Quantum Mechanics I

PHY 3103

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Simple Harmonic Oscillator

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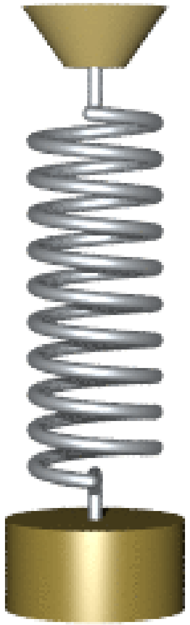
It is one of those few problems that are important to all branches of physics. The harmonic oscillator provides a useful model for a variety of vibrational phenomena that are encountered, for instance, in classical mechanics, electrodynamics, statistical mechanics, solid state, atomic, nuclear, and particle physics. In quantum mechanics, it serves as an invaluable tool to illustrate the basic concepts and the formalism.



The Hamiltonian of SHO

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

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

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

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

Factorizing the Hamiltonian

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

$$a^2 + b^2 = (a - ib)(a + ib)$$

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

Factorizing the Hamiltonian

We now define $$\hat{A} = \hat{x} + \frac{i\hat{p}}{m\omega}$$

and its Hermitian conjugate $$\hat{A}^\dagger = \hat{x} - \frac{i\hat{p}}{m\omega}$$

We therefore have $$\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} = \hat{A}^\dagger\hat{A} + \frac{\hbar}{m\omega}$$

Therefore, the Hamiltonian $$\boxed{\hat{H} = \frac{1}{2}m\omega^2\hat{A}^\dagger\hat{A} + \frac{1}{2}\hbar\omega.}$$

The commutator of $\hat{A}$ and $\hat{A}^\dagger$

$$[\hat{A},\ \hat{A}^\dagger] = \left[\hat{x} + \frac{i\hat{p}}{m\omega},\ \hat{x} - \frac{i\hat{p}}{m\omega}\right]$$

$$= -\frac{i}{m\omega}[\hat{x},\ \hat{p}] + \frac{i}{m\omega}[\hat{p},\ \hat{x}]$$

$$= \frac{2\hbar}{m\omega}$$

$$\left[\sqrt{\frac{m\omega}{2\hbar}}\hat{A},\ \sqrt{\frac{m\omega}{2\hbar}}\hat{A}^\dagger\right] = 1$$

Creation and annihilation operators

Annihilation operator $$\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{A},$$

Creation operator $$\hat{a}^{\dagger} \equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{A}^{\dagger}.$$

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

Creation and annihilation operators

Annihilation operator $\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{A},$

Creation operator $\hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{A}^\dagger.$

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

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

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

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

$$\hat{p} = \frac{1}{i}\sqrt{\frac{m\omega\hbar}{2}}\left(\hat{a} - \hat{a}^\dagger\right)$$

Factorized Hamiltonian of SHO

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

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

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

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

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

On any normalized state ψ

$$\langle \hat{H} \rangle_\psi = (\psi, \hat{H}\psi) = \hbar\omega(\psi, \hat{a}^\dagger \hat{a}\psi) + \frac{1}{2}\hbar\omega(\psi, \psi)$$

$$= \hbar\omega(\hat{a}\psi, \hat{a}\psi) + \frac{1}{2}\hbar\omega \geq \frac{1}{2}\hbar\omega$$

$$(\psi, \psi) \geq 0$$

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

$$E \geq \frac{1}{2}\hbar\omega$$

The ground state wave function

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

$$\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)\psi_0(x) = 0$$

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

$$\frac{\mathrm{d}\psi_0}{\mathrm{d}x} = -\frac{m\omega}{\hbar}x\psi_0$$

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

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

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

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

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

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

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

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

Fist 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

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

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.

Fist excited states

Moreover

$$(\psi_1,\ \psi_1) = (\hat{a}^\dagger\psi_0,\ \hat{a}^\dagger\psi_0) = (\psi_0,\ \hat{a}\hat{a}^\dagger\psi_0)$$

