left(a^\dagger\,a + \frac{1}{2}\right)|\,\psi> = E_n\,|\,\psi>\ .$$

Let $\quad a = \left(\dfrac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} \,+\, i\left(\dfrac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P} \quad$ and $\quad a^\dagger = \left(\dfrac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X}^\dagger \,-\, i\left(\dfrac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}^\dagger\,.$

For reasons that will become apparent, a is called the **lowering operator**, and $a^\dagger$ is known as the **raising operator**. Since $\mathcal{X}$ and $\mathcal{P}$ are Hermitian, $\mathcal{X}^\dagger = \mathcal{X}$ and $\mathcal{P}^\dagger = \mathcal{P}$, so the raising operator can be written

$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}.$$

Remember that $\mathcal{X}$ and $\mathcal{P}$ do not commute. They are fundamentally canonical, $\left[\mathcal{X},\,\mathcal{P}\right] = i\hbar\,.$

$$\begin{aligned}
\hbar\omega\left(a^\dagger\,a + \frac{1}{2}\right) &= \hbar\omega\left\{\left[\left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}\right]\left[\left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}\right] + \frac{1}{2}\right\}\\
&= \hbar\omega\left[\left(\frac{m\omega}{2\hbar}\right)\mathcal{X}^2 + i\left(\frac{1}{4\hbar^2}\right)^{1/2}\mathcal{X}\mathcal{P} - i\left(\frac{1}{4\hbar^2}\right)^{1/2}\mathcal{P}\mathcal{X} + \left(\frac{1}{2m\omega\hbar}\right)\mathcal{P}^2 + \frac{1}{2}\right]\\
&= \hbar\omega\left[\frac{m\omega}{2\hbar}\mathcal{X}^2 + \frac{1}{2m\omega\hbar}\mathcal{P}^2 + \frac{i}{2\hbar}\Big(\mathcal{X}\mathcal{P} - \mathcal{P}\mathcal{X}\Big) + \frac{1}{2}\right]\\
&= \hbar\omega\left[\frac{1}{2m\omega\hbar}\mathcal{P}^2 + \frac{m\omega}{2\hbar}\mathcal{X}^2 + \frac{i}{2\hbar}\Big[\mathcal{X},\,\mathcal{P}\Big] + \frac{1}{2}\right]\\
&= \hbar\omega\left[\frac{1}{2m\omega\hbar}\mathcal{P}^2 + \frac{m\omega}{2\hbar}\mathcal{X}^2 + \frac{i}{2\hbar}\,i\hbar + \frac{1}{2}\right]\\
&= \hbar\omega\left[\frac{1}{2m\omega\hbar}\mathcal{P}^2 + \frac{m\omega}{2\hbar}\mathcal{X}^2 - \frac{1}{2} + \frac{1}{2}\right] = \left[\frac{1}{2m}\mathcal{P}^2 + \frac{m\omega^2}{2}\mathcal{X}^2\right]
\end{aligned}$$

$$\Rightarrow \quad \left[\frac{1}{2m}\mathcal{P}^2 + \frac{m\omega^2}{2}\mathcal{X}^2\right] | \psi> = E_n | \psi> \quad \Longleftrightarrow \quad \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) | \psi> = E_n | \psi> \ .$$

Postscript: The Schrodinger equation is $\left[\mathcal{P}^2 + \mathcal{X}^2\right] | \psi> = E_n | \psi>$, when constant factors are excluded. The sum $\mathcal{P}^2 + \mathcal{X}^2 = \mathcal{X}^2 + \mathcal{P}^2$ would appear to factor as $\left(\mathcal{X} + i\mathcal{P}\right)\left(\mathcal{X} - i\mathcal{P}\right)$, so that

$$\left[\mathcal{P}^2 + \mathcal{X}^2\right] | \psi> = E_n | \psi> \Rightarrow \left[\mathcal{X}^2 + \mathcal{P}^2\right] | \psi> = E_n | \psi> \Rightarrow \left(\mathcal{X} + i\mathcal{P}\right)\left(\mathcal{X} - i\mathcal{P}\right) | \psi> = E_n | \psi> \ .$$

This is only a qualified type of factoring because the order of the "factors" cannot be changed; $\mathcal{X}$ and $\mathcal{P}$ are fundamentally canonical and simply do not commute. Nevertheless, the parallel with common factoring into complex conjugate quantities is part of the motivation for the raising and lowering operators. In fact, some authors refer to this approach as the method of factorization.

Notice that $a^\dagger a = \dfrac{1}{\hbar\omega}\mathcal{H} - \dfrac{1}{2}$.

Notice also that though $\mathcal{X}$ and $\mathcal{P}$ are Hermitian, a and $a^\dagger$ are not.

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3. Show that the commutator $\left[a, \ a^\dagger\right] = 1$.

Problems 3 and 4 are developing tools to approach the eigenvector/eigenvalue problem of the SHO.

