

Simple Harmonic Oscillator

Excited States | Orthonormality of states

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The Hamiltonian of SHO

The total energy $E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$

Here $\omega = \sqrt{k/m}$ is angular frequency of the oscillation.

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

$$V(\hat{x}) = \frac{1}{2}m\omega^2\hat{x}^2$$



Factorized Hamiltonian of SHO

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

$$\hat{N} \equiv \hat{a}^\dagger \hat{a}$$

Number operator

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i\hat{p}}{m\omega} \right)$$

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



The ground state wave function and energy

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

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

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

$$E_0 = \frac{1}{2}\hbar\omega$$



Operator manipulation

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

$$\hat{N} \equiv \hat{a}^\dagger \hat{a}$$

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

$$\hat{N}\psi_0 = \hat{a}^\dagger \hat{a}\psi_0 = 0$$

Thus ψ_0 is an eigenstate of the operator \hat{N} with an eigenvalue $N = 0$. Therefore ψ_0 is an energy eigenstate with energy E_0 given by

$$E_0 = \hbar\omega \left(0 + \frac{1}{2} \right) = \frac{1}{2}\hbar\omega$$



Operator manipulation

$$[\hat{N}, \hat{a}] = [\hat{a}^\dagger \hat{a}, \hat{a}] = \hat{a}^\dagger [\hat{a}, \hat{a}] + [\hat{a}^\dagger, \hat{a}] \hat{a} = -\hat{a}$$

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

Similarly we can show

$$[\hat{N}, \hat{a}^2] = [\hat{N}, \hat{a}\hat{a}] = [\hat{N}, \hat{a}]\hat{a} + \hat{a}[\hat{N}, \hat{a}] = -\hat{a}\hat{a} + \hat{a}(-\hat{a}) = -2\hat{a}^2,$$

$$[\hat{N}, (\hat{a}^\dagger)^2] = [\hat{N}, \hat{a}^\dagger \hat{a}^\dagger] = [\hat{N}, \hat{a}^\dagger]\hat{a}^\dagger + \hat{a}^\dagger[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger \hat{a}^\dagger + \hat{a}^\dagger \hat{a}^\dagger = 2(\hat{a}^\dagger)^2$$



Operator manipulation

$$[\hat{N}, (\hat{a})^k] = -k(\hat{a})^k$$

$$[\hat{N}, (\hat{a}^\dagger)^k] = k(\hat{a}^\dagger)^k$$

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

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

If $\hat{A}\psi = 0$, then $\hat{A}\hat{B}\psi = [\hat{A}, \hat{B}]\psi$



First excited states

Since \hat{a} annihilates ψ_0 consider acting on the ground state with \hat{a}^\dagger . It is clear that \hat{a}^\dagger cannot also annihilate ψ_0 . If that would happen then acting with both sides of the commutator identity $[\hat{a}, \hat{a}^\dagger] = 1$ on ψ_0 would lead to a contradiction: the left-hand side would vanish but the right-hand side would not. Thus consider the wave function

$$\psi_1 \equiv \hat{a}^\dagger \psi_0$$

We are going to show that this is an energy eigenstate.



Fist excited states

$$\hat{N}\psi_1 = \hat{N}\hat{a}^\dagger\psi_0 = [\hat{N}, \hat{a}^\dagger]\psi_0 = \hat{a}^\dagger\psi_0 = \psi_1$$

- ψ_0 is an eigenstate of the operator \hat{N} with eigenvalue $N = 0$.
- ψ_1 is an eigenstate of the operator \hat{N} with eigenvalue $N = 1$.
- \hat{a}^\dagger acting on ψ_0 increases the eigenvalue of \hat{N} by one unit.
- \hat{a}^\dagger is called the *creation* operator or the *raising* operator.



First excited states

Moreover

$$\begin{aligned}(\psi_1, \psi_1) &= (\hat{a}^\dagger \psi_0, \hat{a}^\dagger \psi_0) = (\psi_0, \hat{a} \hat{a}^\dagger \psi_0) \\ &= (\psi_0, [\hat{a}, \hat{a}^\dagger] \psi_0) = (\psi_0, \psi_0) = 1\end{aligned}$$

ψ_1 is normalized and is the wave function of first excited state.

