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 $V(x) = \dfrac{1}{2}\,kx^2$. 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 $V(x_0) = 0$, $\dfrac{dV}{dx}\Big|_{x_0} = 0$ 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

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

Define $x_0 = 0 \;\Rightarrow\; V(x) = \dfrac{1}{2}kx^2$. Since $k = m\omega^2$, this means $V(x) = \dfrac{1}{2}\,m\omega^2 x^2$. 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 $\big(\mathcal{X} + i\mathcal{P}\big)\big(\mathcal{X} - i\mathcal{P}\big)$, so that

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

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

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

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

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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.

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

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

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

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

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 $|\,E_n > \, = \, |\,E_n >$

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

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 $|\,E_n > \, = \, |\,E_n >$

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

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, $\mathcal{H}\left(a^\dagger\,|\,E_n>\right) = \big(E_n + \hbar\omega\big)\left(a^\dagger\,|\,E_n>\right)$ 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 $\mathcal{H}$,

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

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) $C(n)\,|\,n\!> \,=\, a^\dagger\,|\,n\!-\!1\!> \;\Rightarrow\; <\!n\,|\,C^*(n) = <\!n\!-\!1\,|\,\left(a^\dagger\right)^\dagger = <\!n\!-\!1\,|\,a$ 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 $a^\dagger a - a\,a^\dagger = \left[\,a^\dagger\,,\,a\,\right]$,

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

$$\left|C(n)\right|^2 = <n-1\,|\,n-\frac{1}{2}\,|\,n-1> + \frac{1}{2} = <n-1\,|\,n\,|\,n-1> \;-\; <n-1\,\Big|\,\frac{1}{2}\,\Big|\,n-1> + \frac{1}{2}$$
$$= n<n-1\,|\,n-1> \;-\; \frac{1}{2}<n-1\,|\,n-1> + \frac{1}{2} = n - \frac{1}{2} + \frac{1}{2} = n\,,$$
$$\Rightarrow \quad C(n) = \sqrt{n} \quad \Rightarrow \quad \sqrt{n}\,|\,n> = a^\dagger\,|\,n-1>\;.$$

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.

---

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

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

---

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.*,

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

---

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

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

---

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 $a^\dagger$,

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

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

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

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

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

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

---

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, $|\,n> = \frac{1}{\sqrt{n!}} \left(a^\dagger\right)^n |\,0>$, using the position space representation of the raising operator, $a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2} x - \left(\frac{\hbar}{2m\omega}\right)^{1/2} \frac{d}{dx}$. 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, $a^\dagger = \frac{1}{\sqrt{2}} \left(y - \frac{d}{dy}\right)$, 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

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

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.

from a linear combination of Hermite polynomials. The Hermite polynomials, therefore, form an orthogonal basis, and further, form an orthonormal basis when they are normalized.

The infinite set of unit vectors is orthonormal and is complete. The infinite set of sines and cosines used for the infinite square well is orthogonal so can be made orthonormal and is complete. The infinite set of Hermite polynomials used for the SHO is orthogonal so can be made orthonormal and is complete. The infinite sets of Associated Laguerre polynomials, Legendre functions, spherical harmonic functions, and numerous other sets of polynomials and functions are orthogonal so can be made orthonormal and complete. Each of these infinite sets form a basis in the same sense as the unit vectors of chapter 1 form a basis. These infinite sets of polynomials and functions generally require a weighting function to demonstrate orthogonality which, again, is a fact that is not always stated explicitly.

---

19. Given a simple harmonic oscillator potential, graph the first six eigenenergies on an energy versus position plot and superimpose the the first six eigenfunctions on corresponding eigenenergies on the same plot. Plot the probability densities of the first six eigenfunctions in the same manner.

Examine the two graphs below.

Eigenenergies and Eigenfunctions

Eigenenergies and Probability Density

Postscript: Like the infinite square well, it is conventional to graph energy versus position for the eigenenergies and the eigenfunctions are conventionally located at the level of the corresponding eigenenergies where each horizontal line represents zero amplitude for that eigenfunction.

Unlike the infinite square well, the eigenfunctions do not have an amplitude of zero at the boundaries. The eigenfunctions approach zero asymptotically outside the potential well. Further, eigenenergies for the SHO are evenly spaced, the ground state is at $\hbar\omega/2$, and each successive eigenenergy is $\hbar\omega$ higher than the last. Also in contrast, the eigenenergies of the infinite square well scale as n^2, that is $E_1 = E_g$, $E_2 = 4\,E_g$, $E_3 = 9\,E_g$, $E_4 = 16\,E_g$, etc.

Like the infinite square well, the probability densities are non-negative everywhere, there are points inside the well where the probability density is zero, and there are regions of maximal and minimal probability. Unlike the infinite square well and an additional non–classical feature of the SHO is that there are regions of non-zero probability density outside the potential well—there is a finite probability of finding the particle outside of the potential well. That there is a non-zero probability density outside the wall is a feature of all but infinite, vertical potential walls.

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20. Sketch the linear combination $\Psi(x) = 2\,\psi_0(x) + \psi_1(x)$ for the SHO.

A general wavefunction of the SHO is a superposition or linear combination of its eigenfunctions,

$$\Psi(x) = c_0\,\psi_0(x) + c_1\,\psi_1(x) + c_2\,\psi_2(x) + c_3\,\psi_3(x) + \cdots = \sum_{n=0}^{\infty} c_n\,\psi_n(x)\,, \quad \text{in general, or}$$

$$|\,\Psi> = c_0\,|\,0> + \,c_1\,|\,1> + \,c_2\,|\,2> + \,c_3\,|\,3> + \cdots = \sum_{n=0}^{\infty} c_n\,|\,n> \quad \text{for the SHO.}$$

The linear combination given is combined graphically below.

A General State Vector that is the Superposition of two Eigenstates.

Postscript: The c_n are constants that provide the relative contributions of each eigenfunction. The c_n can be any scalars so $\Psi(x)$ can have any shape. As before, if the general wavefunction is normalized, $\Psi(x) = 1$, the relative magnitudes of the c_n are fixed. Also as before, the orthogonality of the eigenfunctions of the SHO ensures that the c_n are unique.

Problems 21 through 26 use the linear combination of two eigenstates,

$$|\,\Psi> = A\left[\;2\,|\,0> + \,5\,|\,2>\;\right],$$

which is the general linear combination of eigenstates for $c_0 = 2\,,\; c_2 = 5\,,$ and all other $c_n = 0\,.$

---

21. (a) Normalize the wavefunction $|\,\Psi>$ using row and column vectors, and

(b) using Dirac notation.

(a) $$< \Psi \,|\, \Psi > = 1 \;\Rightarrow\; (2,\ 0,\ 5,\ 0,\ 0, \cdots)^* A^* A \begin{pmatrix} 2 \\ 0 \\ 5 \\ 0 \\ 0 \\ \vdots \end{pmatrix} = 1$$

$$\Rightarrow\quad (4+25)\,|\,A\,|^2 = 1 \;\Rightarrow\; A = \frac{1}{\sqrt{29}} \;\Rightarrow\; |\,\Psi > = \frac{1}{\sqrt{29}}\Big[\,2\,|\,0> +\, 5\,|\,2>\,\Big].$$

(b) $$< \Psi \,|\, \Psi > = 1 \;\Rightarrow\; \Big[<0\,|\,2^* + <2\,|\,5^* \Big] A^* A \Big[2\,|\,0> + 5\,|\,2> \Big] = 1$$

$$\Rightarrow\quad |\,A\,|^2 \Big[4<0\,|\,0> + 10<0\,|\,2> + 10<2\,|\,0> + 25<2\,|\,2> \Big] = 1\,.$$

Orthonormality, $<i\,|\,j> = \delta_{ij} \;\Rightarrow\; <0\,|\,0> = <2\,|\,2> = 1\,,$ and $<0\,|\,2> = <2\,|\,0> = 0\,,$ so

$$|\,A\,|^2 \Big[4 + 25 \Big] = 1 \;\Rightarrow\; A = \frac{1}{\sqrt{29}} \;\Rightarrow\; |\,\Psi > = \frac{1}{\sqrt{29}}\Big[\,2\,|\,0> +\, 5\,|\,2>\,\Big].$$

Postscript: The row and column vector representation is likely easier to visualize, but normalizing $A\big[\,5\,|\,0> + \,6\,|\,100>\,\big]$ or any large system using the row and column method would be awkward. Both of these approaches are significantly easier than the same calculation in position space that requires evaluation of at least two integrals.

A portion of the utility of abstract Hilbert space is that calculations are dramatically simpler than in any specific representation, such as position space. Abstract Hilbert space also allows maximum generality in that you can represent your work in any appropriate basis at any time. Working in Hilbert space until a representation is necessary is the norm. There is no reason to represent the results of the last examples in any specific basis so they remain in Hilbert space.

---

22. Find the normalized wavefunction $|\,\Psi>$ in position space.

Use the ground state and procedures similar to those seen in problem 17.

$$\psi_2\,(x) = \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4} \left(2\,\frac{m\omega}{\hbar}\,x^2 - 1\right) e^{-m\omega x^2/2\hbar}$$

using table 8–1. Combining with the ground state from problem 17,

$$\Psi\,(x) = \frac{1}{\sqrt{29}}\left[2\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} + 5\left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left(2\,\frac{m\omega}{\hbar}\,x^2 - 1\right) e^{-m\omega x^2/2\hbar}\right]$$
$$= \frac{1}{\sqrt{29}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[2 + \frac{5\sqrt{2}}{2}\left(2\,\frac{m\omega}{\hbar}\,x^2 - 1\right)\right] e^{-m\omega x^2/2\hbar}.$$

---

22. Calculate the probability of measuring $E = \frac{5}{2}\hbar\omega$ for the $|\,\Psi>$ given.

Postulates 3 and 4. The only possible results of a measurement of energy are the eigenvalues $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$. The state vector contains only the two eigenstates $|\,n=0>$ and $|\,n=2>$, so $E_0 = \frac{1}{2}\hbar\omega$ and $E_2 = \frac{5}{2}\hbar\omega$ are the only possible results. Then $P\,(E = E_n) = |\,<n\,|\,\Psi>\,|^2$.

$$P\,(E = E_2) = \left|\, (0,\ 0,\ 1,\ 0, \cdots)\ \frac{1}{\sqrt{29}} \begin{pmatrix} 2 \\ 0 \\ 5 \\ 0 \\ \vdots \end{pmatrix} \right|^2$$

$$= \left|\, \frac{1}{\sqrt{29}}\,(0+0+5+0+\cdots) \right|^2 = \left|\, \frac{5}{\sqrt{29}} \right|^2 = \frac{25}{29}\,,$$

using unit vector notation. The same calculation in Dirac notation looks like

$$P\,(E = E_2) = \left|\, <2\,|\,\Psi>\, \right|^2 = \left|\, <2\,|\,\frac{1}{\sqrt{29}}\Big(2\,|\,0> + \,5\,|\,2>\Big) \right|^2$$

$$= \frac{1}{29}\left|\, 2<2\,|\,0> + \,5<2\,|\,2>\, \right|^2 = \frac{1}{29}\left|\,5\,\right|^2 = \frac{25}{29}\,,$$

where the inner products are $<i\,|\,j> = \delta_{ij}$, meaning $<2\,|\,0> = 0$ and $<2\,|\,2> = 1$.

