Compatible Observables

We say two observables $\hat{A}$ & $\hat{B}$ are compatible if measuring one does not disturb the other.

Example: Momentum & Energy for a Free particle: Let $\psi(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$.

Then $p = \hbar k$ and $E = \frac{(\hbar k)^2}{2m}$

We can measure p, then E, then p again, and we get the exact same values each time. This is because $\frac{1}{\sqrt{2\pi}} e^{ikx}$ is a common eigenstate for both $\hat{p}$ & $\hat{H}$

$\Rightarrow$ We can be 100% certain about p & E at the same time.

Incompatible Observables

If A & B have <u>no common eigenstates</u>, then measuring A leaves the system in a state which is <u>not</u> an eigenstate of B. Then there is uncertainty about the outcome of a measurement of B.

Example : Position and Momentum

If we measure x, then afterwards ψ will be

$\psi(x) = \delta(x-x')$ ← after measurement of x.

AND $\phi(k)$ = momentum space wavefunction $= \frac{1}{\sqrt{2\pi}} e^{ikx'}$

All k are equally likely!

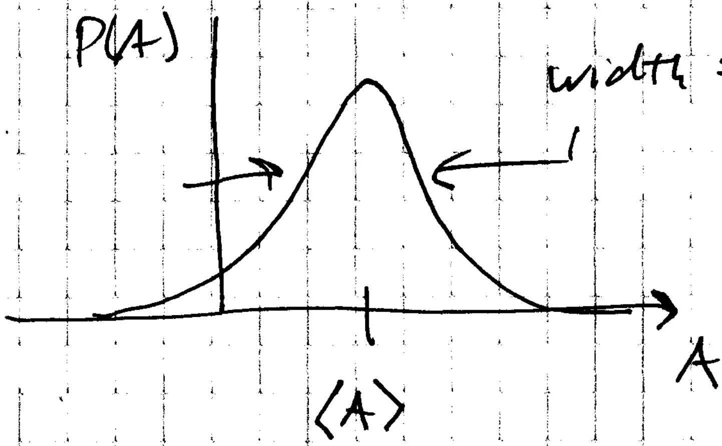
because $P(k) \sim$ constant

k is infinitely uncertain.

Uncertainty Principle – Quantifies how well we can predict the results of measurements of two variables.

- In some cases, the U.P. says that we can predict both variables with perfect accuracy, like p & E for a free particle.
- In other case, the U.P. says that the combined uncertainty will be equal or larger than some minimum value (like p & x).

Recall: We use ΔA to describe the RMS spread in variable A:



Quantitatively, $\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$

In QM, for a state $|\psi\rangle$,

$$\langle A\rangle = \int_{-\infty}^{\infty} \psi^*(x)\,\hat{A}\,\psi(x)\,dx = \langle\psi|\hat{A}|\psi\rangle$$

in Dirac Notation.

and $$\langle A^2\rangle = \int_{-\infty}^{\infty} \psi^*(x)\,\hat{A}^2\,\psi(x)\,dx = \langle\psi|\hat{A}^2|\psi\rangle$$

Therefore

$$\Delta A = \sqrt{\langle\psi|\hat{A}^2|\psi\rangle - \left(\langle\psi|\hat{A}|\psi\rangle\right)^2}$$

and $$\Delta B = \sqrt{\langle\psi|\hat{B}^2|\psi\rangle - \left(\langle\psi|\hat{B}|\psi\rangle\right)^2}$$

If we multiply $\Delta A \times \Delta B$ and do some algebra we get

$$\underbrace{(\Delta A)(\Delta B)}_{\text{"combined uncertainty"}} \geq \frac{1}{2}\overbrace{\left|\underbrace{\langle(\hat{A}\hat{B}-\hat{B}\hat{A})\rangle}_{\text{expectation value}}\right|}^{\text{magnitude}}$$

We call $\hat{A}\hat{B}-\hat{B}A$ "the commutator of $\hat{A}$ & $\hat{B}$",
and we write it as

$$\hat{A}\hat{B}-\hat{B}\hat{A} = \text{"commutator"} \equiv [\hat{A},\hat{B}]$$

Then

$$\boxed{(\Delta A)(\Delta B) \geq \frac{1}{2}\left|\langle [\hat{A},\hat{B}]\rangle\right|}$$

"Generalized Uncertainty Principle".