We want $\left[a, \ a^\dagger\right] = a\,a^\dagger - a^\dagger a$ in terms the definitions of problem 2. Letting

$$C = \left(\frac{m\omega}{2\hbar}\right)^{1/2}, \qquad \text{and} \qquad D = \left(\frac{1}{2m\omega\hbar}\right)^{1/2} \qquad \text{to simplify notation,}$$

$$\begin{aligned}
\left[a, \ a^\dagger\right] &= \left(C\mathcal{X} + iD\mathcal{P}\right)\left(C\mathcal{X} - iD\mathcal{P}\right) - \left(C\mathcal{X} - iD\mathcal{P}\right)\left(C\mathcal{X} + iD\mathcal{P}\right) \\
&= \cancel{C^2\mathcal{X}^2} - iCD\mathcal{X}\,\mathcal{P} + iDC\mathcal{P}\,\mathcal{X} + \cancel{D^2\mathcal{P}^2} - \cancel{C^2\mathcal{X}^2} - iCD\mathcal{X}\,\mathcal{P} + iDC\mathcal{P}\,\mathcal{X} - \cancel{D^2\mathcal{P}^2} \\
&= 2iCD\left(\mathcal{P}\,\mathcal{X} - \mathcal{X}\,\mathcal{P}\right) \\
&= 2i\left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\left[\mathcal{P}, \ \mathcal{X}\right] \\
&= \frac{2i}{2\hbar}\left(-i\hbar\right) = 1, \quad \text{since} \quad \left[\mathcal{P}, \ \mathcal{X}\right] = -\left[\mathcal{X}, \ \mathcal{P}\right] = -i\hbar\,.
\end{aligned}$$

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4. Show that $\mathcal{H}\,a^\dagger = a^\dagger\mathcal{H} + a^\dagger\hbar\omega$.

This is a tool used to solve the eigenvector/eigenvalue problem for the SHO though it should build some familiarity with the raising and lowering operators and commutator algebra.

$$\mathcal{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \quad \Rightarrow \quad \frac{\mathcal{H}}{\hbar\omega} = a^\dagger a + \frac{1}{2}$$

$$\left[a^\dagger,\ \frac{\mathcal{H}}{\hbar\omega} \right] = \left[a^\dagger,\ a^\dagger a + \frac{1}{2} \right] = a^\dagger a^\dagger a + \cancel{a^\dagger \frac{1}{2}} - a^\dagger a a^\dagger - \cancel{\frac{1}{2} a^\dagger}$$

$$= a^\dagger \big(a^\dagger a - a^\dagger a \big) = -a^\dagger \left[a,\ a^\dagger \right] = -a^\dagger$$

$$\Rightarrow \quad \left[a^\dagger,\ \mathcal{H} \right] = -a^\dagger \hbar\omega \quad \Rightarrow \quad a^\dagger \mathcal{H} - \mathcal{H}\, a^\dagger, = -a^\dagger \hbar\omega \quad \Rightarrow \quad \mathcal{H}\, a^\dagger = a^\dagger \mathcal{H} + a^\dagger \hbar\omega\,.$$

Postscript: We will also use the fact that $\mathcal{H}\, a = a\,\mathcal{H} - a\hbar\omega\,,$ though its proof is posed to the student as a problem.

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5. Find the effect of the raising and lowering operators using the results of problem 4.

We have written time–independent Schrodinger equation as $\mathcal{H}\,|\,\psi> \,=\, E_n\,|\,\psi>$ to this point. Since the Hamiltonian is the energy operator, the eigenvalues are necessarily energy eigenvalues. The state vector is assumed to be a linear combination of all energy eigenvectors. If we specifically measure the eigenvalue E_n , then the state vector is necessarily the associated eigenvector which can be written $|\,E_n>$. The time–independent Schrodinger equation written as $\mathcal{H}\,|\,E_n> = E_n\,|\,E_n>$ is likely a better expression for the development that follows.

If $\mathcal{H}\,|\,E_n> = E_n\,|\,E_n>$ where E_n is an energy eigenvalue, then $|\,E_n> \,=\, |\,E_n>$

$$\begin{aligned} \Rightarrow \quad \mathcal{H}\, a^\dagger\,|\,E_n> &= \big(a^\dagger \mathcal{H} + a^\dagger \hbar\omega \big)\,|\,E_n> = a^\dagger \mathcal{H}\,|\,E_n> +\, a^\dagger \hbar\omega\,|\,E_n> \\ &= a^\dagger E_n\,|\,E_n> +\, a^\dagger \hbar\omega\,|\,E_n> = \big(E_n + \hbar\omega \big)\, a^\dagger\,|\,E_n> \quad \text{or} \\ \mathcal{H}\left(a^\dagger\,|\,E_n> \right) &= \big(E_n + \hbar\omega \big)\left(a^\dagger\,|\,E_n> \right). \end{aligned}$$

This means that $a^\dagger\,|\,E_n>$ is an eigenvector of $\mathcal{H}$ with an eigenvalue of $E_n + \hbar\omega$. This is exactly $\hbar\omega$ more than the eigenvalue of the eigenvector $|\,E_n>$. The effect of $a^\dagger$ acting on $|\,E_n>$ is to "raise" the eigenvalue by $\hbar\omega$, thus $a^\dagger$ is known as the raising operator.