---

23. Calculate the expectation value of energy for the $|\,\Psi>$ given.

This problem demonstrates the calculation using the chapter 1 mathematics and is also intended to highlight the relative ease of calculations using matrix and Dirac notation. Setup the calculation in position space just to demonstrate the relative degree of difficulty.

$$<E> = <\mathcal{H}>_\psi = <\psi\,|\,\mathcal{H}\,|\,\psi> \ = \frac{1}{\sqrt{29}}\Big(2,\ 0,\ 5,\ \cdots\Big)^* \begin{pmatrix} \frac{1}{2} & 0 & 0 & \cdots \\ 0 & \frac{3}{2} & 0 & \cdots \\ 0 & 0 & \frac{5}{2} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \hbar\omega\ \frac{1}{\sqrt{29}} \begin{pmatrix} 2 \\ 0 \\ 5 \\ \vdots \end{pmatrix}$$

$$= \frac{\hbar\omega}{29}\Big(2,\ 0,\ 5,\ \cdots\Big) \begin{pmatrix} \frac{1}{2}(2) \\ \\ \frac{3}{2}(0) \\ \\ \frac{5}{2}(5) \\ \\ \vdots \end{pmatrix} = \frac{\hbar\omega}{29}\left(2 + \frac{125}{2}\right) = \frac{129}{58}\,\hbar\omega\,.$$

Notice that we attain the same result if the calculation is done in a three dimensional subspace. The same calculation in Dirac notation using the direct action of the Hamiltonian is

$$\begin{aligned} <E> &= <\psi\,|\,\mathcal{H}\,|\,\psi> \\ &= \left[\frac{1}{\sqrt{29}}\left(<0\,|\,2^* + <2\,|\,5^*\right)\right] \mathcal{H} \left[\frac{1}{\sqrt{29}}\left(2\,|\,0> + 5\,|\,2>\right)\right] & (1) \\ &= \frac{1}{29}\Big[<0\,|\,2 + <2\,|\,5\Big] \left[2\left(\frac{1}{2}\hbar\omega\right)|\,0> + 5\left(\frac{5}{2}\hbar\omega\right)|\,2>\right] & (2) \\ &= \frac{1}{29}\left[2\cdot 2\cdot\left(\frac{1}{2}\hbar\omega\right)<0\,|\,0> + 5\cdot 5\cdot\left(\frac{5}{2}\hbar\omega\right)<2\,|\,2>\right] & (3) \\ &= \frac{\hbar\omega}{29}\left[2 + \frac{125}{2}\right] = \frac{129}{58}\,\hbar\omega, \end{aligned}$$

where the Hamiltonian operating to the right on the two eigenstates in equation (1) results in the eigenvalues times the corresponding eigenstate in equation (2), and the orthonormality of eigenstates results in equation (3) where the inner product of terms that are known to be zero. Excluding known zeros is the norm, and in fact, eigenstates such as $<0\,|\,0> = <2\,|\,2> = 1$ that are known to be one are normally not explicitly written.

Postscript: The calculation of expectation value for the given $|\,\Psi>$ in position space would be

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{29}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[2 + \frac{5\sqrt{2}}{2}\left(2\,\frac{m\omega}{\hbar}\,x^2 - 1\right)\right] e^{-m\omega x^2/2\hbar}\left[\frac{1}{2m}\left(-i\hbar\,\frac{d}{dx}\right)^2 + \frac{1}{2}\,kx^2\right]$$

$$\times\frac{1}{\sqrt{29}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[2 + \frac{5\sqrt{2}}{2}\left(2\,\frac{m\omega}{\hbar}\,x^2 - 1\right)\right] e^{-m\omega x^2/2\hbar}\,dx\,,$$

which is a statement that implies that matrix methods and Dirac notation are worthwhile, in other words, if you want to do this integral, go ahead, we chose to avoid it in favor of modern techniques.

---

24. Calculate the expectation value of energy for the $|\,\Psi>$ given using the ladder operator representation of the Hamiltonian.

This problem is an explicit example of ladder operators calculations. It is not the easiest way to calculate an expectation value. The ladder operators though, are prototypes for the creation and annihilation operators used in field theoretic descriptions of photons, electrons, phonons, etc. In other words, the raising and lowering operators become increasingly important as you progress.

$$\mathcal{H} = \left(a^\dagger a + \frac{1}{2}\right)\hbar\omega,\quad a^\dagger\,|\,n> = \sqrt{n+1}\,|\,n+1>,\quad a\,|\,n> = \sqrt{n}\,|\,n-1>,\quad <E> = <\psi\,|\,\mathcal{H}\,|\,\psi>$$

$$\Rightarrow\ <E>\ = \left[\frac{1}{\sqrt{29}}\left(<0\,|\,2^* + \ <2\,|\,5^*\right)\right]\left[\left(a^{\dagger}a+\frac{1}{2}\right)\hbar\omega\right]\left[\frac{1}{\sqrt{29}}\left(2\,|\,0> + 5\,|\,2>\right)\right]$$

$$= \frac{\hbar\omega}{29}\left[2<0\,|\ +\ 5<2\,|\ \right]\left[2\,a^{\dagger}a\,|\,0> + 5\,a^{\dagger}a\,|\,2> + \frac{2}{2}\ |\,0> + \frac{5}{2}\ |\,2>\right]$$

$$= \frac{\hbar\omega}{29}\left[2<0\,|\ +\ 5<2\,|\ \right]\left[2\cancel{a}^{\dagger}\,\vec{0} + 5\,a^{\dagger}\sqrt{2}\,|\,1> + |\,0> + \frac{5}{2}\,|\,2>\right] \tag{1}$$

$$= \frac{\hbar\omega}{29}\left[2<0\,|\ +\ 5<2\,|\ \right]\left[5\sqrt{2}\cdot\sqrt{2}\,|\,2> + |\,0> + \frac{5}{2}\,|\,2>\right]$$

As before, the raising operator acting on the zero vector is zero so that term is struck in equation (1). The only non-zero contributions are from the $<0\,|\,0>$ and $<2\,|\,2>$ terms since these inner products are 1, the $<0\,|\,2>$ and $<2\,|\,0>$ products are 0, therefore,

$$<E> = \frac{\hbar\omega}{29}\left[2<0\,|\,0> + 5{\cdot}5{\cdot}2<2\,|\,2> + 5{\cdot}\frac{5}{2}<2\,|\,2>\right] = \frac{\hbar\omega}{29}\left[2+5{\cdot}5{\cdot}2+5{\cdot}\frac{5}{2}\right] = \frac{129}{58}\,\hbar\omega\,.$$

---

25. Express the state of the system described by $|\,\Psi>$ at time t,

(a) in Hilbert space in terms of the abstract $|\,n>$'s,

(b) in position space in terms of the $\psi_n(x)$'s,

(c) in momentum space in terms of the $\widehat{\psi}_n(p)$'s, and

(d) in energy space in terms of the $\widetilde{\psi}_n(E)$'s. Do not evaluate the specific $|\,n>$'s, $\psi_n(x)$'s, $\widehat{\psi}_n(p)$'s and $\widetilde{\psi}_n(E)$'s.

Stationary state time dependence is

$$|\,\psi(t)> = \sum_n^{\infty}|\,n><n\,|\,\psi(0)>\ e^{-iE_nt/\hbar} \quad \text{where} \quad |\,\psi(0)> = \frac{1}{\sqrt{29}}\left[2\,|\,0> + 5\,|\,2>\right] \quad \text{here.}$$

(a) $$|\,\psi(t)>\ = \frac{1}{\sqrt{29}}\left[|\,0><0\,|\left(2\,|\,0> + 5\,|\,2>\right)e^{-iE_0t/\hbar} + |\,2><2\,|\left(2\,|\,0> + 5\,|\,2>\right)e^{-iE_2t/\hbar}\right]$$

$$= \frac{1}{\sqrt{29}}\left[|\,0>\left(2<0\,|\,0> + 5<0\cancel{|}2>,\right)e^{-iE_0t/\hbar} + |\,2>\left(2<2\cancel{|}0> + 5<2\,|\,2>\right)e^{-iE_2t/\hbar}\right]$$

$$= \frac{1}{\sqrt{29}}\left[2\,e^{-iE_0t/\hbar}\,|\,0> + 5\,e^{-iE_2t/\hbar}\,|\,2>\right]$$

retaining only the non-zero terms. Using the eigenenergies $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$,

$$|\,\psi(t)> = \frac{1}{\sqrt{29}}\left[2\,|\,0>e^{-i\omega t/2} + 5\,|\,2>e^{-i5\omega t/2}\right].$$

Parts (b) through (d) require only operation on both sides of this equation with the appropriate bra so are essentially exercises in notation.

(b) Remembering that $<x\,|\,\psi(t)> = \psi(x,t)$,

$$<x\,|\,\psi(t)> \;=\; \frac{1}{\sqrt{29}}\left[2<x\,|\,0>e^{-i\omega t/2} + \;5<x\,|\,2>e^{-i5\omega t/2}\right]$$
$$\Rightarrow \quad \psi(x,t) = \frac{1}{\sqrt{29}}\left[2\,\psi_0(x)\,e^{-i\omega t/2} + \;5\,\psi_2(x)\,e^{-i5\omega t/2}\right].$$

(c) To transition to momentum space, $<p\,|\,\psi(t)> = \widehat{\psi}(p,t)$,

$$<p\,|\,\psi(t)> \;=\; \frac{1}{\sqrt{29}}\left[2<p\,|\,0>e^{-i\omega t/2} + \;5<p\,|\,2>e^{-i5\omega t/2}\right]$$
$$\Rightarrow \quad \widehat{\psi}(p,t) = \frac{1}{\sqrt{29}}\left[2\,\widehat{\psi}_0(p)\,e^{-i\omega t/2} + \;5\,\widehat{\psi}_2(p)\,e^{-i5\omega t/2}\right].$$

(d) To find the wavefunction in energy space, remember that $<E\,|\,\psi(t)> = \widetilde{\psi}(E,t)$,

$$<E\,|\,\psi(t)> = \frac{1}{\sqrt{29}}\left[2<E\,|\,0>\;e^{-i\omega t/2} + \;5<E\,|\,2>\;e^{-i5\omega t/2}\right]$$

$$\Rightarrow \quad \widetilde{\psi}(E,t) = \frac{1}{\sqrt{29}}\left[2\,\widetilde{\psi}_0(E,t)\,e^{-i\omega t/2} + \;5\,\widetilde{\psi}_2(E,t)\,e^{-i5\omega t/2}\right].$$

---

26. Calculate the probability of measuring $E = \dfrac{5}{2}\hbar\omega$ at time t for the $|\,\Psi>$ given.

Likely the best choice or representation is the abstract state vector. You will find that the same calculation is much more arduous in position space in one of the problems at the end of this part. Remember that the square of a magnitude is the product of the complex conjugates.