Example: position & momentum.

What is $[\hat{x},\hat{p}]$?

Answer: $(\hat{x}\hat{p}-\hat{p}\hat{x})\,f(x) = x\left(-i\hbar\frac{d}{dx}\right)f(x) + i\hbar\frac{d}{dx}\overbrace{(x\,f(x))}^{\text{chain rule}}$

Any function of x

$$= -i\hbar x f'(x) + i\hbar x f'(x) + i\hbar f(x)$$

cancel

$$= i\hbar f(x)$$

$\therefore$ $[\hat{x},\hat{p}]\,f(x) = i\hbar\, f(x)$

or $\boxed{[\hat{x},\hat{p}] = i\hbar}$ $\quad [\hat{x},\hat{p}]$ = multiply by $i\hbar$.

Then the uncertainty principle for x & p says

$$(\Delta x)(\Delta p) \geq \frac{1}{2}\left|\langle i\hbar\rangle\right|$$

What is $\langle i\hbar\rangle$? Answer: $\langle i\hbar\rangle = \langle\psi|i\hbar|\psi\rangle = i\hbar\overbrace{\langle\psi|\psi\rangle}^{1}$

$$= i\hbar$$

$\therefore \quad (\Delta x)(\Delta p) \geq \frac{1}{2} \left| \underbrace{i\hbar}_{} \right|$

a complex number:

$$i\hbar = \underbrace{\hbar}_{\text{magnitude} \equiv \hbar} e^{i\pi/2}$$

$$|i\hbar| = \hbar$$

$$\boxed{(\Delta x)(\Delta p) \geq \frac{\hbar}{2}}$$ Uncertainty Principle for x & p.

Comments

1) The uncertainty principle says the combined uncertainty will be equal to or larger than a minimum value. For most quantum states, the combined uncertainty is larger than the minimum value.

2) If $[\hat{A}, \hat{B}] = \emptyset$, then the U.P. says

$(\Delta A)(\Delta B) \geq \frac{1}{2} |\langle \emptyset \rangle| = \emptyset$. ← This means A & B are compatible observables. Then we can find a common eigenstate for A & B.

Example: $[\hat{P}, \hat{H}_{\text{free particle}}] = ?$

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$$\left(\hat{p}\,\hat{H}_{Free} - \hat{H}_{Free}\,\hat{p}\right) f(x) = \left[\left(-i\hbar\frac{d}{dx}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) + \left(+\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\left(-i\hbar\frac{d}{dx}\right)\right] f(x)$$

$$= \phi.$$

$\therefore\ (\Delta p)(\Delta E) = \phi$ for a free particle.

Common set of Base ~~Set~~ States in QM.

1. $\{|n\rangle\}$: Bound state energy eigenstates. Discrete
2. $\{|x\rangle\}$: Position eigenstates, Continuous
3. $\{|k\rangle\}$: momentum eigenstates, Continuous for a free particle.

We can project these states into the position basis. This gives us their spatial wavefunctions:

$$\langle x|n\rangle = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad \langle x|x^*\rangle = \delta(x-x^*)$$

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

For each of these bases, we have completeness and orthonormality:

orthonormality | completeness

$\langle m|n\rangle = \delta_{mn} \leftarrow$ Kronecker Delta, $\quad \hat{I} = \sum_n |n\rangle\langle n|$

$\langle x|x^*\rangle = \delta(x-x^*) \leftarrow$ Dirac Delta, $\quad \hat{I} = \int |x\rangle\langle x|$

$\langle k|k^*\rangle = \delta(k-k^*) \leftarrow$ Dirac Delta, $\quad \hat{I} = \int |k\rangle\langle k|$

We can use the completeness statement to calculate the Dirac Bracket of arbitrary states, if we know how those states are represented in one of these bases:

$$\langle a|b\rangle = \langle a|\underset{\text{Identity}}{\hat{I}}|b\rangle = \langle a|\left(\sum_n |n\rangle\langle n|\right)|b\rangle$$

$$= \sum_n \langle a|n\rangle \langle n|b\rangle$$

we can use this if we know the $\{a_n\}$ & $\{b_n\}$ $\rightarrow$ $= \sum_n a_n^* b_n$