Again, given that $\mathcal{H}\,|\,E_n> = E_n\,|\,E_n>$ and starting with $|\,E_n> \,=\, |\,E_n>$

$$\begin{aligned} \Rightarrow \quad \mathcal{H}\, a\,|\,E_n> &= \big(a\mathcal{H} - a\hbar\omega \big)\,|\,E_n> = a\mathcal{H}\,|\,E_n> -\, a\hbar\omega\,|\,E_n> \\ &= aE_n\,|\,E_n> -\, a\hbar\omega\,|\,E_n> = \big(E_n - \hbar\omega \big)\, a\,|\,E_n> \quad \text{or} \\ \mathcal{H}\left(a\,|\,E_n> \right) &= \big(E_n - \hbar\omega \big)\left(a\,|\,E_n> \right). \end{aligned}$$

Here $a\,|\,E_n>$ is an eigenvector of $\mathcal{H}$ with an eigenvalue of $E_n - \hbar\omega$. This is $\hbar\omega$ less than the eigenvalue of the eigenvector $|\,E_n>$. The effect of a acting on $|\,E_n>$ is to "lower" the eigenvalue by $\hbar\omega$, thus a is known as the lowering operator.

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6. What is the effect of the lowering operator on the ground state, E_g ?

This is another step toward finding the eigenvalues of the SHO.

Given $\mathcal{H}\,|\,E_g\!> = E_g\,|\,E_g\!>$, the effect of the lowering operator is to lower the eigenvalue by $\hbar\omega$, $\mathcal{H}\,a\,|\,E_g\!> = \big(E_g - \hbar\omega\big)\,|\,E_g\!>$. This is physically impossible; there cannot be an energy less than ground state energy. The only physical possibility of the lowering operator acting on the ground state is zero...this means that there is no physical system.

Postscript: Zero, the absence of a physical system, is not the same as the zero vector, $|\,0\!>$. The quantum number $n = 0$ is the ground state of the SHO. The quantum number of the SHO is sufficient to uniquely identify the eigenstate so $|\,E_3\!> = |\,3\!>$, $|\,E_7\!> = |\,7\!>$, and $|\,E_0\!> = |\,0\!>$.

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7. Calculate a value for the ground state energy of the SHO.

Remember that $a\,|\,0\!> = 0$ from the previous problem. Orthogonality of eigenstates is required, and any system that is orthogonal can be made orthonormal. The strategy is to calculate the expectation value of the ground state two different ways.

$$\mathcal{H}\,|\,0\!> = E_0\,|\,0\!> \;\Rightarrow\; <\!0\,|\,\mathcal{H}\,|\,0\!> = <\!0\,|\,E_0\,|\,0\!> \;\Rightarrow\; <\!0\,|\,\mathcal{H}\,|\,0\!> = \; E_0 <\!0\,|\,0\!> = E_0$$

because $<\!0\,|\,0\!> = 1$ due to the orthonormality of eigenstates. This expectation value can also be expressed in terms of the raising and lowering operators

$$\begin{aligned} E_0 = <\!0\,|\,\mathcal{H}\,|\,0\!> &= <\!0\,|\,\hbar\omega\left(a^\dagger a + \frac{1}{2}\right)|\,0\!> = <\!0\,|\,\hbar\omega a^\dagger a + \frac{\hbar\omega}{2}\,|\,0\!> \\ &= <\!0\,|\,\hbar\omega a^\dagger a\,|\,0\!> \;+\; <\!0\,|\,\frac{\hbar\omega}{2}\,|\,0\!> \\ &= <\!0\,|\,\hbar\omega a^\dagger\Big(a\,|\,0\!>\Big) \;+\; \frac{\hbar\omega}{2} <\!0\,|\,0\!> = 0 + \frac{\hbar\omega}{2} = \frac{\hbar\omega}{2} \end{aligned}$$

is the ground state energy of the SHO.

Postscript: Orthonormality is an assumption based upon the requirement for orthogonality that proves to be warranted for the ground state.

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8. Derive the eigenenergies of the SHO

Per problem 5, $\mathcal{H}\Big(a^\dagger\,|\,E_n\!>\Big) \;= \big(E_n + \hbar\omega\big)\Big(a^\dagger\,|\,E_n\!>\Big)$ so $a^\dagger\,|\,E_n\!>$ is an eigenvector of $\mathcal{H}$ with the eigenvalue $E_n + \hbar\omega$. Similarly, that $a^\dagger\,|\,E_n\!>$ is an eigenvector of $\mathcal{H}$,

$$\Rightarrow \;\; \mathcal{H}\,\Big[a^\dagger\Big(a^\dagger\,|\,E_n\!>\Big)\Big] \;= \big(E_n + \hbar\omega + \hbar\omega\big)\,\Big[a^\dagger\Big(a^\dagger\,|\,E_n\!>\Big)\Big]$$

so $a^\dagger\Big(a^\dagger\,|\,E_n>\Big) = a^\dagger a^\dagger\,|\,E_n>$ is an eigenvector of $\mathcal{H}$ with the eigenvalue $E_n + 2\hbar\omega$. Successively applying the raising operator yields successive eigenvalues. The eigenvalue of the ground state is fixed at $\hbar\omega/2$ so all the eigenvalues can be attained in terms of the ground–state eigenvalue.