Since the state vector is normalized, probability is $P\,(E = E_n) = |<n\,|\,\psi(t)>|^2$, then

$$P\,(E = E_2) = \left|\;<2\,|\,\frac{1}{\sqrt{29}}\left[2\,|\,0>e^{-i\omega t/2} + \;5\,|\,2>e^{-i5\omega t/2}\right]\;\right|^2$$
$$= \frac{1}{29}\left|\,2\;\cancel{<2\,|\,0>}\,e^{-i\omega t/2} + \,5\;<2\,|\,2>e^{-i5\omega t/2}\,\right|^2,$$

where the first term is struck because the eigenstates of the SHO are orthonormal so the inner product of unlike vectors is zero. Orthonormality also means that $<2\,|\,2> = 1$. Then

$$P\,(E = E_2) = \frac{1}{29}\left|\,5\,e^{-i5\omega t/2}\,\right|^2 = \frac{1}{29}\left(5\,e^{i5\omega t/2}\right)\left(5\,e^{-i5\omega t/2}\right) = \frac{1}{29}\left(25\,e^0\right) = \frac{25}{29},$$

necessarily identical to the time independent case for all startionary state probability calculations.

---

27. Calculate $<\mathcal{P}>$ using the state vector

$$|\,\Phi\,(t)> \;=\; \frac{1}{\sqrt{30}}\left[2\,|\,0>e^{-i\omega t/2} + \,|\,1>e^{-i3\omega t/2} + \;5\,|\,2>e^{-i5\omega t/2}\right].$$

Time never appears in any probability of a stationary state. The exponential stationary state time dependence does affect other calculations, however, such as an expectation value of a dynamic variable. We pick $<\mathcal{P}> \,=\, <\Phi\,(t)\,|\,\mathcal{P}\,|\,\Phi\,(t)>$ to demonstrate both (a) vector/matrix operator and (b) Dirac notation/ladder operator calculation of an expectation value that is time dependent. The principles are the same for $<\mathcal{H}>$, $<\mathcal{X}>$, $<\mathcal{P}^2/2m>$, and $<m\omega^2\mathcal{X}^2/2>$, or other classically dynamical variables. The state vector is changed to the three-dimensional $|\,\Phi>$ because the two-dimensional $|\,\Psi>$ used for the last six problems leads to too many zeros to be a good example.

(a) Using the matrix operator representation of $\mathcal{P}$ for the SHO found earlier,

$$<\mathcal{P}> \,=\, <\Phi(t)\,|\,i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & -\sqrt{5} & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}\frac{1}{\sqrt{30}}\begin{pmatrix} 2e^{-i\omega t/2} \\ e^{-i3\omega t/2} \\ 5e^{-i5\omega t/2} \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$$

$$= \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(2\,e^{+i\omega t/2},\; e^{+i3\omega t/2},\; 5\,e^{+i5\omega t/2},\; 0, \cdots\right)\begin{pmatrix} -e^{-i3\omega t/2} \\ 2\,e^{-i\omega t/2} - 5\sqrt{2}\,e^{-i5\omega t/2} \\ \sqrt{2}\,e^{-i3\omega t/2} \\ 5\sqrt{3}\,e^{-i5\omega t/2} \\ \vdots \end{pmatrix}$$

$$= \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(-2\,e^{-i\omega t} + 2\,e^{+i\omega t} - 5\sqrt{2}\,e^{-i\omega t} + 5\sqrt{2}\,e^{+i\omega t} + 0\right)$$

$$= \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2} 2i\left(2\frac{(e^{+i\omega t} - e^{-i\omega t})}{2i} + 5\sqrt{2}\,\frac{(e^{+i\omega t} - e^{-i\omega t})}{2i}\right)$$

$$= -\frac{1}{15}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(2\sin(\omega t) + 5\sqrt{2}\sin(\omega t)\right) = -\left(\frac{2+5\sqrt{2}}{15}\right)\left(\frac{m\omega\hbar}{2}\right)^{1/2}\sin(\omega t)\,.$$

(b) The momentum operator is $\mathcal{P} = i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(a^\dagger - a)$ in terms of the ladder operators, so

$$\begin{aligned} <\mathcal{P}> &= <\Phi\,(t)\,\big|\,\mathcal{P}\,\big|\Phi\,(t)> \\ &= <\Phi\,(t)\,|\,i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(a^\dagger - a)\big|\frac{1}{\sqrt{30}}\left(2\,|\,0>e^{-i\omega t/2} + \,|\,1>e^{-i3\omega t/2} + 5\,|\,2>e^{-i5\omega t/2}\right) \\ &= <\Phi\,(t)\,|\,i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\frac{1}{\sqrt{30}}\Big(2\,a^\dagger\,|\,0>e^{-i\omega t/2} - 2\,a\,|\,0>e^{-i\omega t/2} + a^\dagger\,|\,1>e^{-i3\omega t/2} \\ &\qquad - a\,|\,1>e^{-i3\omega t/2} + 5\,a^\dagger\,|\,2>e^{-i5\omega t/2} - 5\,a\,|\,2>e^{-i5\omega t/2}\Big) \end{aligned}$$

$$= <\Phi(t)\,|\, i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\frac{1}{\sqrt{30}}\Big(2\sqrt{1}\,|\,1>e^{-i\omega t/2} - 0 + \sqrt{2}\,|\,2>e^{-i3\omega t/2} - \sqrt{1}\,|\,0>e^{-i3\omega t/2}$$
$$+ 5\sqrt{3}\,|\,3>e^{-i5\omega t/2} - 5\sqrt{2}\,|\,1>e^{-i5\omega t/2}\Big)$$
$$= <\Phi(t)\,|\, i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\frac{1}{\sqrt{30}}\Big(-\,|\,0>e^{-i3\omega t/2} + |\,1>\left[2\,e^{-i\omega t/2} - 5\sqrt{2}\,e^{-i5\omega t/2}\right]$$
$$+ \,|\,2>\sqrt{2}\,e^{-i3\omega t/2} + \,|\,3>5\sqrt{3}\,e^{-i5\omega t/2}\Big)$$
$$= \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(2<0\,|\,e^{+i\omega t/2} + <1\,|\,e^{+i3\omega t/2} + 5<2\,|\,e^{+i5\omega t/2}\right)\times$$
$$\left(|\,0>\left[-e^{-i3\omega t/2}\right] + |\,1>\left[2e^{-i\omega t/2} - 5\sqrt{2}\,e^{-i5\omega t/2}\right] + |\,2>\left[\sqrt{2}\,e^{-i3\omega t/2}\right] + |\,3>\left[5\sqrt{3}\,e^{-i5\omega t/2}\right]\right)$$

$$= \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(-2e^{-i\omega t} + 2\,e^{+i\omega t} - 5\sqrt{2}\,e^{-i\omega t} + 5\sqrt{2}\,e^{+i\omega t}\right) \tag{1}$$
$$= \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2} 2i\left(2\,\frac{(e^{+i\omega t} - e^{-i\omega t})}{2i} + 5\sqrt{2}\,\frac{(e^{+i\omega t} - e^{-i\omega t})}{2i}\right)$$
$$= -\left(\frac{2+5\sqrt{2}}{15}\right)\left(\frac{m\omega\hbar}{2}\right)^{1/2}\sin(\omega t)\,.$$

Postscript: This calculation is made shorter by dropping all but the $|\,0>$, $|\,1>$, and $|\,2>$ terms right after letting the ladder operators act. Only these terms will survive when the inner products are calculated. Orthonormality of eigenstates is used to attain equation (1) though other economies are ignored in order to show the new "machinery" explicitly in this example.

Practice Problems

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

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

Practice in using the raising and lowering operators. See problem 2.

---

29. Show that a and $a^\dagger$ are not Hermitian.

More practice in using the raising and lowering operators. Does $a^\dagger = a$?

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30. Show that $\mathcal{H}\, a = a\,\mathcal{H} - a\hbar\omega$.

Parallel problem 4.

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

See problem 10.

---

32. Show that $\mathcal{H}\,|\,3\!> = \frac{7}{2}\hbar\omega\,|\,3\!>$ by explicit matrix multiplication.

Use the unit vector $|\,3\!>$ and matrix representation of $\mathcal{H}$ given in problem 12.

---

33. Express the matrix elements (a) $<\!n\,|\,a\,|\,m\!>$, (b) $<\!n\,|\,a^\dagger|\,m\!>$, (c) $<\!n\,|\,\mathcal{X}\,|\,m\!>$, (d) $<\!n\,|\,\mathcal{P}\,|\,m\!>$, and (e) $<\!n\,|\,\mathcal{H}\,|\,m\!>$, in terms of quantum numbers and Kronecker deltas.

The condition of orthonormality, $<\!i\,|\,j\!> = \delta_{i,\,j}$, can also be expressed $<\!n\,|\,m-1\!> = \delta_{n,\,m-1}$. The action of $a^\dagger$ on a general ket $|\,m\!>$ is given by $a^\dagger|\,m\!> = \sqrt{m+1}\,|\,m+1\!>$. Then consider the inner product with the bra $<\!n\,|$ to obtain

$$<\!n\,|\,a^\dagger|\,m\!> = <\!n\,|\,\sqrt{m+1}\;|\,m+1\!> = \sqrt{m+1}\,<\!n\,|\,m+1\!> = \sqrt{m+1}\;\delta_{n,\,m+1}\,.$$

In other words, $<\!n\,|\,a^\dagger|\,m\!> = \sqrt{m+1}$ for $n = m+1$, and $<\!n\,|\,a^\dagger|\,m\!> = 0$ otherwise. Part (b) is now done for you. Part (a) is done in problem 13. Parts (c) through (e) are similar in concept because all operators can be expressed in terms of the ladder operators. You should find

$$<\!n\,|\,\mathcal{X}\,|\,m\!> = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(\sqrt{m+1}\;\delta_{n,\,m+1} + \sqrt{m}\;\delta_{n,\,m-1}\right) \quad \text{for instance.}$$

---

34. Use the results of the previous problem to calculate the matrix elements (a) $<\!7\,|\,a\,|\,8\!>$, (b) $<\!7\,|\,a^\dagger|\,8\!>$, (c) $<\!7\,|\,\mathcal{X}\,|\,8\!>$, (d) $<\!7\,|\,\mathcal{P}\,|\,8\!>$, and (e) $<\!14\,|\,\mathcal{H}\,|\,14\!>$.

This problem illustrates that it may be convenient to have skills using Kronecker deltas. It is impractical to build matrices large enough to attain the requested elements. See problem 13.

---

35. (a) Develop the matrix representation of the raising operator for the SHO.

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

(c) demonstrate the equivalence $a^\dagger \,|\, n> = \sqrt{n+1}\,|\, n+1>$.

Parallel the procedures in problem 13. Also see problem 33. The matrix operator representation of the raising operator is seen in many places in this chapter.