Similarly,

$$\langle a|b\rangle = \langle a|\hat{I}|b\rangle = \langle a|\left(\int |x\rangle\langle x|dx\right)|b\rangle$$

$$= \int \langle a|x\rangle\langle x|b\rangle\, dx$$

We can use this if we know the spatial wavefunctions for ~~a~~ $|a\rangle$ & $|b\rangle$. →

$$= \int \psi_a^*(x)\,\psi_b(x)\, dx$$

And

$$\langle a|b\rangle = \langle a|\hat{I}|b\rangle = \langle a|\left(\int |k\rangle\langle k|dk\right)|b\rangle$$

$$= \int \underbrace{\langle a|k\rangle}_{\phi_a^*(k)}\ \underbrace{\langle k|b\rangle}_{\phi_b(k)}\, dk$$

We can use this if we know the momentum space wavefunction for $|a\rangle$ & $|b\rangle$.

$$= \int \phi_a^*(k)\,\phi_b(k)\, dk$$

In all three cases we are <u>projecting</u> these abstract bra & ket vectors onto a particular basis. This makes them more down-to-earth, and ~~they~~ allows us to use their <u>explicit</u> forms, in these bases.

Note: most people & textbooks use the symbol "$|\psi\rangle$" to represent an arbitrary QM state. Remember, "ψ" is a label. Strictly speaking

a real variable

$$\langle x|\psi\rangle = \psi(x)$$

a label

a label

a complex #

Dictionary for translating Wave Mechanics Into Dirac Notation

	Wave Mech.	Dirac Notation
~~Eigenfunction Eqn~~		
Eigenvalue Eq:	$\hat{A}\,\alpha = a\,\alpha$	$\hat{A}\,\|\alpha\rangle = a\,\|\alpha\rangle$
Momentum Eigenstates:	$\alpha(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$	$\langle x\|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$
TISE:	$\hat{H}\,\alpha_n = E_n\,\alpha_n$	$\hat{H}\,\|n\rangle = E_n\,\|n\rangle$
General Solution $e\ t=\emptyset$:	$\psi(x) = \sum_n a_n \alpha_n(x)$	$\|\psi\rangle = \sum_n a_n \|n\rangle$
For all t:	$\Psi(x,t) = \sum_n a_n \alpha_n(x) e^{-i\omega_n t}$	$\|\Psi\rangle = \sum_n a_n \|n\rangle e^{-i\omega_n t}$
Fourier's Trick	$a_n = \int \alpha_n^* \psi(x)\,dx$	$a_n = \langle n\|\psi\rangle$
orthonormality for bound state	$\int \alpha_m^*(x)\,\alpha_n(x)\,dx = \delta_{mn}$	$\langle m\|n\rangle = \delta_{mn}$
Orthonormality for momentum eigenstates	$\frac{1}{2\pi}\int_{-\infty}^{\infty} \left(e^{ikx}\right)^* \left(e^{ik'x}\right) dx = \delta(k-k')$	$\langle k\|k'\rangle = \delta(k-k')$
Orthonormality for position eigenstates	$\frac{1}{2\pi}\int_{-\infty}^{\infty} \left(e^{ikx}\right)^* \left(e^{ikx'}\right) dk = \delta(x-x')$	$\langle x\|x'\rangle = \delta(x-x')$
Free Particle	$\psi(x) = \frac{1}{\sqrt{2\pi}} \int \phi(k) e^{ikx}\,dk$	$\|\psi\rangle = \int \|k\rangle\,\phi(k)\,dk$
Expectation Value	$\langle C\rangle = \int \psi^*(x)\,\hat{C}\,\psi(x)\,dx$	$\langle\psi\|\hat{C}\|\psi\rangle$

~~$|\alpha\rangle = \int |k\rangle\langle k|\psi\rangle\,dk$~~ (with $\phi(k)$ written above $\langle k|\psi\rangle$)

