

SHO Energy Levels, Wave functions via Operator Formalism

The energy eigenvalues for a one-dimensional quantum harmonic oscillator (QHO) using the algebraic ladder operator method. are shown. This approach, centered on creation and annihilation operators, elegantly reveals the quantized energy spectrum without solving the Schrödinger eigenvalue equation directly, solution of wave functions are easier to obtain.

1 The Hamiltonian and Dimensionless Operators

The Hamiltonian for a 1-dimensional simple harmonic oscillator is given by:

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

where \hat{p} and \hat{x} are the momentum and position operators, with canonical commutation relation $[\hat{x}, \hat{p}] = i\hbar$.

To simplify the algebra, we employ the dimensionless position & momentum operators, \hat{Q} and \hat{P} :

$$\hat{Q} = \sqrt{\frac{m\omega}{\hbar}}\hat{x} \quad \text{and} \quad \hat{P} = \frac{1}{\sqrt{m\omega\hbar}}\hat{p}$$

Their commutator is:

$$[\hat{Q}, \hat{P}] = \left[\sqrt{\frac{m\omega}{\hbar}}\hat{x}, \frac{1}{\sqrt{m\omega\hbar}}\hat{p} \right] = \frac{1}{\hbar}[\hat{x}, \hat{p}] = \frac{1}{\hbar}(i\hbar) = i$$

In terms of these new operators, the Hamiltonian becomes:

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{P}^2 + \hat{Q}^2)$$

2 Ladder Operators

We now define the *annihilation operator* \hat{a} and the *creation operator* \hat{a}^\dagger . While they are schematically combinations of position and momentum, their precise, standard definitions are:

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{Q} + i\hat{P}) \tag{1}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{Q} - i\hat{P}) \tag{2}$$

Note that \hat{a}^\dagger is the Hermitian conjugate of \hat{a} .

2.1 Commutation Relation

The commutator of \hat{a} and \hat{a}^\dagger is fundamental to this method:

$$\begin{aligned} [\hat{a}, \hat{a}^\dagger] &= \frac{1}{2}[(\hat{Q} + i\hat{P}), (\hat{Q} - i\hat{P})] \\ &= \frac{1}{2}([\hat{Q}, \hat{Q}] - i[\hat{Q}, \hat{P}] + i[\hat{P}, \hat{Q}] - i^2[\hat{P}, \hat{P}]) \\ &= \frac{1}{2}(0 - i(i) + i(-i) - (-1)(0)) \\ &= \frac{1}{2}(1 + 1) = 1 \end{aligned}$$

So, we have the crucial result:

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

2.2 Hamiltonian in Terms of Ladder Operators

We can express the Hamiltonian in terms of \hat{a} and \hat{a}^\dagger . First, let's find the product $\hat{a}^\dagger \hat{a}$:

$$\begin{aligned}\hat{a}^\dagger \hat{a} &= \frac{1}{2}(\hat{Q} - i\hat{P})(\hat{Q} + i\hat{P}) \\ &= \frac{1}{2}(\hat{Q}^2 + i\hat{Q}\hat{P} - i\hat{P}\hat{Q} - i^2\hat{P}^2) \\ &= \frac{1}{2}(\hat{Q}^2 + \hat{P}^2 + i[\hat{Q}, \hat{P}]) \\ &= \frac{1}{2}(\hat{Q}^2 + \hat{P}^2 + i(i)) = \frac{1}{2}(\hat{Q}^2 + \hat{P}^2 - 1)\end{aligned}$$

Rearranging this gives $\hat{Q}^2 + \hat{P}^2 = 2\hat{a}^\dagger \hat{a} + 1$. Substituting this into our expression for the Hamiltonian yields:

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

We define the ***number operator*** as $\hat{N} = \hat{a}^\dagger \hat{a}$. The Hamiltonian is thus:

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right)$$

Since \hat{H} and \hat{N} differ only by constants, they share the same eigenvectors. If $|n\rangle$ is an eigenvector of \hat{N} with eigenvalue n , then it is also an eigenvector of \hat{H} with eigenvalue $E_n = \hbar\omega(n + 1/2)$.