$$= (\psi_0,\ [\hat{a},\ \hat{a}^\dagger]\psi_0) = (\psi_0,\ \psi_0) = 1$$

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

Energy of the first exited 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

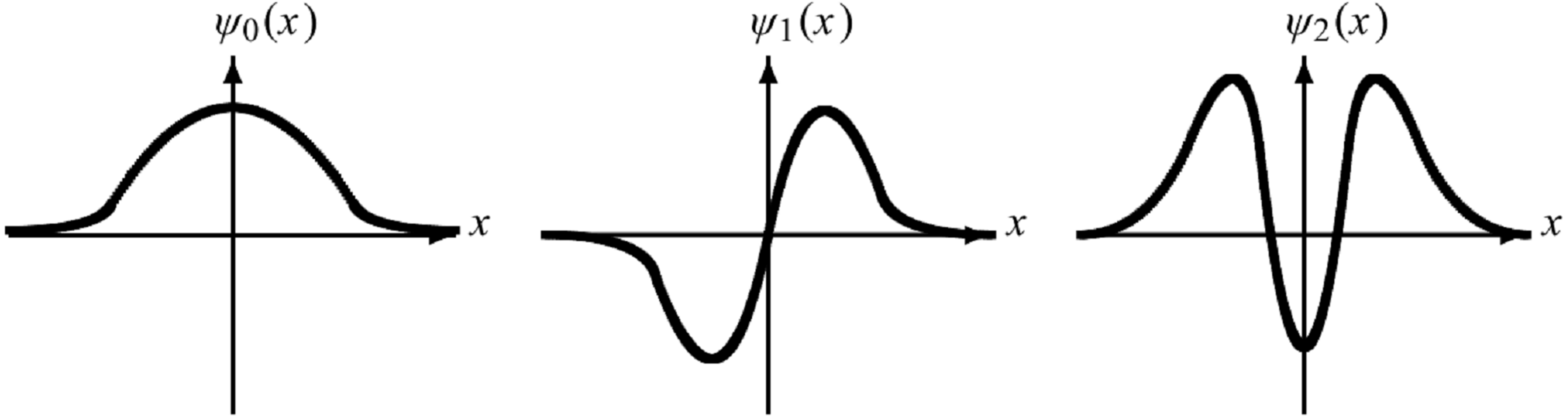
The properly normalized wave function is

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

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

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

Shapes of the first three wave functions of the SHO



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

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

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

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

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

Properties of of $\hat{a}$ and $\hat{a}^\dagger$

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

$$= \frac{n}{\sqrt{n!}}\sqrt{(n-1)!}\,\psi_{n-1} = \sqrt{n}\,\psi_{n-1}$$

$$\hat{a}^\dagger\psi_n = \hat{a}^\dagger\frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\psi_0 = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^{n+1}\psi_0$$

$$= \frac{1}{\sqrt{n!}}\sqrt{(n+1)!}\,\psi_{n+1} = \sqrt{(n+1)}\,\psi_{n+1}$$

Orthonormality of eigenstates

Eigenstates are orthonormal: $$(\psi_m, \psi_n) = \delta_{mn}$$

Kronecker delta

$$\delta_{mn} = \begin{cases} 1 & \text{if} \quad m = n, \\ 0 & \text{if} \quad m \neq n. \end{cases}$$

$$\begin{aligned} \hat{a}\psi_n &= \sqrt{n}\,\psi_{n-1}, \\ \hat{a}^\dagger\psi_n &= \sqrt{(n+1)}\,\psi_{n+1}. \end{aligned}$$

Expectation values of operators

$$
\begin{aligned}
\langle \hat{x} \rangle_{\psi_n} &= (\psi_n,\, \hat{x}\psi_n) = \sqrt{\frac{\hbar}{2m\omega}}\,(\psi_n,\, (\hat{a}+\hat{a}^\dagger)\psi_n) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\,(\psi_n,\, \hat{a}\psi_n + \hat{a}^\dagger\psi_n) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\,(\psi_n,\, \hat{a}\psi_n) + \sqrt{\frac{\hbar}{2m\omega}}\,(\psi_n,\, \hat{a}^\dagger\psi_n) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\,(\psi_n,\, \sqrt{n}\,\psi_{n-1}) + \sqrt{\frac{\hbar}{2m\omega}}\,(\psi_n,\, \sqrt{(n+1)}\,\psi_{n+1}) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\,\sqrt{n}(\psi_n,\, \psi_{n-1}) + \sqrt{\frac{\hbar}{2m\omega}}\,\sqrt{(n+1)}(\psi_n,\, \psi_{n+1}) \\
&= 0.
\end{aligned}
$$