$$\begin{aligned}
\mathcal{H}\,|\,0> = E_0\,|\,0> = \frac{\hbar\omega}{2}\,|\,0> \quad &\Rightarrow \quad \mathcal{H}\,a^\dagger\,|\,0> = \left(\frac{\hbar\omega}{2} + \hbar\omega\right)\,|\,0> \\
&\Rightarrow \quad \mathcal{H}\,a^\dagger a^\dagger\,|\,0> = \left(\frac{\hbar\omega}{2} + 2\hbar\omega\right)\,|\,0> \\
&\Rightarrow \quad \mathcal{H}\,a^\dagger a^\dagger a^\dagger\,|\,0> = \left(\frac{\hbar\omega}{2} + 3\hbar\omega\right)\,|\,0> \quad \text{and in general} \\
&\Rightarrow \quad \mathcal{H}\,\left(a^\dagger\right)^n\,|\,0> = \left(\frac{\hbar\omega}{2} + n\hbar\omega\right)\,|\,0>
\end{aligned}$$

from which we ascertain

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad \text{are the eigenenergies of the SHO.}$$

Postscript: This argument does not specify the eigenvectors $a^\dagger\,|\,0>,\ a^\dagger a^\dagger\,|\,0>, \ldots, \left(a^\dagger\right)^n\,|\,0>$.

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9. Find energy space representations for the eigenvectors of the SHO.

Explicit eignvalues given $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ are $E_0 = \frac{1}{2}\hbar\omega,\ E_1 = \frac{3}{2}\hbar\omega,\ E_2 = \frac{5}{2}\hbar\omega,\ E_3 = \frac{7}{2}\hbar\omega, \ldots, E_n = \left(n + \frac{1}{2}\right)\hbar\omega$. The eigenvector/eigenvalue equations must remain $\mathcal{H}\,|\,0> = E_0\,|\,0>,\ \mathcal{H}\,|\,1> = E_1\,|\,1>,\ \mathcal{H}\,|\,2> = E_2\,|\,2>,\ \mathcal{H}\,|\,3> = E_3\,|\,3>, \ldots, \mathcal{H}\,|\,n> = E_n\,|\,n>$. Combining these eigenvalue/eigenvector relations with those attained earlier using the raising operator provides the ability to explicitly respresent the eigenvectors.

$$\begin{aligned}
\mathcal{H}\,|\,1> = \frac{3}{2}\hbar\omega\,|\,1> = \mathcal{H}\,a^\dagger\,|\,0> \quad &\Rightarrow \quad |\,1> \propto a^\dagger\,|\,0> \\
\mathcal{H}\,|\,2> = \frac{5}{2}\hbar\omega\,|\,2> = \mathcal{H}\,a^\dagger a^\dagger\,|\,0> \quad &\Rightarrow \quad |\,2> \propto a^\dagger a^\dagger\,|\,0> \propto a^\dagger\,|\,1> \\
\mathcal{H}\,|\,3> = \frac{7}{2}\hbar\omega\,|\,3> = \mathcal{H}\,a^\dagger a^\dagger a^\dagger\,|\,0> \quad &\Rightarrow \quad |\,3> \propto a^\dagger a^\dagger a^\dagger\,|\,0> \propto a^\dagger\,|\,2> \quad \text{and} \\
\mathcal{H}\,|\,n> = \left(n + \frac{1}{2}\right)\hbar\omega\,|\,n> = \mathcal{H}\,\left(a^\dagger\right)^n\,|\,0> \quad &\Rightarrow \quad |\,n> \propto \left(a^\dagger\right)^n\,|\,0> \propto a^\dagger\,|\,n-1>
\end{aligned}$$

$$\Rightarrow \quad C\,(n)\,|\,n> = a^\dagger\,|\,n-1> \quad \text{in general, where } C\,(n) \text{ is a proportionality constant.}$$

Postscript: The relation of proportionality is appropriate for this argument because of the nature of the eigenvalue/eigenvector equation. Any vector that is proportional to the eigenvector will work in the eigenvalue/eigenvector equation. Consider

$\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}$ whose eigenvalues are 2 and 1, corresponding to the eigenvectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

$$\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 2\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} 2 \\ 0 \end{pmatrix} = \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \quad \text{but any vector}$$

proportional to $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ also yields a true statement in the eigenvalue/eigenvector equation, *e.g.*,

$$\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 2 \\ 0 \end{pmatrix} = 2\begin{pmatrix} 2 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} 4 \\ 0 \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \end{pmatrix}.$$

In fact, the proportionality condition is equivalent to the normalization condition in this case.

The n in the equation $C(n)\,|\,n\!> \,= \, a^\dagger\,|\,n-1\!>$ is one eigenstate higher than $n-1$. The raising operator acting on an eigenstate increases the state to the next higher eigenstate.

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10. Normalize $C(n)\,|\,n\!> \,= \, a^\dagger\,|\,n-1\!>$.

This problem is a good example of (a) forming adjoints and applying the normalization condition, (b) using commutator algebra, and (c) using eigenvalue/eigenvector equations. Remember orthonormality requires that $<\!n\,|\,n\!> \,=\, <\!n-1\,|\,n-1\!> \,= 1$, and that $\left[\,a\,,\,a^\dagger\,\right] = 1$.