~~$\psi(x) = \langle x|\psi\rangle = \int \langle x|k\rangle\,\phi(k)\,dk$~~

~~$\frac{1}{\sqrt{2\pi}}\int e^{ikx}\,\phi(k)\,dk$~~

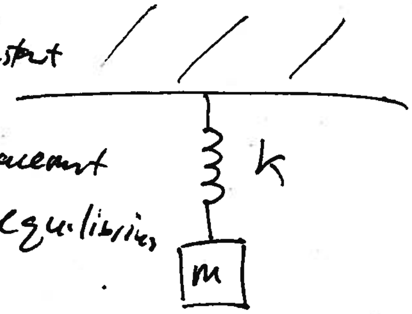
Simple Harmonic Oscillator (SHO)

A mass on a spring is a classical example of a SHO:

$$F = -kx$$

spring constant

displacement from equilibrium



Newton's 2nd Law says

$$-kx = m\ddot{x} = m\frac{d^2x}{dt^2}$$

$$\frac{dx^2}{dt^2} + \frac{k}{m}x = \emptyset \qquad \text{Define } \omega_0 = \sqrt{k/m} = \text{natural frequency}$$

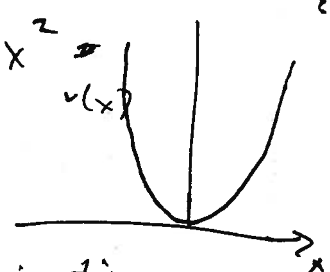
$$\frac{d^2x}{dt^2} + \omega_0^2 x = \emptyset$$

arbitrary constants (determined by initial conditions)

Classical Solution: $x(t) = A\cos(\omega_0 t + \delta)$

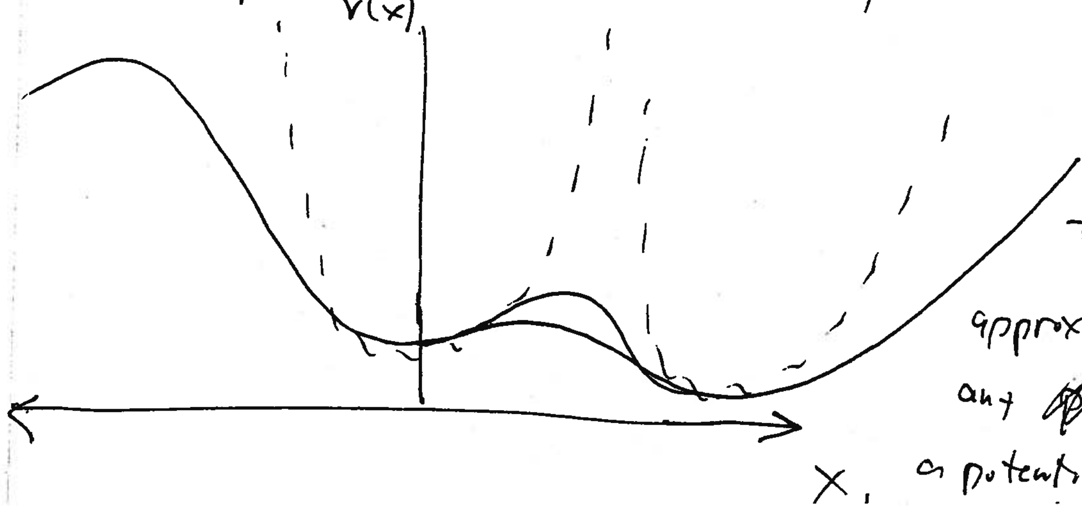
$$KE = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 = \frac{1}{2}m\dot{x}^2 = \frac{p^2}{2m}$$

Potential energy $V(x) = +\int_0^x kx'\,dx' = \frac{1}{2}kx^2$



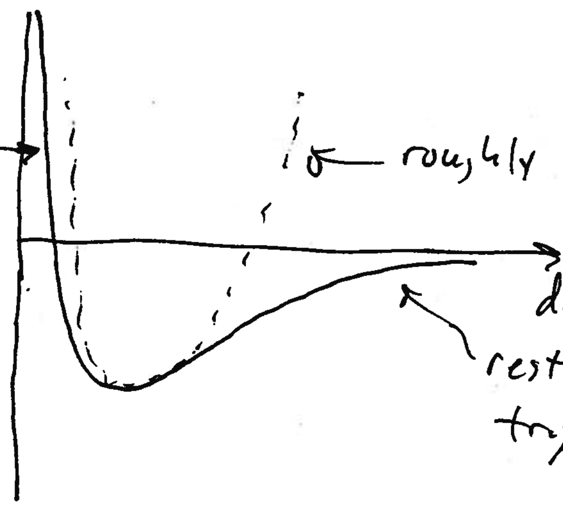
Total Energy $= \frac{p^2}{2m} + \frac{1}{2}kx^2$

~~[illegible]~~, the SHO makes a good approximation for the potential near almost any potential minimum.