Energy of the first excited state

$$E_1 = \hbar\omega \left(1 + \frac{1}{2} \right) = \frac{3}{2} \hbar\omega$$



Second Excited states

Next consider the state $\psi'_2 \equiv \hat{a}^\dagger \hat{a}^\dagger \psi_0$.

$$\hat{N}\psi'_2 = \hat{N}\hat{a}^\dagger \hat{a}^\dagger \psi_0 = [\hat{N}, \hat{a}^\dagger \hat{a}^\dagger] \psi_0 = 2\hat{a}^\dagger \hat{a}^\dagger \psi_0 = 2\psi'_2$$

ψ'_2 is a state with number $N = 2$ and energy $E_2 = \frac{5}{2}\hbar\omega$.

$$\begin{aligned} (\psi'_2, \psi'_2) &= (\hat{a}^\dagger \hat{a}^\dagger \psi_0, \hat{a}^\dagger \hat{a}^\dagger \psi_0) = (\psi_0, \hat{a} \hat{a} \hat{a}^\dagger \hat{a}^\dagger \psi_0) = (\psi_0, \hat{a} [\hat{a}, \hat{a}^\dagger \hat{a}^\dagger] \psi_0) \\ &= (\psi_0, 2\hat{a} \hat{a}^\dagger \psi_0) = 2(\psi_0, \psi_0) = 2. \end{aligned}$$



Excited state wave functions

The properly normalized wave function is

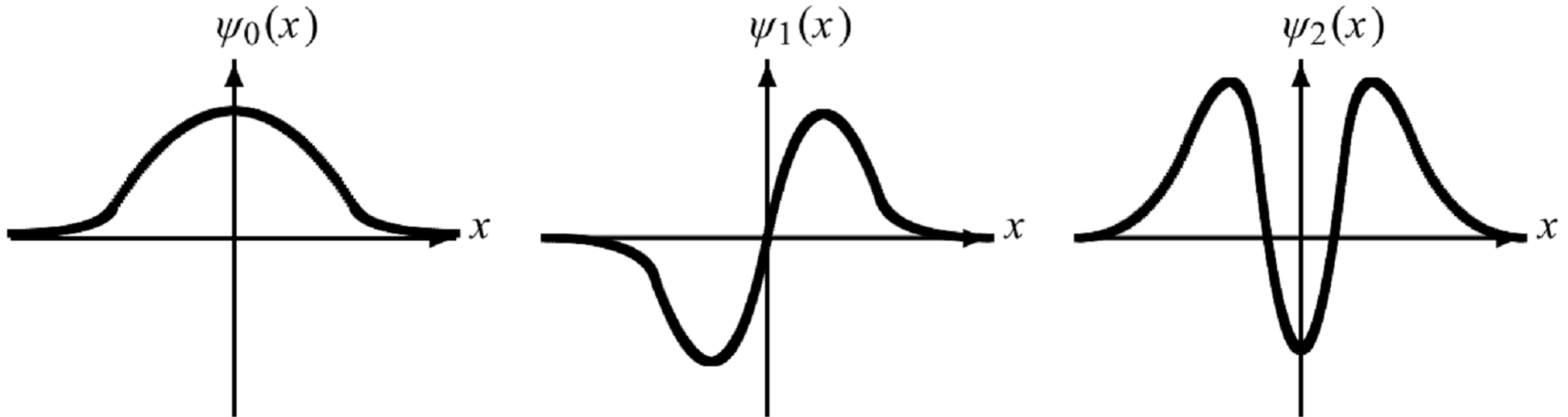
$$\psi_2 \equiv \frac{1}{\sqrt{2}} \hat{a}^\dagger \hat{a}^\dagger \psi_0.$$

$$\psi_3 \equiv \frac{1}{\sqrt{2}} \frac{1}{\sqrt{3}} \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \psi_0 = \frac{1}{\sqrt{3!}} (\hat{a}^\dagger)^3 \psi_0$$

$$\psi_n \equiv \frac{1}{\sqrt{n!}} \underbrace{\hat{a}^\dagger \cdots \hat{a}^\dagger}_n \psi_0 = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n \psi_0.$$



Shapes of the first three wave functions of the SHO



$$\psi_n \equiv \frac{1}{\sqrt{n!}} \underbrace{\hat{a}^\dagger \cdots \hat{a}^\dagger}_n \psi_0 = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n \psi_0.$$

Eigenvalue of ψ_n for the operators \hat{N} and \hat{H}

$$\begin{aligned}\hat{N}\psi_n &= \frac{1}{\sqrt{n!}}\hat{N}(\hat{a}^\dagger)^n\psi_0 = \frac{1}{\sqrt{n!}}\hat{a}^\dagger\hat{a}(\hat{a}^\dagger)^n\psi_0 \\ &= \frac{1}{\sqrt{n!}}\hat{a}^\dagger[\hat{a},(\hat{a}^\dagger)^n]\psi_0 = \frac{1}{\sqrt{n!}}\hat{a}^\dagger n(\hat{a}^\dagger)^{n-1}\psi_0 \\ &= \frac{n}{\sqrt{n!}}(\hat{a}^\dagger)^n\psi_0 = n\psi_n\end{aligned}$$

Since for the operator \hat{N} the eigenvalue of ψ_n is n , the energy eigenvalue E_n is given by

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



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