(a) $\quad C(n)\,|\,n\!> \,= \, a^\dagger\,|\,n-1\!> \;\Rightarrow\; <\!n\,|\,C^*(n) = \,<\!n-1\,|\left(a^\dagger\right)^\dagger = \,<\!n-1\,|\,a$ is the adjoint equation

$$\Rightarrow \;<\!n\,|\,C^*(n)\,C(n)\,|\,n\!> \,=\, <\!n-1\,|\,a\,a^\dagger\,|\,n-1\!> \quad \text{are the innner products.}$$

We have an expression for $a^\dagger a$, but need to develop an expression for $a\,a^\dagger$.

(b) $$\mathcal{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \;\Rightarrow\; a^\dagger a = \frac{\mathcal{H}}{\hbar\omega} - \frac{1}{2} \;\Rightarrow\; a^\dagger a - a\,a^\dagger = \frac{\mathcal{H}}{\hbar\omega} - \frac{1}{2} - a\,a^\dagger$$

subtracting $a\,a^\dagger$ from both sides. $\left[\,a\,,\,a^\dagger\,\right] = 1 \;\Rightarrow\; \left[\,a^\dagger\,,\,a\,\right] = -1$, and $a^\dagger a - a\,a^\dagger = \left[\,a^\dagger\,,\,a\,\right]$,

$\Rightarrow \;\left[\,a^\dagger\,,\,a\,\right] = \dfrac{\mathcal{H}}{\hbar\omega} - \dfrac{1}{2} - a\,a^\dagger \;\Rightarrow\; -1 = \dfrac{\mathcal{H}}{\hbar\omega} - \dfrac{1}{2} - a\,a^\dagger \;\Rightarrow\; a\,a^\dagger = \dfrac{\mathcal{H}}{\hbar\omega} + \dfrac{1}{2}$. Returning to part (a),

(c) $$\left|\,C(n)\,\right|^2 <\!n\,|\,n\!> \,=\, <\!n-1\,|\,\frac{\mathcal{H}}{\hbar\omega} + \frac{1}{2}\,|\,n-1\!>$$

$$\Rightarrow \;\left|\,C(n)\,\right|^2 = \,<\!n-1\,|\,\frac{\mathcal{H}}{\hbar\omega}\,|\,n-1\!> + <\!n-1\,|\,\frac{1}{2}\,|\,n-1\!>$$

$$\Rightarrow \;\left|\,C(n)\,\right|^2 = \,<\!n-1\,|\,\frac{1}{\hbar\omega}\left(n-1+\frac{1}{2}\right)\hbar\omega\,|\,n-1\!> + \frac{1}{2} <\!n-1\,|\,n-1\!>$$

where $\mathcal{H}$ acts on $|\,n-1>$ resulting in the eigenvalue in the first term on the right. Then

$$\begin{aligned}\big|\,C\,(n)\,\big|^2 &= <n-1\,|\,n-\frac{1}{2}\,|\,n-1> + \frac{1}{2} = <n-1\,|\,n\,|\,n-1> \;-\; <n-1\,\Big|\,\frac{1}{2}\,\Big|\,n-1> + \frac{1}{2}\\ &= n<n-1\,|\,n-1> \;-\; \frac{1}{2}<n-1\,|\,n-1> + \frac{1}{2} = n - \frac{1}{2} + \frac{1}{2} = n\,,\end{aligned}$$

$$\Rightarrow \quad C\,(n) = \sqrt{n} \quad \Rightarrow \quad \sqrt{n}\,|\,n> = a^\dagger\,|\,n-1> \;.$$

Postscript: An alternate way of writing this result is $a^\dagger\,|\,n> = \sqrt{n+1}\,|\,n+1>$. The effect of the lowering operator is $a\,|\,n> = \sqrt{n}\,|\,n-1>$, and is left to the student as a problem.

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11. Find a general relation for an arbitrary eigenstate of the SHO in terms of the ground state and the raising operator.

A useful relation and a numerical example of the use of the raising operator follow.

The general relation for one state in terms of the higher adjacent state and the raising operator is $a^\dagger\,|\,n> = \sqrt{n+1}\,|\,n+1>$. Applying this relation to the ground state and adjacent states,

$$\begin{aligned} a^\dagger\,|\,0> &= \sqrt{0+1}\,|\,0+1> = \sqrt{1}\,|\,1>\\ \left(a^\dagger\right)^2|\,0> &= a^\dagger\sqrt{1}\,|\,1> = \sqrt{1}\;a^\dagger\,|\,1> = \sqrt{1}\sqrt{1+1}\,|\,1+1> = \sqrt{1}\sqrt{2}\,|\,2>\\ \left(a^\dagger\right)^3|\,0> &= a^\dagger\sqrt{1}\sqrt{2}\,|\,2> = \sqrt{1}\sqrt{2}\;a^\dagger\,|\,2> = \sqrt{1}\sqrt{2}\sqrt{2+1}\,|\,2+1> = \sqrt{1}\sqrt{2}\sqrt{3}\,|\,3>\;.\end{aligned}$$

For arbitrary n this pattern yields

$$\begin{aligned}\left(a^\dagger\right)^n|\,0> &= a^\dagger\sqrt{1}\sqrt{2}\sqrt{3}\sqrt{4}\cdots\sqrt{n-1}\,|\,n-1>\\ &= \sqrt{1}\sqrt{2}\sqrt{3}\sqrt{4}\cdots\sqrt{n-1}\;a^\dagger\,|\,n-1>\\ &= \sqrt{1}\sqrt{2}\sqrt{3}\sqrt{4}\cdots\sqrt{n-1}\sqrt{n}\,|\,n>\\ &= \sqrt{n!}\,|\,n>\\ \Rightarrow \qquad |\,n> &= \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n|\,0>\;.\end{aligned}$$

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12. Develop a matrix operator representation of the Hamiltonian of the SHO.