---

36. Find the matrix representation of $\mathcal{P}$ for the SHO.

See problem 14, and in particular, see the postscript to problem 14, and problem 33.

---

37. Use explicit matrix operations to find the matrix representation of the Hamiltonian operator.

Use the matrix representations of $a^\dagger$ and a in $\mathcal{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$ to attain the same result as problem 12. Remember that a scalar in a matrix equation means multiply that scalar by the identity matrix of the same dimension as the matrices with which this "scalar" is intended to operate. An infinite dimensional identity matrix is appropriate for the scalar "1/2" in this problem.

---

38. Normalize the ground state eigenfunction of the SHO in position space.

Apply the normalization condition to the result of problem 15 to attain the result presented in the postscript of problem 15. Gaussian integrals have been addressed in both chapters 1 and 3.

Problems 39 through 47 concern a simple harmonic oscillator that is initially in the state

$$|\,\psi\,(t=0)\,> = N\left[\,3\,|\,0> + \,2\,|\,1> + \,1\,|\,5>\,\right].$$

---

39. Calculate the normalization constant using (a) row and column vectors, and (b) Dirac notation.

See problem 21.

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40. Energy is measured at $t = 0$. What results are possible and what is the probability of each possibility? Calculate probabilities using (a) row and column vectors, and (b) Dirac notation.

What are postulates 3 and 4. See problem 22.

---

41. (a) Find the expectation value $<E>$ by calculating $<\psi\,|\,\mathcal{H}\,|\,\psi>$ using matrix methods.

(b) Show that $a^\dagger a \,|\, n> \,= n \,|\, n>$.

(c) Use the result of part (b) to calculate $<E>$ using ladder operator methods.

Use the matrix representation of the Hamiltonian derived in problem 12 for part (a). Operate on $a \,|\, n> \,= \sqrt{n} \,|\, n-1>$ with $a^\dagger$ for part (b). Remember that $a^\dagger \,|\, n> \,= \sqrt{n+1} \,|\, n+1>$. The operator $a^\dagger a$ is often called "the number operator," often denoted $\mathcal{N}$, because it's eigenvalues are the index numbers of the SHO eigenvectors. Problem 23 should also be helpful.

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42. (a) Find the standard deviation of energy using matrix methods.

(b) Show that $\mathcal{N}^2 \,|\, n> \,= n^2 \,|\, n>$ where $\mathcal{N}^2 = a^\dagger a \, a^\dagger a$.

(c) Use the result of part (b) to find the standard deviation of energy by ladder operator methods.

Remember that $\Delta E = \sqrt{<\psi \,|\, (\mathcal{H} - <\mathcal{H}>)^2 \,|\, \psi>}$ for part (a). Multiply $<\mathcal{H}>$ from the previous problem by the identity matrix to attain the matrix form of $<\mathcal{H}>$. Subtract this from $\mathcal{H}$ and square the result. You should find

$$(\mathcal{H} - \; <\mathcal{H}>)^2 = \begin{pmatrix} \frac{81}{196} & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & \frac{25}{196} & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & \frac{361}{196} & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \frac{1089}{196} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \frac{2209}{196} & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \frac{3721}{196} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \hbar^2\omega^2 .$$

Next calculate $\Delta E^2 = \,<\psi \,|\, (\mathcal{H} - \; <\mathcal{H}>)^2 \,|\, \psi>$, and the square root to find

$$\Delta E = \sqrt{<\psi \,|\, (\mathcal{H} - \; <\mathcal{H}>)^2 \,|\, \psi>} \;= \sqrt{\frac{325}{196}\hbar^2\omega^2} \;\approx 1.288 \,\hbar\omega .$$

You have previously shown $\mathcal{N} \,|\, n> \,= n \,|\, n>$. Operate on both sides with the lowering operator, then operate on both sides of the result with the raising operator to complete part (b). You need to determine $\mathcal{H}^2$ in terms of $\mathcal{N}$ so that you can calculate $<\psi \,|\, \mathcal{H}^2 \,|\, \psi>$ for part (c). Since

$$\mathcal{H} = \left(a^\dagger a + \frac{1}{2} \right) \hbar\omega = \left(\mathcal{N} + \frac{1}{2} \right) \hbar\omega, \quad \text{you should find that} \quad \mathcal{H}^2 = \left(\mathcal{N}^2 + \mathcal{N} + \frac{1}{4} \right) \hbar^2\omega^2.$$

You should then find that $<\psi \,|\, \mathcal{H}^2 \,|\, \psi> \,= 83\,\hbar^2\omega^2/28$ for the given wavefunction. All the pieces for $\Delta E = \left[\, <\psi \,|\, \mathcal{H}^2 \,|\, \psi> - <\psi \,|\, \mathcal{H} \,|\, \psi>^2 \, \right]^{1/2}$ are present. It must, of course, agree with part (a).

---

43. Verify your earlier results by calculating

$$\text{(a)} \quad <E> \,= \sum_i P(E_i)\, E_i \qquad \text{and} \qquad \text{(b)} \quad \Delta E = \sqrt{\sum_i P(E_i) \left[E_i - <E> \right]^2} .$$

Another way to get $<E>$, also denoted $<\mathcal{H}>$, is to multiply each of the possible eigenvalues by the probability of measuring that eigenvalue and add the products. Calculating standard deviation using probabilities is common. Of course, you must attain the same answers.

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44. Plot your calculated probabilities $P(E_i)$ versus E. Show your expectation value and standard deviation on the plot. Discuss what this plot shows, *i.e.*, explain how the expectation value and the standard deviation are related to the outcome of a series of energy measurements.

The range of probability is 0 to 1 on the vertical axis. Use units of $\hbar\omega$ on the horizontal axis. The requested graph has only three discrete spikes at the energies of the eigenvalues, a discrete value at $<E>$, and a discrete value at ΔE. Expectation value and standard deviation mean the same as they did when presented in chapter 2. It is important that you not lose the foundational elements as they are applied to new systems, like the SHO.

---

45. Calculate the state of the system at time t. Express your answer

(a) in the Hilbert space in terms of the abstract $|n>$'s,

(b) in position space in terms of the $\psi_n(x)$'s,

(c) in momentum space in terms of the $\widehat{\psi}_n(p)$'s, and

(d) in energy space in terms of the $\widetilde{\psi}_n(E)$'s. Do not evaluate the specific $|n>$'s, $\psi_n(x)$'s, $\widehat{\psi}_n(p)$'s or $\widetilde{\psi}_n(E)$'s.

Notation, how things are written and what the symbols mean, can be formidable in any endeavor, particularly when the subject material is new. This problem is designed to help you assimilate the notation of quantum mechanics using an SHO state vector as a vehicle. It is largely an exercise in notation. Per postulate 1, the state of a system is described by a state vector. This problem is asking only for the form of the state vector in different spaces. See problem 25.

---

46. Calculate the following time-dependent expectation values for (a) $<\mathcal{H}>$, (b) $<\mathcal{P}>$, (c) $<\mathcal{X}>$, (d) $<\mathcal{P}^2/2m>$, (e) $<m\omega^2\mathcal{X}^2/2>$.

This problem demonstrates that the phase, the factor $e^{-iE_nt/\hbar}$ in this case, can be consequential even for stationary states. There are multiple options to calculate the five requested expectation values. Matrix arguments are likely the most straightforward. Part (a) is $<\psi(t)|\mathcal{H}|\psi(t)>$ where $\mathcal{H}$ is seen in problem 12. In ket form, the state vector is

$$\psi(t) = \frac{1}{\sqrt{14}} \begin{pmatrix} 3\,e^{-i\omega t/2} \\ 2\,e^{-i3\omega t/2} \\ 0 \\ 0 \\ 0 \\ e^{-i11\omega t/2} \\ \vdots \end{pmatrix}.$$

$<\mathcal{H}>$ is independent of time and the same as previously calculated. You should find that $<\mathcal{P}^2/2m> = <m\omega^2\mathcal{X}^2/2> = 4\hbar\omega/7$. You will also find

$$<\mathcal{P}> = -\frac{6}{7}\left(\frac{m\hbar\omega}{2}\right)^{1/2}\sin(\omega t) \quad \text{and} \quad <\mathcal{X}> = \frac{6}{7}\left(\frac{\hbar}{2m\omega}\right)^{1/2}\cos(\omega t)$$

See problem 27. See problem 14 for matrices to use matrix methods for part (b) through (e).

---

47. (a) Show that this state vector obeys the quantum mechanical virial theorem for the SHO, which states that the expectation value of the kinetic energy is equal to the expectation value of the potential energy, $<T> = <V>$.

(b) Show that your values of $<T>$ and $<V>$ are consistent with previous calculations of $<E>$.

The general virial theorem is deeper than the statement given here, but this is a simple example that the expectation value of the kinetic energy will equal the expectation value of the potential energy in this circumstance. Examine the parts (d) and (e) of the last problem. If you can recognize kinetic and potential energy in those expectation values, you have essentially completed both parts (a) and (b). Part (b) means that the expectation values of kinetic and potential energies must sum to the expectation value of the total energy which you have from problem 41.

---

48. (a) Write the time-independent Schrodinger equation for the SHO in position space.

(b) Write the time-independent Schrodinger equation for the SHO in momentum space.

Again, notation and representation are important. You have done this problem and problems like it in chapter 2. It is also preparation for part 2 of this chapter for which the position space representation of the SHO is central. Remember that in position space,

$$\mathcal{P} \longrightarrow -i\hbar \frac{\partial}{\partial x} \qquad \text{and} \qquad \mathcal{X} \longrightarrow x\,,$$

the time-independent Schrodinger equation is $\mathcal{H}\,|\,\psi> = E\,|\,\psi>$ where $|\,\psi> \rightarrow \psi\,(x)$ in position space, and that the Hamiltonian is the total energy operator $\mathcal{H} = \mathcal{T} + \mathcal{V}$. In momentum space,

$$\mathcal{P} \longrightarrow p \qquad \text{and} \qquad \mathcal{X} \longrightarrow i\hbar \frac{\partial}{\partial p} \qquad \text{and} \qquad |\,\psi> \longrightarrow \widehat{\psi}\,(p).$$

---

49. Calculate the ground state energy for a 1 gram mass on a $k = 0.1\ N/m$ spring. Calculate the approximate quantum number of this oscillator if its energy is $k_B T/2$ where $T = 300\ K$ and k_B is Boltzmann's constant. At what temperature would this oscillator be in its ground state?

This numerical problem should give you some appreciation of the magnitudes involved. Ground state energy, also known as zero point energy, means $n = 0$ for an SHO. You should find that the ground state energy is on the order of $10^{-34}\ J$ for this system, and that ground state temperature is on the order of $10^{-11}\ K$. $T = 300\ K$ is approximately room temperature where the quantum number is just less than 2×10^{12}. Notice that n is inversely proportional to $\hbar\omega$ to calculate the quantum number at large n, *i.e.*, at 300 K. MKS units are likely easiest given that the spring constant is in N/m. $k_B = 1.38 \times 10^{-23}\ J/K$ and $\hbar = 1.06 \times 10^{-34}\ J \cdot s$ in MKS units. The assumption that the energy is $k_B T/2$ is a statement of the equipartition theorem[2]. Finally, remember that $\omega = \sqrt{k/m}$, $E = k_B T/2$, and $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$.