3 Derivation of Energy Eigenvalues

To understand the action of \hat{a} and \hat{a}^\dagger , we compute their commutators with the Hamiltonian:

$$\begin{aligned}[\hat{H}, \hat{a}] &= [\hbar\omega(\hat{a}^\dagger \hat{a} + 1/2), \hat{a}] = \hbar\omega[\hat{a}^\dagger \hat{a}, \hat{a}] = \hbar\omega[\hat{a}^\dagger, \hat{a}]\hat{a} = \hbar\omega(-1)\hat{a} = -\hbar\omega\hat{a} \\ [\hat{H}, \hat{a}^\dagger] &= [\hbar\omega(\hat{a}^\dagger \hat{a} + 1/2), \hat{a}^\dagger] = \hbar\omega[\hat{a}^\dagger \hat{a}, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger(1) = +\hbar\omega\hat{a}^\dagger\end{aligned}$$

Now, let $|E\rangle$ be an energy eigenstate with eigenvalue E , so $\hat{H}|E\rangle = E|E\rangle$. Consider the state $\hat{a}|E\rangle$:

$$\hat{H}(\hat{a}|E\rangle) = (\hat{a}\hat{H} - \hbar\omega\hat{a})|E\rangle = \hat{a}(E|E\rangle) - \hbar\omega(\hat{a}|E\rangle) = (E - \hbar\omega)(\hat{a}|E\rangle)$$

This shows that if $|E\rangle$ is an energy eigenstate, then $\hat{a}|E\rangle$ is also an energy eigenstate with its energy **lowered** by $\hbar\omega$. Similarly, for $\hat{a}^\dagger|E\rangle$:

$$\hat{H}(\hat{a}^\dagger|E\rangle) = (\hat{a}^\dagger\hat{H} + \hbar\omega\hat{a}^\dagger)|E\rangle = \hat{a}^\dagger(E|E\rangle) + \hbar\omega(\hat{a}^\dagger|E\rangle) = (E + \hbar\omega)(\hat{a}^\dagger|E\rangle)$$

This shows that $\hat{a}^\dagger|E\rangle$ is an energy eigenstate with its energy raised by $\hbar\omega$.

The energy of the harmonic oscillator cannot be infinitely negative, as the Hamiltonian is a sum of two positive-definite operators. Therefore, there must exist a lowest energy state, or ***ground state***, which we will call $|0\rangle$. This state cannot be lowered further, which implies:

$$\hat{a}|0\rangle = 0$$

The energy of this ground state, E_0 , can be found by applying the Hamiltonian:

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

The ground state energy is $E_0 = \frac{1}{2}\hbar\omega$ which is called zero point energy.

All other energy states, or excited states, are generated by successively applying the creation operator \hat{a}^\dagger to the ground state.

- The first excited state has energy $E_1 = E_0 + \hbar\omega = \frac{3}{2}\hbar\omega$.
- The second excited state has energy $E_2 = E_1 + \hbar\omega = \frac{5}{2}\hbar\omega$.

In general, the energy of the n -th state is:

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

3.1 Derivation of SHO Wave Functions in Operator Formalism

3.1.1 Ground State Wave Function ($n = 0$)

The ground state is defined by the condition that the annihilation operator acting on it gives zero:

$$\hat{a}|\psi_0\rangle = 0$$

In the position representation, this becomes a first-order differential equation:

$$\sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{\hbar}{m\omega} \frac{d}{dx}\right) \psi_0(x) = 0$$

This can be rearranged to:

$$\frac{d\psi_0(x)}{dx} = -\frac{m\omega}{\hbar} x \psi_0(x)$$

Solving this separable differential equation by integration, $\int \frac{d\psi}{\psi} = -\frac{m\omega}{\hbar} \int x dx \Rightarrow \ln(\psi_0(x)) = -\frac{m\omega}{2\hbar} x^2 + C'$. Normalizing this gives the same result as the conventional method:

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

3.1.2 First Excited State Wave Function ($n = 1$)

The first excited state is created by applying the creation operator to the ground state:

$$|\psi_1\rangle = \hat{a}^\dagger |\psi_0\rangle$$

In the position representation, this is:

$$\psi_1(x) = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{\hbar}{m\omega} \frac{d}{dx}\right) \psi_0(x)$$

Substituting $\psi_0(x) = C_0 e^{-m\omega x^2/2\hbar}$, where $C_0 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}$, we get:

$$\frac{d\psi_0(x)}{dx} = C_0 \left(-\frac{m\omega}{\hbar} x\right) e^{-m\omega x^2/2\hbar}$$

$$\psi_1(x) = C_0 \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{\hbar}{m\omega} \left(-\frac{m\omega}{\hbar} x\right)\right) e^{-m\omega x^2/2\hbar} = C_0 \sqrt{\frac{m\omega}{2\hbar}} (2x) e^{-m\omega x^2/2\hbar}$$