It is convenient to use unit vectors to express eigenstates for the SHO. The first few are written

$$|\,0> = \begin{pmatrix}1\\0\\0\\0\\0\\\vdots\end{pmatrix}, \quad |\,1> = \begin{pmatrix}0\\1\\0\\0\\0\\\vdots\end{pmatrix}, \quad |\,2> = \begin{pmatrix}0\\0\\1\\0\\0\\\vdots\end{pmatrix}, \quad |\,3> = \begin{pmatrix}0\\0\\0\\1\\0\\\vdots\end{pmatrix}.$$

Notice that all the eigenkets are of infinite dimension and that they are orthonormal. This problem is an application of the mathematics of part 2 of chapter 1 applied to a realistic system.

The Hamiltonian is Hermitian and has unit vectors as basis vectors. The Hamiltonian must, therefore, be diagonal with the eigenvalues on the main diagonal, *i.e.*,

$$\mathcal{H} = \hbar\omega \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 3/2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 5/2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 7/2 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 9/2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

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13. (a) Develop the matrix representation of the lowering operator for the SHO.

(b) Lower the third excited state of the SHO using explicit matrix multiplication, and

(c) demonstrate equivalence to $a\,|\,n> \,=\, \sqrt{n}\;|\,n-1>$.

An individual element of any matrix can be calculated using Dirac notation by sandwiching the operator between the bra representing the row of interest and the ket representing the column of interest. In general for the lowering operator,

$$\begin{aligned} <n\,|\,a\,|\,m> \; &= \; <n\,|\,\sqrt{m}\,|\,m-1> \\ &= \sqrt{m}\; <n\,|\,m-1> \\ &= \sqrt{m}\;\delta_{n,\,m-1}, \end{aligned}$$

where the lowering operator acted to the right in the first line. The Kronecker delta reflects orthonormality. It says that the element in row n and column $m-1$ is zero unless $n = m-1$.

(a) Trying a few values on the main diagonal,

$$\begin{aligned} <0\,|\,a\,|\,0> \; &= \sqrt{0}\;\delta_{0,-1} = \sqrt{0}\,(0) = 0\,, \\ <1\,|\,a\,|\,1> \; &= \sqrt{1}\;\delta_{1,\,0} = \sqrt{1}\,(0) = 0\,, \quad \text{and} \\ <2\,|\,a\,|\,2> \; &= \sqrt{2}\;\delta_{2,\,1} = \sqrt{2}\,(0) = 0\,. \end{aligned}$$

In fact, all elements on the main diagonal are zero. The Kronecker delta indicates that the column must be one greater than the row to be non–zero, so

$$\begin{aligned} <0\,|\,a\,|\,1> \; &= \sqrt{1}\;\delta_{0,\,0} = \sqrt{1}\,(1) = \sqrt{1}\,, \\ <1\,|\,a\,|\,2> \; &= \sqrt{2}\;\delta_{1,\,1} = \sqrt{2}\,(1) = \sqrt{2}\,, \\ <2\,|\,a\,|\,3> \; &= \sqrt{3}\;\delta_{2,\,2} = \sqrt{3}\,(1) = \sqrt{3}\,, \end{aligned}$$

and the pattern continues to yield

$$a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

(b) $$a\,|\,3> = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \sqrt{3} \\ 0 \\ 0 \\ \vdots \end{pmatrix} = \sqrt{3} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} = \sqrt{3}\,|\,2>\,,$$

(c) which is the same as $a\,|\,3> = \sqrt{3}\,|\,3-1> = \sqrt{3}\,|\,2>$. (Of course, these must be the same. The relation used for part (c) is also the relation upon which the matrix representation is built).

Postscript: The upper left element of matrix operators used to describe the SHO is row zero, column zero. This is because the zero is an allowed quantum number for the SHO and $|\,0>$ is the ground state. The upper left element in most other matrices is row one, column one.

The matrix representation of the raising operator is similarly developed and is

$$a^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

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14. Find the matrix representation of $\mathcal{X}$ for the SHO.

The operators $\mathcal{X}$, $\mathcal{P}$, and $\mathcal{H}$, correspond to position, momentum, and energy, which are dynamical variables in classical mechanics, but operators in quantum mechanics. Remember

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}\,,$$
$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}\,.$$

are the definition of the "ladder" operators in terms of the position and momentum operators. Since we have matrix representations of a and $a^\dagger$, the matrix representation of $\mathcal{X}$, $\mathcal{P}$, and $\mathcal{H}$, are a matter of chapter 1 matrix addition and multiplicative constants.