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[2] Atkins *Quanta* (Oxford University Press, Oxford, 1991), pp 111-112.

50. (a) Find $\psi_2(x)$ for the SHO using the Hermite polynomials given in Table 8–1.

(b) Verify this eigenfunction using the generating function of problem 16.

Hermite polynomials are well known so part (a) is likely an easier method to attain an excited state of the SHO in position space than using the generating function. See problem 17.

Nevertheless, the generating function for the second excited state in position space is

$$\psi_2(y) = \frac{1}{\sqrt{2!}}\left(\frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)\right)^2 \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-y^2/2} = \frac{1}{2\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(y - \frac{d}{dy}\right)^2 e^{-y^2/2}.$$

The two terms in the operator $\left(y - \frac{d}{dy}\right)^2$ do not commute. The operator can be applied as

$$\left(y - \frac{d}{dy}\right)\left(y - \frac{d}{dy}\right) \quad \text{or} \quad y^2 - y\frac{d}{dy} - \frac{d}{dy}y + \frac{d}{dy}\frac{d}{dy}, \quad \text{but not as} \quad y^2 - 2y\frac{d}{dy} - \frac{d^2}{dy^2}.$$

Remember that $y = \sqrt{\frac{m\omega}{\hbar}}\,x$ to attain the final form. Parts (a) and (b) must agree, of course.

---

51. Show that $H_1(\xi)$ is orthogonal to $H_3(\xi)$ when both are weighted with the factor $e^{-\xi^2/2}$.

To be useful for quantum mechanics, a basis must be orthonormal. If the basis is orthogonal, it can be made orthonormal. The intent of this problem is to demonstrate orthogonality for a selected pair of Hermite polynomials. When weighted by $e^{-\xi^2/2}$, the recurrence relation immediately below table 8–1 leads to a differential equation that is self-adjoint and the solutions to a self-adjoint differential equation are orthogonal[3]. Byron and Fuller show by methods of integration that Hermite polynomials are orthogonal in general when weighted by $e^{-\xi^2/2}$ per footnote 1.

Per problem 18, weighting each Hermite polynomial by $e^{-\xi^2/2}$ means to multiply both $H_1(\xi)$ and $H_3(\xi)$ by $e^{-\xi^2/2}$ in the orthogonality condition which may be written

$$\int_{-\infty}^{\infty} H_1(\xi)\, e^{-\xi^2/2}\, H_3(\xi)\, e^{-\xi^2/2}\, d\xi\,.$$

This results in a difference of two integrals that are both even. An even integral is equal to twice the same integrand from the limits zero to infinity. Both integrals can be evaluated using

$$\int_0^{\infty} x^{2n}\, e^{-p\xi^2}\, dx = \frac{(2n-1)!!}{2\,(2p)^n}\sqrt{\frac{\pi}{p}}\,, \quad p > 0\,, \quad n = 0\,,1\,,2\,,\ldots$$

---

52. Express the position space state function

$$\Psi(x,t) = \frac{1}{\sqrt{14}}\left[3\,\psi_0(x)\, e^{-i\omega t/2} + 2\,\psi_1(x)\, e^{-i3\omega t/2} + \psi_5(x)\, e^{-i11\omega t/2}\right]$$

[3] Arfken *Mathematical Methods for Physicists* (Academic Press, New York, 1970, 2nd ed.), pp 424-432 and 611.

in functional form in terms of the independent variable x.

The given $\Psi(x,t)$ is the answer to problem 45 (b). Express the three $\psi_n(x)$'s in terms of x. You have $\psi_0(x)$ and $\psi_1(x)$ from previous problems. You need only to find $\psi_5(x)$, which is likely easiest using table 8–1, and then substitute the three eigenfunctions into the given wavefunction. Though the calculation is not very difficult, you may be surprised at the length. You should find

$$\Psi(x,t) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}\left\{\frac{3}{\sqrt{14}}\,e^{-i\omega t/2} + \frac{4}{\sqrt{14}}\left(\frac{m\omega}{2\hbar}\right)^{1/2} x\,e^{-i3\omega t/2}\right.$$
$$\left. + \frac{1}{\sqrt{210}}\left[2\left(\frac{m\omega}{\hbar}\right)^{5/2} x^5 - 10\left(\frac{m\omega}{\hbar}\right)^{3/2} x^3 + \frac{15}{2}\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right] e^{-i11\omega t/2}\right\}.$$

---

53. Express the state function of the last problem in functional form in terms of the variable p.

The intent of this problem is to practice a change of basis from position space to momentum space. It should also demonstrate an application of the raising operator. The most obvious idea is to employ a quantum mechanical Fourier transform to change the solution of problem 52 to momentum space. The Fourier transform of $\Psi(x)$ is given by the integral

$$\widehat{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x)\,e^{-ipx/\hbar}\,dx\,.$$

Obtaining $\widehat{\psi}_0(p)$ from $\psi_0(x)$ this way is straight forward. You can also do the Fourier transform of $\psi_1(x)$, but this is actually a fairly difficult integration. If you want to Fourier transform $\psi_5(x)$, you likely want (or need) to use a software package like Maple or Mathematica, and validating the results of the software calculation may then be a problem.

A paper and pencil method is to use the raising operator in momentum space which is

$$a^{\dagger} = i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\frac{\partial}{\partial p} - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} p = i\left[\left(\frac{\alpha}{2}\right)^{1/2}\frac{\partial}{\partial p} - \left(\frac{1}{2\alpha}\right)^{1/2} p\right]$$

where $\alpha = m\omega\hbar$ is used to reduce clutter. Calculate $\widehat{\psi}_1(p)$ using this raising operator on $\widehat{\psi}_0(p)$,

$$\widehat{\psi}_1(p) = a^{\dagger}\,\widehat{\psi}_0(p) = i\left[\left(\frac{\alpha}{2}\right)^{1/2}\frac{\partial}{\partial p} - \left(\frac{1}{2\alpha}\right)^{1/2} p\right]\widehat{\psi}_0(p)$$

and then attain $\widehat{\psi}_2(p)$ from $\widehat{\psi}_1(p)$, $\widehat{\psi}_3(p)$ from $\widehat{\psi}_2(p)$, and so on until you arrive at $\widehat{\psi}_5(p)$. You should find

$$\widehat{\psi}_2(p) = \frac{\sqrt{2}}{(\pi)^{1/4}(m\omega\hbar)^{3/4}}\left[\left(\frac{m\omega\hbar}{2}\right)^{1/2} - \left(\frac{2}{m\omega\hbar}\right)^{1/2} p^2\right] e^{-p^2/2m\omega\hbar}, \quad \text{for instance, and eventually}$$

$$\widehat{\psi}_5(p) = \frac{-i\sqrt{2}}{(\pi)^{1/4}(m\omega\hbar)^{3/4}}\left[\frac{4p^5}{(m\omega\hbar)^2} - \frac{20p^3}{m\omega\hbar} + 15p\right] e^{-p^2/2m\omega\hbar}, \quad \text{so that}$$

$$\widehat{\Psi}(p,t) = \frac{e^{-p^2/2m\omega\hbar}}{\sqrt{14}\,(\pi m\omega\hbar)^{1/4}}\left\{3\,e^{-i\omega t/2} - \frac{i\,2\sqrt{2}\,p}{(m\omega\hbar)^{1/2}}\,e^{-i3\omega t/2}\right.$$
$$\left. - \frac{i\sqrt{2}}{(m\omega\hbar)^{1/2}}\left[\frac{4\,p^5}{(m\omega\hbar)^2} - \frac{20\,p^3}{m\omega\hbar} + 15\,p\right] e^{-i11\omega t/2}\right\}.$$

The Simple Harmonic Oscillator, Part 2

Meet! What meet? Might as well be a track meet as far as I'm concerned...maybe my man will come through...at least the pigeons seem to be enjoying this popcorn...I should be in Atlantic City where the slots are friendly and...Charles! "Gave the case to another gal. Black, average height, slender like the mark, dressed in a brown business suit, no purse, no hat. Drove off in a gold Mercedes. Had a New York vanity plate." "A gold Mercedes with a vanity plate, wow, not exactly low profile. What did the plate say Charles?" "HERMEET."

---

1. Show that Schrodinger's equation in position space can be written

$$\frac{d^2\,\psi(x)}{dx^2} + \left(\lambda - \alpha^2 x^2\right)\psi(x) = 0 \quad \text{for an SHO in one dimension.}$$

Part 2 should amplify and reinforce the results of part 1, however, it emphasizes the procedures for solving an ordinary differential equation (ODE) using power series. The SHO potential is only the first ODE that we will solve with a power series solution. Further, power series solutions to ODE's are useful in numerous areas of physics.

The Schrodinger equation for the SHO potential in one dimension in position space is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2\right)\psi(x) = E\,\psi(x) \quad \Rightarrow \quad \frac{d^2\,\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\psi(x) = 0\,.$$

$$\text{Let}\ \ \lambda = \frac{2mE}{\hbar^2} \ \ \text{and}\ \ \alpha^2 = \frac{mk}{\hbar^2} \quad \Rightarrow \quad \frac{d^2\,\psi(x)}{dx^2} + \left(\lambda - \alpha^2 x^2\right)\psi(x) = 0\,.$$

---

2. Discuss the procedures for solving an ODE using a power series solution.

Power series solutions to ODE's are longer problems. Breaking longer problems into smaller segments will often make the overall solution more accessible, so here is a six step procedure.

Power Series Solution Road Map

1. Find the solution as x approaches infinity, *i.e.*, the asymptotic solution.
2. Assume that the product of the asymptotic solution and an arbitrary function, $f(x)$, is a solution. Use this solution in the homogeneous ODE and simplify.
3. Assume the arbitrary function can be expressed as an infinite power series, *i.e.*,

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots = \sum_{i=0}^{\infty} a_i x^i\,.$$

4. Evaluate the derivatives where $f(x)$ is expressed as the power series of step 3, and substitute these into the ODE.
5. Group like powers of x such that each power of x has its own coefficient.
6. The expressions that are the coefficients must vanish individually. Express this fact as a recursion relation in closed form if possible.

Postscript: The fact given in step 6 "The expressions that are the coefficients must vanish individually," is not obvious. Each power of x may be viewed as a basis vector. The different basis vectors cannot mix, so in the homogeneous series $a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots = 0$, each a_i must be zero individually. The coefficients are usually expressions and not individual scalars, like $\big(\lambda - n\big)$ or more sophisticated expressions, so that each coefficient can vanish individually. Arfken[3] provides a more formal discussion. Problem 7 will likely be illustrative.