Expectation values of operators

$$\begin{aligned}
\langle \hat{x}^2 \rangle_{\psi_n} &= (\psi_n,\, \hat{x}^2 \psi_n) = \frac{\hbar}{2m\omega} (\psi_n,\, (\hat{a} + \hat{a}^\dagger)^2 \psi_n) \\
&= \frac{\hbar}{2m\omega} (\psi_n,\, (\hat{a} + \hat{a}^\dagger)(\hat{a} + \hat{a}^\dagger) \psi_n) \\
&= \frac{\hbar}{2m\omega} (\psi_n,\, (\hat{a}\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a} + \hat{a}^\dagger \hat{a}^\dagger) \psi_n) \\
&= \frac{\hbar}{2m\omega} (\psi_n,\, (\hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a}) \psi_n) \\
&= \frac{\hbar}{2m\omega} (\psi_n,\, (1 + 2\hat{N}) \psi_n) \\
&= \frac{\hbar}{2m\omega} (1 + 2n)
\end{aligned}$$

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

Expectation values of operators

$$\langle \hat{p} \rangle_{\psi_n} = 0$$

$$\langle \hat{p}^2 \rangle_{\psi_n} = \frac{m\hbar\omega}{2}(1+2n).$$

$$\langle \hat{x} \rangle_{\psi_n} = 0$$

$$\langle \hat{x}^2 \rangle_{\psi_n} = \frac{\hbar}{2m\omega}(1+2n)$$

$$\frac{m\omega^2}{2}\langle \hat{x}^2 \rangle_{\psi_n} = \frac{1}{2m}\langle \hat{p}^2 \rangle_{\psi_n} = \frac{1}{2}\langle \hat{H} \rangle_{\psi_n}$$

Uncertainty principle

$$\langle \hat{x} \rangle_{\psi_n} = 0$$

$$\langle \hat{x}^2 \rangle_{\psi_n} = \frac{\hbar}{2m\omega}(1 + 2n)$$

$$\langle \hat{p} \rangle_{\psi_n} = 0$$

$$\langle \hat{p}^2 \rangle_{\psi_n} = \frac{m\hbar\omega}{2}(1 + 2n).$$

$$\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2}$$

$$\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2}$$

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

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Harmonic oscillator in 3D

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)\right]\psi(x,y,z) = E\psi(x,y,z)$$

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$V(x,y,z) = V_x(x) + V_y(y) + V_z(z)$$

$$\left[\hat{H}_x + \hat{H}_y + \hat{H}_z\right]\psi(x,y,z) = E\psi(x,y,z)$$

Harmonic oscillator in 3D

$$\hat{H}_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_x(x)$$

$$\hat{H}_y = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + V_y(y)$$

$$\hat{H}_z = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V_z(z)$$

$$\boxed{\psi(x, y, z) = X(x)Y(y)Z(z)}$$

Harmonic oscillator in 3D

$$\left[-\frac{\hbar^2}{2m}\frac{1}{X}\frac{\mathrm{d}^2X}{\mathrm{d}x^2}+V_x(x)\right]+\left[-\frac{\hbar^2}{2m}\frac{1}{Y}\frac{\mathrm{d}^2Y}{\mathrm{d}y^2}+V_y(y)\right]+\left[-\frac{\hbar^2}{2m}\frac{1}{Z}\frac{\mathrm{d}^2Z}{\mathrm{d}z^2}+V_z(z)\right]=E$$

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V_x(x)\right]X(x)=E_xX(x)$$

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}y^2}+V_y(y)\right]Y(y)=E_yY(y)$$

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+V_z(z)\right]Z(z)=E_zZ(z)$$

$$E_x+E_y+E_z=E$$

Anisotropic harmonic oscillator

$$V(x,y,z) = \frac{1}{2}m\,\omega_x^2\,\hat{x}^2 + \frac{1}{2}m\,\omega_x^2\,\hat{y}^2 + \frac{1}{2}m\,\omega_x^2\,\hat{z}^2$$

$$E_{n_x\,n_y\,n_z} = E_{n_x} + E_{n_y} + E_{n_z} = \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y + \left(n_z + \frac{1}{2}\right)\hbar\omega_z$$

$$\psi_{n_x\,n_y\,n_z}(x,y,z) = X_{n_x}(x)\,Y_{n_y}(y)\,Z_{n_z}(z)$$

Isotropic harmonic oscillator

$$\omega_x = \omega_y = \omega_z = \omega$$

$$E_{n_x\, n_y\, n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega$$

n	$2E_n/(\hbar\omega)$	$(n_x n_y n_z)$	g_n
0	3	(000)	1
1	5	(100), (010), (001)	3
1	7	(200), (020), (002)	6
		(110), (101), (001)	
3	9	(300), (030), (003)	10
		(210), (201), (021)	
		(120), (102), (012)	
		(111)	