After proper normalization, this leads to:

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

3.1.3 Second Excited State Wave Function ($n = 2$)

The second excited state is found by applying the creation operator twice:

$$|\psi_2\rangle = \frac{1}{\sqrt{2!}}(\hat{a}^\dagger)^2|\psi_0\rangle = \frac{1}{\sqrt{2}}\hat{a}^\dagger|\psi_1\rangle$$

In the position representation:

$$\psi_2(x) = \frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right)\psi_1(x)$$

We need to find $\frac{d\psi_1(x)}{dx}$ which is

$$\frac{d\psi_1(x)}{dx} = C_1\sqrt{\frac{2m\omega}{\hbar}}\left(1 \cdot e^{-m\omega x^2/2\hbar} + x\left(-\frac{m\omega}{\hbar}x\right)e^{-m\omega x^2/2\hbar}\right) = C_1\sqrt{\frac{2m\omega}{\hbar}}\left(1 - \frac{m\omega}{\hbar}x^2\right)e^{-m\omega x^2/2\hbar}$$

Substituting this back into the expression for $\psi_2(x)$ and simplifying:

$$\psi_2(x) = \frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{2\hbar}}\left[x - \frac{\hbar}{m\omega}\left(1 - \frac{m\omega}{\hbar}x^2\right)\right]\psi_1(x) = C_2\left(4\frac{m\omega}{\hbar}x^2 - 2\right)e^{-m\omega x^2/2\hbar}$$

After normalization, this results in the same form as the conventional method, confirming consistency between the two approaches. The Hermite polynomial, $H_0(\xi) = 1$, $H_1(\xi) = 2\xi$, $H_2(\xi) = 4\xi^2 - 2$ naturally arises from this process. In general, $\psi_n(x) = N_n H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-\frac{m\omega}{2\hbar}x^2}$.

4 Visualization

Potential $V(x) = \frac{1}{2}m\omega^2 x^2$ along with the wavefunctions $\psi_0(x)$, $\psi_1(x)$, and $\psi_2(x)$, each centered on its corresponding energy level. We use dimensionless units where $m = \omega = \hbar = 1$.

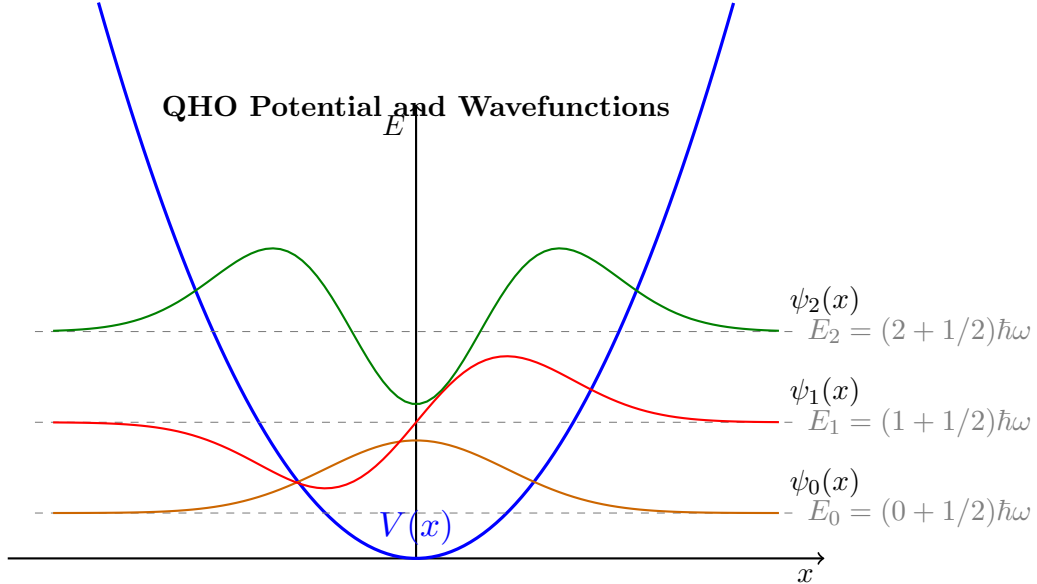


Figure 1: The parabolic potential well of the quantum harmonic oscillator. The dashed lines show the quantized energy levels. The wavefunctions for the ground state ($n = 0$, orange), first excited state ($n = 1$, red), and second excited state ($n = 2$, green) are shown, vertically shifted to their respective energy levels.