---

3. Find the asymptotic solution to $\dfrac{d^2\,\psi\,(x)}{dx^2} + \big(\lambda - \alpha^2 x^2\big)\,\psi\,(x) = 0\,.$

An asymptotic solution means the solution as $|\,x\,| \gg 0$. The solution that is sought is a wavefunction. A wavefunction must be normalizable so must approach zero as $|\,x\,| \gg 0$.

$$|\,x\,| \gg 0 \quad\Rightarrow\quad \alpha^2 x^2 \gg \lambda\,, \quad \text{so at large } x \text{ the ODE approaches} \quad \frac{d^2\,\psi\,(x)}{dx^2} - \alpha^2 x^2 \psi\,(x) = 0\,. \tag{1}$$

The solution to this asymptotic form of the rearranged time independent Schrodinger equation is

$$\psi\,(x) = A\,e^{-\alpha x^2/2} + \cancel{B\,e^{\alpha x^2/2}} = A\,e^{-\alpha x^2/2}, \tag{2}$$

where $B = 0$ because the exponential term with the positive argument approaches infinity so is not normalizable and is discarded. To show that equation (2) is a solution to equation (1),

$$\frac{d}{dx}\,\psi\,(x) = -\alpha x A\,e^{-\alpha x^2/2} \quad\Rightarrow\quad \frac{d^2}{dx^2}\,\psi\,(x) = \frac{d}{dx}\left(-\alpha x A\,e^{-\alpha x^2/2}\right) = \alpha^2 x^2 A\,e^{-\alpha x^2/2} - \cancel{\alpha A\,e^{-\alpha x^2/2}}$$

where the last term is struck because it is negligible under the assumption $x \gg 0$. Substituting into equation (1) yields $\alpha^2 x^2 A\,e^{-\alpha x^2/2} - \alpha^2 x^2 A\,e^{-\alpha x^2/2} = 0$, so equation (2) is the asymptotic form sought. Now we know the "long distance" behavior. Step 1 of the road map is complete.

Postscript: Other terminology used to convey the fact that a function is not normalizable is that it is not square integrable or that the function is non-physical.

---

4. Reduce $\dfrac{d^2\,\psi\,(x)}{dx^2} + \big(\lambda - \alpha^2 x^2\big)\,\psi\,(x) = 0$ to an equivalent ODE valid over the entire domain.

The domain is $-\infty < x < \infty$. Step 2 is substitute $\psi\,(x) = A\,e^{-\alpha x^2/2} f\,(x)$ and reduce.

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[3] Arfken *Mathematical Methods for Physicists* (Academic Press, New York, 1970, 2nd ed.), pp 267–270.

$$\frac{d^2}{dx^2}\, e^{-\alpha x^2/2} f\,(x) + \big(\lambda - \alpha^2 x^2\big)\, e^{-\alpha x^2/2} f\,(x) = 0\,, \tag{1}$$

where we have divided both sides by the constant A so it does not appear. The second derivative of the composite function is required, so

$$\frac{d^2}{dx^2}\, e^{-\alpha x^2/2} f\,(x) = \frac{d}{dx}\left(-\alpha x\, e^{-\alpha x^2/2} f\,(x) + e^{-\alpha x^2/2}\, \frac{d}{dx}\, f\,(x)\right)$$

$$= -\alpha\, e^{-\alpha x^2/2} f\,(x) + \alpha^2 x^2 e^{-\alpha x^2/2} f\,(x) - \alpha x\, e^{-\alpha x^2/2} f'\,(x) - \alpha x\, e^{-\alpha x^2/2}\, \frac{d}{dx}\, f\,(x) + e^{-\alpha x^2/2} f''\,(x)\,.$$

Using this in equation (1),

$$-\alpha\, e^{-\alpha x^2/2} f\,(x) + \alpha^2 x^2 e^{-\alpha x^2/2} f\,(x) - \alpha x\, e^{-\alpha x^2/2}\, \frac{d}{dx}\, f\,(x) - \alpha x\, e^{-\alpha x^2/2}\, \frac{d}{dx}\, f\,(x)$$
$$+\, e^{-\alpha x^2/2}\, \frac{d^2}{dx^2}\, f\,(x) + \big(\lambda - \alpha^2 x^2\big)\, e^{-\alpha x^2/2} f\,(x) = 0$$

Each of the six terms on the left contains the same exponential. Dividing both sides by the exponential and striking terms that sum to zero,

$$-\alpha f\,(x) + \alpha^2 \cancel{x^2} f\,(x) - 2\alpha\, x \frac{d}{dx}\, f\,(x) + \frac{d^2}{dx^2}\, f\,(x) + \lambda f\,(x) - \alpha^2 \cancel{x^2} f\,(x) = 0$$

$$\Rightarrow \quad \frac{d^2}{dx^2}\, f\,(x) - 2\alpha x\, \frac{d}{dx}\, f\,(x) + \big(\lambda - \alpha\big) f\,(x) = 0\,, \quad \text{and that concludes step 2.}$$

---

5. Change the variable in $\dfrac{d^2}{dx^2}\, f\,(x) - 2\alpha x\, \dfrac{d}{dx}\, f\,(x) + \big(\lambda - \alpha\big) f\,(x) = 0$ to $\xi = \sqrt{\alpha}\, x\,.$

A change of variables is used to caste an expression or equation into a more favorable form. This is an optional technique prior to step 3 that should expose some of the existing body of mathematics.

$$\xi = \sqrt{\alpha}\, x \quad \Rightarrow \quad d\xi = \sqrt{\alpha}\, dx \quad \Rightarrow \quad \frac{d\xi}{dx} = \sqrt{\alpha}\,.$$

To change variables, also needed is $\dfrac{d}{dx}\, f\,(x) = \dfrac{d}{d\xi}\, \dfrac{d\,\xi}{dx}\, f\,(\xi) = \dfrac{d}{d\xi}\, \sqrt{\alpha}\, f\,(\xi) = \sqrt{\alpha}\, \dfrac{d}{d\xi}\, f\,(\xi)$

$$\Rightarrow \quad \frac{d^2}{dx^2}\, f\,(x) = \frac{d}{dx}\, \sqrt{\alpha}\, \frac{d}{d\xi}\, f\,(\xi) = \frac{d}{d\xi}\, \frac{d\xi}{dx}\, \sqrt{\alpha}\, \frac{d}{d\xi}\, f\,(\xi) = \frac{d}{d\xi}\, \alpha\, \frac{d}{d\xi}\, f\,(\xi) = \alpha\, \frac{d^2}{d\xi^2}\, f\,(\xi)\,,$$

therefore, $\dfrac{d^2}{dx^2}\, f\,(x) - 2\alpha x\, \dfrac{d}{dx}\, f\,(x) + \big(\lambda - \alpha\big) f\,(x) = 0$ becomes

$$\alpha\, \frac{d^2}{d\xi^2}\, f\,(\xi) - 2\alpha\, \frac{\xi}{\sqrt{\alpha}}\, \sqrt{\alpha}\, \frac{d}{d\xi}\, f\,(\xi) + \big(\lambda - \alpha\big) f\,(\xi) = 0$$

$$\Rightarrow \quad \frac{d^2}{d\xi^2} f(\xi) - 2\xi \frac{d}{d\xi} f(\xi) + \left(\frac{\lambda}{\alpha} - 1\right) f(\xi) = 0 \,,$$

and this is **Hermite's equation**. The arbitrary function $f(\xi)$ is often represented $H_n(\xi)$, or

$$\frac{d^2}{d\xi^2} H_n(\xi) - 2\xi \frac{d}{d\xi} H_n(\xi) + \left(\frac{\lambda}{\alpha} - 1\right) H_n(\xi) = 0 \,.$$

The solutions to Hermite's equation are the Hermite polynomials denoted $H_n(\xi)$.

---

6. Express Hermite's equation in terms of an infinite power series.

Solutions to Schrodinger's equation with the SHO potential are $\psi(x) = H_n(\xi)$ where a normalization constant A and an exponential factor $e^{-\alpha x^2/2}$ have been divided from the ODE. The $H_n(\xi)$ are the solutions so the rest of the road map is unnecessary. We continue the process only to illustrate the further procedures of completing a power series solution. Generally, we assume

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots = \sum_{i=0}^{\infty} a_i x^i \,, \quad \text{but in terms of } \xi \,,$$

$$f(\xi) = a_0 + a_1 \xi + a_2 \xi^2 + a_3 \xi^3 + \cdots = \sum_{i=0}^{\infty} a_i \xi^i \,.$$

$$\frac{d}{d\xi} f(\xi) = a_1 + 2a_2 \xi + 3a_3 \xi^2 + 4a_4 \xi^3 + \cdots = \sum_{i=1}^{\infty} i\, a_i\, \xi^{i-1},$$

$$\frac{d^2}{d\xi^2} f(\xi) = 1 \cdot 2a_2 + 2 \cdot 3a_3 \xi + 3 \cdot 4a_4 \xi^2 + 4 \cdot 5a_5 \xi^3 + \cdots = \sum_{i=2}^{\infty} (i-1) i\, a_i\, \xi^{i-2}.$$

Inserting these derivatives into Hermite's equation,

$$1 \cdot 2a_2 + 2 \cdot 3a_3 \xi + 3 \cdot 4a_4 \xi^2 + 4 \cdot 5a_5 \xi^3 + \cdots - 2\xi \left(a_1 + 2a_2 \xi + 3a_3 \xi^2 + 4a_4 \xi^3 + \cdots\right)$$
$$+ \left(\frac{\lambda}{\alpha} - 1\right) \left(a_0 + a_1 \xi + a_2 \xi^2 + a_3 \xi^3 + \cdots\right) = 0 \,,$$

is the power series form of Hermite's equation, completing steps 3 and 4.

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7. Find the coefficient of each power of ξ in the power series form of Hermite's equation then develop a recursion relation summarizing all coefficients.