Adding the equations for a and $a^\dagger$,

$$a + a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} + i\left(\cancel{\frac{1}{2m\omega\hbar}}\right)^{1/2}\mathcal{P} + \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} - i\left(\cancel{\frac{1}{2m\omega\hbar}}\right)^{1/2}\mathcal{P} = 2\left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X}$$

$$\Rightarrow \quad \mathcal{X} = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(a + a^\dagger\right)$$

$$= \left(\frac{\hbar}{2m\omega}\right)^{1/2} \left[\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \right]$$

$$= \left(\frac{\hbar}{2m\omega}\right)^{1/2} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Postscript: Subtract a from $a^\dagger$ to find the matrix representation of $\mathcal{P}$, which is

$$\mathcal{P} = i\left(\frac{m\omega\hbar}{2}\right)^{1/2} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

---

15. Use the position space representations of the position and momentum operators in the lowering operator to derive the ground state eigenfunction of the SHO in position space.

The position space representation of the lowering operator is

$$\begin{aligned} a &= \left(\frac{m\omega}{2\hbar}\right)^{1/2} \mathcal{X} + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} \mathcal{P} \\ &= \left(\frac{m\omega}{2\hbar}\right)^{1/2} x + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} \left(-i\hbar\frac{d}{dx}\right) \\ &= \left(\frac{m\omega}{2\hbar}\right)^{1/2} x + \left(\frac{\hbar}{2m\omega}\right)^{1/2} \frac{d}{dx}. \end{aligned}$$

The idea is to use this to attain a position space representation. The ground state will follow.

Just to simplify the notation, we are going to change variables. Let

$$y = \left(\frac{m\omega}{\hbar}\right)^{1/2} x \quad \Rightarrow \quad dy = \left(\frac{m\omega}{\hbar}\right)^{1/2} dx$$

$$\Rightarrow \quad x = \left(\frac{\hbar}{m\omega}\right)^{1/2} y \qquad \text{and} \qquad dx = \left(\frac{\hbar}{m\omega}\right)^{1/2} dy$$

$$\Rightarrow \quad a = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\frac{\hbar}{m\omega}\right)^{1/2} y + \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(\frac{m\omega}{\hbar}\right)^{1/2}\frac{d}{dy} \quad \Rightarrow \quad a = \frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right).$$

The eigenkets $|\,n>$ in abstract Hilbert space and $\psi_n\,(y)$ in position space are equivalent expressions, and we used the fact that $a\,|\,0> = 0$ to attain eigenenergies earlier, so

$$|\,n> = \psi_n\,(y) \quad \Rightarrow \quad a\,|\,n> = a\,\psi_n\,(y) \quad \Rightarrow \quad a\,|\,0> = a\,\psi_0\,(y) \quad \Rightarrow \quad a\,\psi_0\,(y) = 0\,, \quad \text{therefore}$$

$$\frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right)\psi_0\,(y) = 0$$

$$\Rightarrow \quad \frac{d\,\psi_0\,(y)}{\psi_0\,(y)} = -y\,dy$$

$$\Rightarrow \quad \ln\psi_0\,(y) = -\frac{1}{2}\,y^2 + C$$

$$\Rightarrow \quad \psi_0\,(y) = A_0\,e^{-y^2/\,2}$$

where the variable of integration is absorbed into the constant A_0. Returning to the variable x,

$$\psi_0\,(x) = A_0\,e^{-m\omega x^2/\,2\hbar}$$

is the unnormalized ground state eigenfunction of the SHO in position space.

Postscript: Notice that the ground state eigenfunction of the SHO in position space is a Gaussian function. The normalized ground state eigenfunction is

$$\psi_0\,(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/\,2\hbar}.$$

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16. (a) Find a generating function for the eigenstates of the SHO in position space in general.

(b) Find the eigenfunction for the first excited state of the SHO in position space.

Employ the result of problem 11, $|\,n> = \dfrac{1}{\sqrt{n!}}\left(a^\dagger\right)^n|\,0>$, using the position space representation of the raising operator, $a^\dagger = \left(\dfrac{m\omega}{2\hbar}\right)^{1/2} x - \left(\dfrac{\hbar}{2m\omega}\right)^{1/2}\dfrac{d}{dx}$. This is cleaner using y as defined in problem 15. Use the result and eliminate y to express ψ_1 in terms of x for part (b).

(a) Using y as defined in problem 15, $a^\dagger = \dfrac{1}{\sqrt{2}}\left(y - \dfrac{d}{dy}\right)$, so the result of problem 11 is

$$\psi_n\,(y) = \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)\right)^n \psi_0\,(y) \quad \Rightarrow \quad \psi_n\,(y) = \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)\right)^n\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-y^2/2}.$$

(b) The first excited state of the SHO means $n = 1$, so

$$\psi_1\,(y) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{1!}}\left(\frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)\right)^1 e^{-y^2/\,2} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2}}\left(y\,e^{-y^2/\,2} - \frac{d}{dy}\,e^{-y^2/\,2}\right)$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2}}\left(y\,e^{-y^2/\,2} - (-y)\,e^{-y^2/\,2}\right) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2}}\,2y\,e^{-y^2/\,2}$$

$$\Rightarrow \quad \psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{2}\, \left(\frac{m\omega}{\hbar}\right)^{1/2} x\, e^{-m\omega x^2/2\hbar} = \left(\frac{4}{\pi}\left(\frac{m\omega}{\hbar}\right)^3\right)^{1/4} x\, e^{-m\omega x^2/2\hbar}.$$

---

17. Find the eigenfunction for the ground state and first excited state of the SHO in position space using Hermite polynomials.