To a good approximation, almost any ~~spot~~ minimum in a potential function

~~SHO~~ In QM, the SHO is a good model for most molecules. Imagine 2 atoms bound together, like 2 Hydrogen atoms bound into H_2: The potential is roughly



The Hamiltonian is taken from the classical energy:

$$E_{classical} = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

End here 10/21/09 →

$$\therefore \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2}kx^2$$

The TISE is

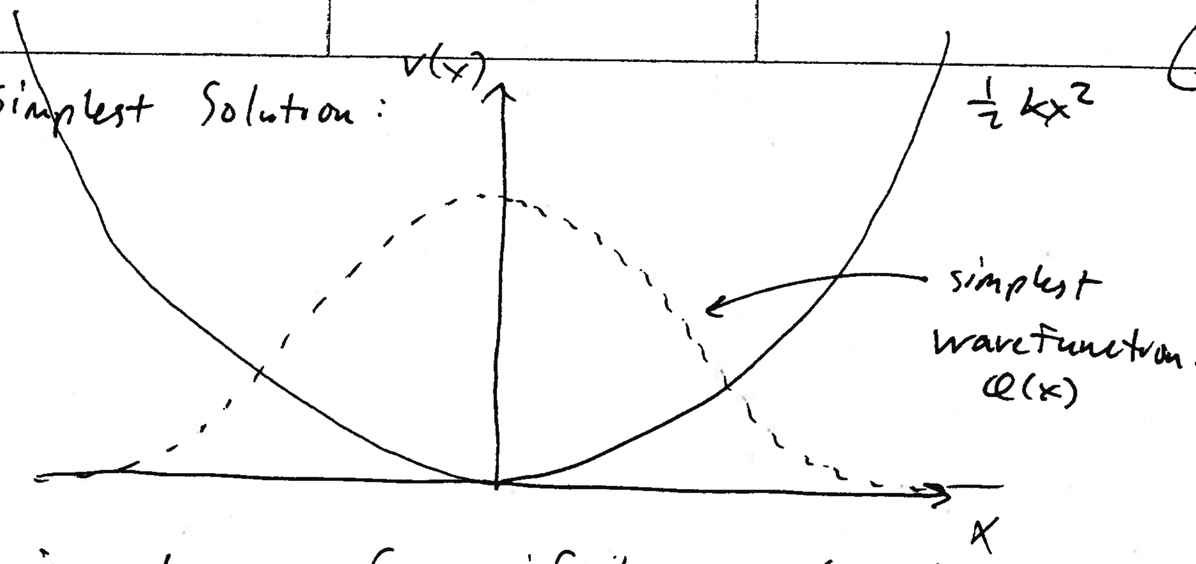
$$\hat{H}\psi = E\psi \leftarrow \text{e.v. equation for } \hat{H}.$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x)$$

The simplest solution to this differential eq. is a Gaussian

$$\psi(x) = A e^{-\beta^2x^2/2}, \text{ where } \beta^2 = \frac{m\omega_0}{\hbar} = \frac{m}{\hbar}\sqrt{\frac{k}{m}} = \frac{\sqrt{km}}{\hbar}$$