Steps 5 and 6 in the power series solution road map follows.

$$1 \cdot 2a_2 + 2 \cdot 3a_3 \xi + 3 \cdot 4a_4 \xi^2 + 4 \cdot 5a_5 \xi^3 + \cdots$$

$$-2\xi\, a_1 - 2\xi\, 2a_2\, \xi - 2\xi\, 3a_3\, \xi^2 - 2\xi\, 4a_4\, \xi^3 - \cdots$$
$$+ \left(\frac{\lambda}{\alpha} - 1\right) a_0 + \left(\frac{\lambda}{\alpha} - 1\right) a_1\, \xi + \left(\frac{\lambda}{\alpha} - 1\right) a_2\, \xi^2 + \left(\frac{\lambda}{\alpha} - 1\right) a_3\, \xi^3 + \cdots = 0$$

$$\Rightarrow \quad 1 \cdot 2a_2 + 2 \cdot 3a_3\, \xi + 3 \cdot 4a_4\, \xi^2 + 4 \cdot 5a_5\, \xi^3 + \cdots$$
$$-2\, a_1\, \xi - 2 \cdot 2a_2\, \xi^2 - 2 \cdot 3a_3\, \xi^3 - 2 \cdot 4a_4\, \xi^4 - \cdots$$
$$+ \left(\frac{\lambda}{\alpha} - 1\right) a_0 + \left(\frac{\lambda}{\alpha} - 1\right) a_1\, \xi + \left(\frac{\lambda}{\alpha} - 1\right) a_2\, \xi^2 + \left(\frac{\lambda}{\alpha} - 1\right) a_3\, \xi^3 + \cdots = 0\,.$$

Examining each power of ξ reveals

$$\begin{array}{ll}
\text{coefficient of } \xi^0: & 1 \cdot 2a_2 + \left(\dfrac{\lambda}{\alpha} - 1\right) a_0 \\
\text{coefficient of } \xi^1: & 2 \cdot 3a_3 + \left(\dfrac{\lambda}{\alpha} - 1 - 2\right) a_1 \\
\text{coefficient of } \xi^2: & 3 \cdot 4a_4 + \left(\dfrac{\lambda}{\alpha} - 1 - 2 \cdot 2\right) a_2 \\
\text{coefficient of } \xi^3: & 4 \cdot 5a_5 + \left(\dfrac{\lambda}{\alpha} - 1 - 2 \cdot 3\right) a_3 \\
\vdots & \vdots
\end{array}$$

The pattern can be written $\quad (n+1)(n+2)\, a_{n+2} + \left(\frac{\lambda}{\alpha} - 1 - 2 \cdot n\right) a_n \quad$ for $\quad n = 0, 1, 2, 3, \ldots\,.$

Each coefficient must vanish individually, or $\quad (n+1)(n+2)\, a_{n+2} + \left(\frac{\lambda}{\alpha} - 1 - 2 \cdot n\right) a_n = 0$

$$\Rightarrow \quad a_{n+2} = -\frac{\left(\lambda/\alpha - 1 - 2 \cdot n\right)}{(n+1)(n+2)}\, a_n \quad \text{for} \quad n = 0\,,\ 1\,,\ 2\,,\ 3\,,\ \ldots\,.$$

is the recursion relation that completes step 6.

Postscript: The statement that says each coefficient must vanish individually is

$$(n+1)\,(n+2)\, a_{n+2} + \left(\frac{\lambda}{\alpha} - 1 - 2 \cdot n\right) a_n = 0\,.$$

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8. Find the eigenenergies of the SHO from the recursion relation.

The eigenfunctions do not approach zero at $|\,x\,| \gg 0$ quickly enough to be normalizable if the series does not terminate[4], so termination is a requirement. It follows that $\lambda/\alpha - 1 - 2n = 0$, as can be seen from the recursion relation found in the previous problem.

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[4] Gasiorowicz *Quantum Physics* (John Wiley & Sons, New York, 1974), pp 101–105.

$$\frac{\lambda}{\alpha} - 1 - 2n = 0 \quad \Rightarrow \quad \lambda_n = \big(2n+1\big)\,\alpha\,. \quad \text{Also} \quad \lambda = \frac{2mE}{\hbar^2} \quad \text{and} \quad \alpha^2 = \frac{mk}{\hbar^2} \quad \text{from problem 1}$$

$$\Rightarrow \quad \frac{2mE_n}{\hbar^2} = \big(2n+1\big)\,\frac{\sqrt{mk}}{\hbar} \quad \Rightarrow \quad E_n = \big(2n+1\big)\,\frac{1}{\hbar}\,\frac{\hbar^2}{2m}\sqrt{mk}$$

$$\Rightarrow \quad E_n = \left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\,, \qquad \text{or} \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega\,.$$

Practice Problems

9. Consider the three-dimensional SHO with the potential $V\,(r) = \frac{1}{2}m\omega^2 r^2\,.$ Separate the three-dimensional, time-dependent Schrodinger equation into time and spatial variables in (a) spherical coordinates, (b) Cartesian coordinates, and then (c) solve the time-dependent portion of the separated equation. Discuss the meaning of the differential equation dependent only on time.

10. Solve the time-independent Schrodinger equation in Cartesian coordinates by separating spatial variables. Find the eigenenergies and the degree of degeneracy for a three-dimensional SHO in the arbitrary excited state n.

11. Solve the time-independent Schrodinger equation in spherical coordinates in three dimensions for the SHO. Separate radial and angular dependence. Solve the radial equation using a power series solution. Find the eigenenergies a three-dimensional SHO in the arbitrary excited state n.

12. Compare your solutions for the Cartesian and spherical models by showing that the eigenenergies and total degeneracy are the same. Relate the eigenstates expressed in Cartesian coordinates and the eigenstates expressed in spherical coordinates.

We are going to address these four problems as one problem with 21 parts. This problem set is designed to guide you through two different differential equation solutions to the three-dimensional harmonic oscillator problem, namely the solution in Cartesian coordinates which is precisely like solving the one-dimensional problem three times, and the solution in spherical coordinates which involves a separation of the radial and angular degrees of freedom which is very similar to our solution of the hydrogen atom—specifically, there is an effective radial potential governing the radial dependence, and the spherical harmonics govern the angular dependence. This problem contains several important pedagogical issues:

(1) You should be able to separate the time and space dependence of the wavefunction. You should understand how the energy eigenvalues emerge as the separation constant during this separation of time and space, and how this separation of variables leads from the time-dependent Schrodinger equation to the time-independent Schrodinger equation.

As we saw for the one-dimensional harmonic oscillator, only special values of the separation constant terminate the power series—these special solutions to the time-independent Schrodinger equation are the "stationary states". When you solve the time-independent Schrodinger equation to get the stationary states, remember that there are only a few special values of the separation constant (the energy eigenvalues) that produce these very special time and space separated stationary solutions. For an arbitrary energy, you cannot separate the wavefunction into a single function of space times a single function of time! In fact, there are infinitely many linear combinations of the stationary states with any given expectation value of the energy. However, you can always uniquely separate any given initial state (which will always have a definite expectation value of its energy E at $t = 0$) into a sum of the stationary states times their respective time dependences. Of course, that's why we spent so much time expanding the initial $t = 0$ wavefunction in terms of the energy eigenstates...

(2) You should be able to separate three-dimensional problems in Cartesian coordinates or in spherical coordinates. The $3D$ SHO is one of the few problems that is so easily soluble in both coordinate systems, and it gives us a good chance to compare the two approaches.

(3) You should be able to make the separated differential equation dimensionless. Once you have a dimensionless equation, you should be able to solve it in the asymptotic limit. Then you should be able to separate the asymptotic behavior. Finally, you must be able to solve for the dimensionless asymptotic-behavior-removed stationary state wavefunctions. Of course, the point is that by making the equation dimensionless, and by removing the asymptotic behavior, you will find a complete set of finite polynomials that solve your problem. The special values of the separation constant that terminate these otherwise infinite series solutions are the dimensionless energy eigenvalues. And, of course, you must be able to use the recursion relations you obtain to deduce the polynomials and the corresponding energy eigenvalues.

(4) Finally, you should realize that no matter what set of coordinates you use to solve the problem, you must get the same answer! For this problem your answers will look very different, but there is nevertheless a fairly simple way to relate them to each other: linear combinations of the Cartesian stationary states are the energy eigenfunctions of the radial and angular momentum description, and, of course, linear combinations of the radial and angular momentum stationary states are the energy eigenfunctions of the Cartesian description...

9. Separating Variables for the 3d SHO

(a) Write down the time-dependent Schrodinger equation in the position space representation using $V(r) = \frac{1}{2} m\omega^2 r^2$. Then separate the time and space dependence of this equation using separable product eigenfunctions of the form $\Psi_n(\vec{\mathbf{r}}, t) = \psi_n(\vec{\mathbf{r}})\, g_n(t)$.

(b) Use $r^2 = x^2 + y^2 + z^2$ and the Cartesian form of the Laplacian to express the time-dependent Schrodinger equation in Cartesian coordinates. Then separate the time and space dependence using separable product eigenfunctions of the form $\Psi_n(x, y, z, t) = \psi_n(x, y, z)\, g_n(t)$. The resulting time dependent $g_n(t)$ must be the same as part (a).

Parts (a) and (b) illustrate how the time-independent Schrodinger equation can be constructed from the time-dependent Schrodinger equation in a position representation. The time-independent Schrodinger equation only applies to the stationary states—all wavefunctions obey the time-dependent Schrodinger equation, but only the stationary states obey the time-independent Schrodinger equation!

(c) Show that the time-dependent functions are given by $g_n(t) = e^{-iE_n t/\hbar}$ by solving the differential equation that you obtained for $g_n(t)$ when you separated the time and space dependence. This is the differential equation version of the origin of the exponential phase describing time-dependence of the stationary states!

10. The 3d SHO in Cartesian Coordinates

(d) Express your time-independent Schrodinger equation in Cartesian coordinates, *i.e.,* in terms of x, y, z, p_x, p_y, and p_z, and then separate the x, y, and z dependence of this equation with eigenfunctions of the form $\psi_n(\vec{\mathbf{r}}) = \psi_n(x,y,z) = f(x)\, g(y)\, h(z)$. This is a little trickier than parts (a) and (b) since we considered only two degrees of freedom but have three degrees of freedom and a constant term here. Consider the Hamiltonian for the SHO

$$\mathcal{H} = \mathcal{H}_x + \mathcal{H}_y + \mathcal{H}_z = \left(\frac{\mathcal{P}_x^2}{2m} + \frac{1}{2}m\omega^2 x^2\right) + \left(\frac{\mathcal{P}_y^2}{2m} + \frac{1}{2}m\omega^2 y^2\right) + \left(\frac{\mathcal{P}_z^2}{2m} + \frac{1}{2}m\omega^2 z^2\right)$$

and you should be able to conclude what the separation constants must be. The final form of your separated equations for $f(x)$, $g(y)$, and $h(z)$ are time-independent Schrodinger equations for the one-dimensional SHO.

(e) Show that the eigenenergies for the three-dimensional harmonic oscillator are just the sum of the eigenenergies for the three separated directions, *i.e.,* show that

$$E_n = E\,(n_x,\, n_y,\, n_z) = \left(n + \frac{3}{2}\right)\hbar\omega, \quad \text{where} \quad n = n_x + n_y + n_z\,.$$

(f) Make a table of all possible combinations of the component and total quantum numbers for the ground state and for the first three excited states. Show that the degeneracy of the n-th state is $d(n) = \frac{1}{2}(n+1)(n+2)$ and list n_x, n_y, and n_z. This can be tricky. You may want to use form 1.2.2.1 in the *Handbook of Mathematical Formulas and Integrals* by Jeffrey,

$$\sum_{\mathrm{k}=0}^{m-1}(a + kd) = \frac{m}{2}\Big[2a + (m-1)\,d\Big]\,.$$

11. The 3d SHO in Spherical Coordinates

(g) Express your time-independent Schrodinger equation in spherical coordinates, *i.e.,* in terms of r, θ, and ϕ. Use the Laplacian in spherical coordinates,

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,.$$

Separate the radial dependence and the angular dependence of this equation using product eigenfunctions consisting of radial wavefunctions times the spherical harmonics, *i.e.,*

$$\psi_{klm}(\vec{\mathbf{r}}) = \psi_{klm}(r,\theta,\phi) = R_{kl}(r)\, Y_{lm}(\theta,\phi)\,.$$

The subscripts are important but not particularly useful at this point so just use $\psi = RY$. Spherical harmonics are another family of orthogonal polynomials dependent only on polar and azimuthal angle for the moment. We will discuss the spherical harmonics in chapter 8. Use $l(l+1)$ as the separation constant. The reason for this choice should become clear in chapters 8 and 9.