Eigenstates of the SHO can be expressed using Hermite polynomials. The n^{th} eigenstate is

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}\, H_n(\xi)\, e^{-\xi^2/2} \qquad \text{where} \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}\, x \tag{1}$$

and the H_n are Hermite polynomials. The first few Hermite polynomials are

$$\begin{aligned}
H_0(\xi) &= 1 \\
H_1(\xi) &= 2\xi \\
H_2(\xi) &= 4\xi^2 - 2 \\
H_3(\xi) &= 8\xi^3 - 12\xi \\
H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12 \\
H_5(\xi) &= 32\xi^5 - 160\xi^3 + 120\xi \\
H_6(\xi) &= 64\xi^6 - 480\xi^4 + 720\xi^2 - 120 \\
H_7(\xi) &= 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi \\
H_8(\xi) &= 256\xi^8 - 3584\xi^6 + 13440\xi^4 - 13440\xi^2 + 1680 \\
H_9(\xi) &= 512\xi^9 - 9216\xi^7 + 48384\xi^5 - 80640\xi^3 + 30240\xi
\end{aligned}$$

Table 6 − 1. The First Ten Hermite Polynomials.

Hermite polynomials can be generated using the recurrence relation

$$H_{n+1}(\xi) = 2x\, H_n(\xi) - 2n\, H_{n-1}(\xi).$$

The Schrodinger equation in position space for the SHO is a naturally occurring form of Hermite's equation. The solutions to Hermite's equation are the Hermite polynomials. We will solve this differential equation thereby deriving the Hermite polynomials using a power series solution in part 2 of this chapter. Using equation (1) with the appropriate Hermite polynomial is likely the easiest way to attain a position space eigenfunction for the quantum mechanical SHO.

$$\begin{aligned}
\psi_0(x) &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^0\, 0!}}\, H_0\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-m\omega x^2/2\hbar} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} (1)\, e^{-m\omega x^2/2\hbar} \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}, \quad \text{in agreement with our earlier calculation.}
\end{aligned}$$

$$\psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^1\, 1!}}\, H_1\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-m\omega x^2/2\hbar} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}}\, 2\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-m\omega x^2/2\hbar}$$

$$= \left(\frac{4}{\pi} \left(\frac{m\omega}{\hbar} \right)^3 \right)^{1/4} x\, e^{-m\omega x^2/2\hbar}, \quad \text{also in agreement with our earlier calculation.}$$

Postscript: Charles Hermite's most important work completed in 1873 was to prove that Euler's number e could not be a solution to any polynomial equation. Thus, e was not considered an "algebraic number" but was considered to have "transcended" the algebraic. Euler's number was the first proven to be a transcendental number. Of course, the adjective form of Hermite's name is Hermitian, as in Hermitian operator...and the polynomials used to describe the eigenfunctions of the SHO also bear his name. Hermite was Professor of Higher Algebra at the University of Paris .

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18. Show that $H_1(\xi)$ is orthogonal to $H_2(\xi)$.

The Hermite polynomials are orthogonal when both are weighted by $e^{-\xi^2/2}$. Multiplication by this weighting function is equivalent to an adjustment in the length of the eigenket.

Including the weighting functions, the orthogonality condition is

$$\int_{-\infty}^{\infty} H_1(\xi)\, e^{-\xi^2/2}\, H_2(\xi)\, e^{-\xi^2/2}\, d\xi = \int_{-\infty}^{\infty} 2\xi \left(4\xi^2 - 2\right) e^{-\xi^2}\, d\xi$$

$$= \int_{-\infty}^{\infty} \left(8\xi^3 - 4\xi\right) e^{-\xi^2}\, d\xi = 8 \int_{-\infty}^{\infty} \xi^3\, e^{-\xi^2}\, d\xi - 4 \int_{-\infty}^{\infty} \xi\, e^{-\xi^2}\, d\xi\,.$$

The integrands are both odd functions integrated between symmetric limits. The integrands are therefore, both zero, so their difference is zero. Since

$$\int_{-\infty}^{\infty} H_1(\xi)\, e^{-\xi^2/2}\, H_2(\xi)\, e^{-\xi^2/2}\, d\xi = 0, \quad H_1(\xi) \text{ is orthogonal to } H_2(\xi)\,.$$

Postscript: This is a calculation for two specific Hermite polynomials. To show the Hermite polynomials are orthogonal in general, we need to show

$$|A|^2 \int_{-\infty}^{\infty} H_n(\xi)\, e^{-\xi^2/2}\, H_m(\xi)\, e^{-\xi^2/2}\, d\xi = \delta_{n,m}.$$

This calculation is done in Byron and Fuller[1], and other texts. The weighting function is necessary to demonstrate orthogonality which is a fact that is not always stated explicitly.

A set of eigenstates also needs to be complete, to span the entire space, to be useful. The infinite set of Hermite polynomials is complete. Any eigenfunction in the space can be constructed

[1] Byron and Fuller *Mathematics of Classical and Quantum Physics* (Dover Publications, New York, 1970), pp 261-273.