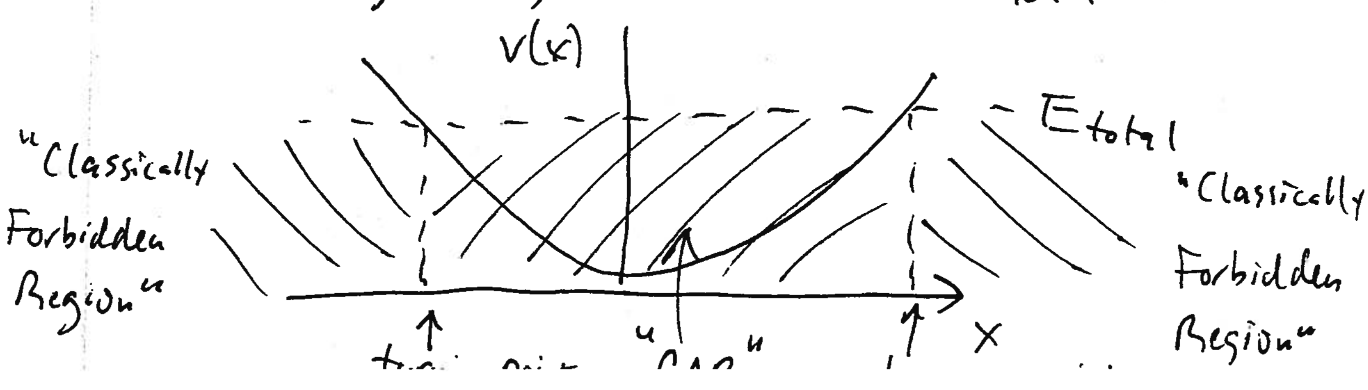
Simplest Solution:



This is only one of an infinite # of solutions. In fact, this one turns out to be the <u>ground state</u>, or state of lowest energy.

> Also, recall from the uncertainty principle that a Gaussian Wavefunction coincidentally minimizes $\Delta x \Delta p$. For this wavefunction $\Delta x \Delta p = \hbar/2$, the absolute minimum

One interesting thing about this wavefunction is that it ~~is~~ extends all the way to $x \to \pm\infty$. That means there is some <u>non-zero probability</u> to find the particle <u>anywhere</u> on the x-axis, although usually it will be found near $x = \emptyset$. In fact, we might find the particle outside the "Classically Allowed Region" ("CAR"), where $V(x) \leq E_{total}$.



So a QM ~~SHO~~ particle might be observed at a location which is forbidden by energy conservation in classical mechanics. In QM, however, if we measured an "illegal" position, and then measured the energy (to try to confirm the violation of energy conservation) the position measurement would disturb the energy state. We then expect a spectrum of possible energy measurements, and we ~~could say~~ would learn nothing about the energy of the particle before we measured the position.

Operator Solution to the QM SHO

We could find the other, more complicated solutions to the D.E. by continuing to guess them. But a better way uses the "creation" & "annihilation" operators.

Define

$$\hat{a} \equiv \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right), \quad \beta \equiv \sqrt{\frac{m\omega_0}{\hbar}}$$

What is the Hermitian Conjugate of $\hat{a}$? Well,

$$\hat{x} \rightarrow \hat{x}^{+} = \hat{x}, \quad \hat{p} \rightarrow \hat{p}^{+} = \hat{p}, \quad \& \; (i) \rightarrow (-i)$$

$$\therefore \quad \hat{a}^{+} \equiv \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)$$

Using $[\hat{x}, \hat{p}] = i\hbar$, we can prove that $[\hat{a}, \hat{a}^{+}] = 1$

or $\hat{a}\hat{a}^{+} = 1 + \hat{a}^{+}\hat{a}$

We can also write

$$\hat{x} = \frac{\hat{a} + \hat{a}^+}{\sqrt{2\beta}} \quad , \quad \hat{p} = -im\omega_0 \left(\frac{\hat{a} - \hat{a}^+}{\sqrt{2\beta}} \right)$$

In terms of $\hat{a}$ & $\hat{a}^+$, the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \hbar\omega_0 \left(\hat{a}^+\hat{a} + \frac{1}{2} \right)$$

We also define $\hat{N} = \hat{a}^+\hat{a}$, so that $\hat{H} = \hbar\omega_0 (\hat{N} + \frac{1}{2})$.

$\hat{N}$ is Hermitian and has real eigenvalues (n).
We don't yet know that (n) will be an integer, but it will turn out that way. Also, since $\hat{H} = \hbar\omega_0(\hat{N} + \frac{1}{2})$, if $|n\rangle$ is an eigenstate of $\hat{N}$, it is also an eigenstate of $\hat{H}$.

So let $|n\rangle$ stand for an eigenstate of $\hat{N}$ & $\hat{H}$.
If we let (n) stand for the $\hat{N}$ eigenvalue, then

$$\hat{N} \, |n\rangle = n \, |n\rangle .$$