(h) Show that your separated radial equation has the form

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}\,r + \frac{1}{2}m\omega^2 r^2 + \frac{l(l+1)\,\hbar^2}{2\,mr^2}\right] R_{kl}(r) = E_{kl}\,R_{kl}(r)\,.$$

Again, the subscripts are important but since we have placed little emphasis on their meaning to this point, they are largely cosmetic.

(i) Set $R_{kl}(r) = r^{-1}\,u_{kl}(r)$ and $\epsilon_{kl} = 2mE_{kl}/\hbar^2$ to obtain the corresponding dimensionless energy version of the time-independent Schrodinger equation

$$\left[\frac{d^2}{dr^2} - \beta^4\,r^2 - \frac{l(l+1)}{r^2} + \epsilon_{kl}\right] u_{kl}(r) = 0\,, \quad \text{where} \quad \beta = \sqrt{\frac{m\omega}{\hbar}}\,.$$

(j) Show that at large r, your asymptotic differential equation becomes

$$\left[\frac{d^2}{dr^2} - \beta^4\,r^2\right] u_{kl}(r) = 0\,.$$

Solve this asymptotic differential equation to obtain the asymptotic solutions $e^{\beta^2 r^2/2}$ and $e^{-\beta^2 r^2/2}$. Discard the solution that diverges at infinity since the wavefunction must go to zero at infinity. It is likely easiest to "guess" a proposed solution and differentiate to show that it is, in fact, a solution. See problem 3.

(k) Separate variables again to remove the Gaussian asymptotic behavior by substituting

$$u_{kl}(r) = e^{-\beta^2 r^2/2}\,y_{kl}(r)$$

into the differential equation for u_{kl} to obtain the corresponding differential equation for y_{kl},

$$\left[\frac{d^2}{dr^2} - 2\,\beta^2\,r\,\frac{d}{dr} + \epsilon_{kl} - \beta^2 - \frac{l(l+1)}{r^2}\right] y_{kl}(r) = 0\,.$$

Again, it is good that you see the subscripts, but they are still cosmetic at this point.

(l) Now substitute the power series $y_{kl}(r) = r^s \sum a_q r^q$ into the differential equation to obtain the recursion relation for the coefficients. See problem 6.

(m) Show that $\big[s(s-1) - l(l+1) \big] a_0 = 0$, and that this requires $s = l+1$ so that $a_0 \neq 0$.

(n) Show that $\big[s(s+1) - l(l+1) \big] a_1 = 0$, and that this requires $a_1 = 0$.

(o) Show that for the coefficient of the r^{q+s} term to be equal to zero we must have

$$\big[(q+s+2)(q+s+1) - l(l+1) \big] a_{q+2} + \big[\epsilon_{kl} - \beta^2 - 2\beta^2 (q+s) \big] \; a_q = 0$$

or equivalently, after using $s = l+1$, that

$$\big[(q+2)(q+2l+3) \big] a_{q+2} = \big[(2q+2l+3)\beta^2 - \epsilon_{kl} \big] a_q \, .$$

(p) Show that all the coefficients with odd subscripts q are zero.

(q) Explain why the interesting values of the separation constants are those that terminate the series. Then show that the series terminates when $\epsilon_{kl} = (2k+2l+3)\beta^2$ where k and l are non-negative integers.

(r) Show that the eigenenergies are given by

$$E_{kl} = \left(k + l + \frac{3}{2} \right) \hbar\omega = \left(n + \frac{3}{2} \right) \hbar\omega \, .$$

(s) Show that the allowed values of $\{k, l\}$ for a given n depend on whether n is even or odd and are given by

For n even: $\{k, l\} = \{0, n\}, \; \{2, n-2\}, \; \ldots\,, \; \{n-2, 2\}, \; \{n, 0\}$.

For n odd: $\{k, l\} = \{0, n\}, \; \{2, n-2\}, \; \ldots\,, \; \{n-3, 3\}, \; \{n-1, 1\}$.

12. Comparison of the Cartesian and Spherical Solutions

(t) Show that when the $2l+1$ degeneracy of the angular momentum states is included, the total degeneracy of each state of the three-dimensional harmonic oscillator described in spherical coordinates is exactly the same as the degeneracy that you already calculated in Cartesian coordinates, $g(n) = \frac{1}{2}(n+1)(n+2)$. Use the formula for a finite arithmetic progression given in part (f). You must cast these sums into the same form where the index starts at zero and is consecutive. The forms that are comparable to the given finite arithmetic sum are

$$\sum_{l \,\text{even}}^{n} (2l+1) = \sum_{i}^{n/2} (4i+1) \qquad \text{and} \qquad \sum_{l \,\text{odd}}^{n} (2l+1) = \sum_{i}^{(n-1)/2} (4i+3) \, .$$

(u) We would like to have you show that you can form a linear combination of the Cartesian stationary states to produce one of the spherical stationary states and vice versa, but we will not ask that here. We will ask you to do this problem after we have discussed spherical harmonics. In the interim, please be assured that the Cartesian stationary states are simply a linear combination of the spherical stationary states and vice versa. Not surprisingly, likely the easiest way to show this is using Dirac notation...

a = [a,H] = aH-Ha—oh, my, gotcha!!!

The ladder operator solution to the simple harmonic oscillator problem is subtle, exquisite, and rather slippery—so I thought you might appreciate a recapitulation of what I said in class . . . . You might want to go through the argument line-by-line until it clicks!

There were three steps in the argument:

1. The first step was to show that the eigenvalues of the Hamiltonian H are equal to $\hbar\omega$ times $\frac{1}{2}$ plus the eigenvalues of the number operator $N = a^\dagger a$ (which will turn out to be n, so we will end up with $(n + \frac{1}{2})\hbar\omega$). We did this by showing that the Hamiltonian H is $\hbar\omega$ times the sum of the number operator plus one half the identity operator,

$$H \ = \ \big(a^\dagger a + \frac{1}{2}\big)\ \hbar\omega.$$

We showed this by defining the $a^\dagger$ and a operators, and then calculating $a^\dagger a$. Note that once we found that $H = (a^\dagger a + \frac{1}{2})\ \hbar\omega$, we immediately knew that the eigenvectors of H would be the same as the eigenvalues of $a^\dagger a$—because every vector is an eigenvector of the identity operator! We also immediately knew that the eigenvalues of H would be equal to $\hbar\omega$ times the eigenvalues of the $a^\dagger a$ operator plus $\frac{1}{2}\hbar\omega$.

2. The second step was to show that when the $a^\dagger$ and a operators act on any eigenvector of H, we get back another eigenvector of H one step up or down the ladder of states. We showed this by calculating the three commutators:

$$\begin{aligned}
[a, a^\dagger] &= +1 \\
[a, H] &= +a \\
[a^\dagger, H] &= -a^\dagger
\end{aligned}$$

and considering the action of the last two commutators on any eigenvector of the Hamiltonian

$$\begin{aligned}
[a, H]\ |\text{eigenvector of H}\!> &= +a\ \ |\text{eigenvector of H}\!> \\
[a^\dagger, H]\ |\text{eigenvector of H}\!> &= -a^\dagger\ |\text{eigenvector of H}\!>.
\end{aligned}$$

By expanding the commutators, we found

$$\begin{aligned}
\big(aH - Ha\big)\ |\text{eigenvector of H}\!> &= +a\ \ |\text{eigenvector of H}\!> \\
\big(a^\dagger H - Ha^\dagger\big)\ |\text{eigenvector of H}\!> &= -a^\dagger\ |\text{eigenvector of H}\!>.
\end{aligned}$$

which allowed us to conclude that

$$\begin{aligned}
a\ |\epsilon\!> &= (\epsilon - 1)\ |\epsilon - 1\!> \\
a^\dagger\ |\epsilon\!> &= (\epsilon + 1)\ |\epsilon + 1\!>.
\end{aligned}$$

This showed us that the eigenvalues of H are separated by $\pm\hbar\omega$. Combining this with the $\frac{1}{2}\hbar\omega$ from step one, we then concluded that the eigenvalues of the Hamiltonian are given by

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

where n is any integer (*i.e.,* positive, negative, or zero!!!). However, in step three, we found the smallest eigenvalue of the number operator is equal to zero.

So the only other thing we did not know yet was whether the raising and lowering operators return normalized eigenvectors of the Hamiltonian, *i.e.,* are the vectors $a|\epsilon>$ and $a^\dagger|\epsilon>$ normalized eigenvectors of H? We did know that they are eigenvectors of H with eigenvalues of $(\epsilon-1)\hbar\omega$ and $(\epsilon+1)\hbar\omega$, respectively, but we did not know whether they are normalized—and, in fact, they are not!

3. The third step was to calculate the normalization coefficients. To do this we started with two adjacent normalized states, $|n> \equiv |E = (n+\frac{1}{2})\hbar\omega>$ and $|n-1> \equiv |E = ((n-1)+\frac{1}{2})\hbar\omega>$ and then we calculated the expectation value of the number operator in two different ways:

(i) First, we started with the lowering operator equation

$$a\;|n> = \;c_n\;|n-1>$$

and then we calculated the adjoint of this equation

$$<n|\;a^\dagger \;\;= <n-1|\;c_n^*.$$

We combined these to evaluate the expectation value of the number operator

$$\begin{aligned} <n|\;a^\dagger a\;|n> \;&= <n-1|\;c_n^* c_n\;|n-1> = \;|c_n|^2\;\;<n-1|n-1> \\ &= \;|c_n|^2. \end{aligned}$$

(ii) Second, we replaced $a^\dagger a$ by $\widehat{H} - \frac{1}{2}$ and recalculated the expectation value of N

$$\begin{aligned} <n|\;\widehat{H} - \frac{1}{2}\;|n> \;&= <n-1|\;\big[\;(n+\frac{1}{2}) + \frac{1}{2}\;\big]\;|n> = \;n\;\;<n|n> \\ &= \;n. \end{aligned}$$

By combining these two calculations, we found

$$\begin{aligned} |c_n|^2 = n \;\Rightarrow\; c_n = \sqrt{n} \\ \Rightarrow\; a\;|n> = \sqrt{n}\;|n-1>\,. \end{aligned}$$

Finally, to see that the lowest eigenvalue of the number operator is zero, we considered

$$a\;|0> = \;\sqrt{0}\;|0-1> = \;0\;|-1> = \;\vec{0}.$$

So $|0>$ is the bottom rung on the ladder (lowering it we obtain the zero vector), and consequently the lowest eigenvalue of H is $\frac{1}{2}\hbar\omega$, which is the zero point energy of the oscillator.