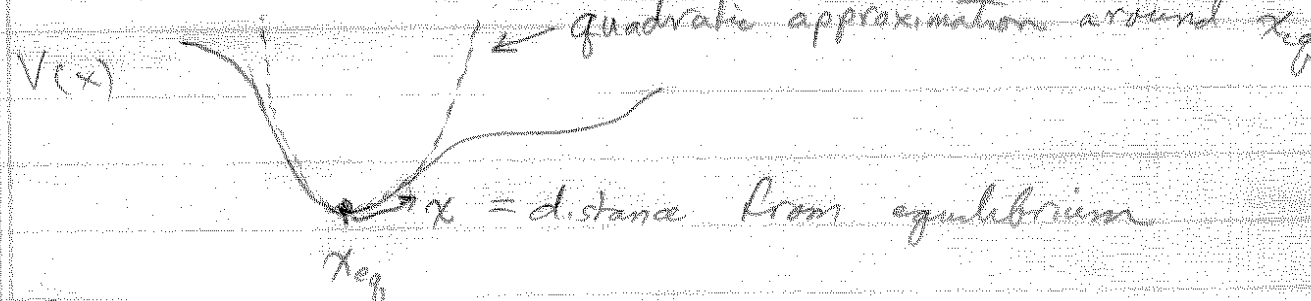
Physics 491: Quantum Mechanics I

Introduction to the Simple Harmonic Oscillator

The simple harmonic oscillator (SHO) is one of (if not <u>the</u>) most important problems in physics. It describes the oscillation of a system slightly displaced from a point of stable equilibrium. The ubiquitous phenomenon of <u>resonance</u> is easily seen for a SHO. The SHO is central to understanding such systems as

- Molecular vibrations
- Crystal phonons
- Quantum fields (normal modes)

If there is a stable equilibrium point x_{eq}



<u>Classical picture</u>

Hooke's law (restoring force) $\quad F = -kx$

(<u>linear</u>)

$$F = m\ddot{x} = -kx \Rightarrow \ddot{x} + \frac{k}{m}x = 0$$

Let $\omega = \sqrt{k/m}$

Solution $\Rightarrow x(t) = A\cos(\omega t + \phi) = x(0)\cos\omega t + \frac{\dot{x}(0)}{\omega}\sin\omega t$

Hamiltonian formulation:

$$H = \frac{p^2}{2m} + V(x)$$

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

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial H}{\partial x} = -m\omega^2 x$$

$$\Rightarrow \ddot{x} = \frac{\dot{p}}{m} = -\omega^2 x \quad \text{SHO} \checkmark$$

Make dimensionless:

Let us suppose there is a characteristic energy scale E_c

$\Rightarrow$ Characteristic momentum: $\frac{p_c^2}{2m} = E_c \Rightarrow p_c = \sqrt{2mE_c}$

Characteristic position: $\frac{1}{2} m\omega^2 x^2 = E_c \Rightarrow x_c = \sqrt{\frac{2E_c}{m\omega^2}}$

Let $h = \frac{H}{E_c}$, $\quad \underline{P} = \frac{p}{p_c} \quad \underline{X} = \frac{x}{x_c}$

$$\Rightarrow \boxed{h = \underline{X}^2 + \underline{P}^2}$$

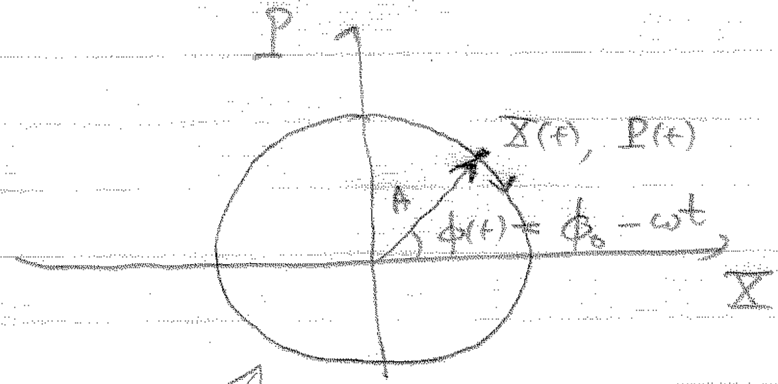
$\underline{X}$ and $\underline{P}$ look the same

Hamilton's Equations: $\dot{\underline{X}} = \omega \underline{P}$, $\quad \dot{\underline{P}} = -\omega \underline{X}$

$$\Rightarrow \underline{X}(t) = \underline{X}(0)\cos\omega t + \underline{P}(0)\sin\omega t$$

$$\underline{P}(t) = \underline{P}(0)\sin\omega t - \underline{X}(0)\cos\omega t$$

Phase Space



h = constant = circle

$$X(t) = A\cos(\phi_0 - \omega t) = \mathrm{Re}\big(\underbrace{\underbrace{Ae^{i\phi_0}}_{\alpha_0}\; e^{-i\omega t}}_{\alpha(t)}\big)$$

$$\mathrm{Re}(\alpha_0) = A\cos\phi_0 = X(0)$$
$$\mathrm{Im}(\alpha_0) = A\sin\phi_0 = P(0)$$

Let $\alpha(t) = X(t) + iP(t) = Ae^{i\phi(t)}$
$= \alpha(0)\, e^{-i\omega t}$ = phasor

Note $h = X^2 + P^2 = |\alpha(t)|^2$

$h = \alpha^* \alpha$ (amplitude squared = energy)

The phasor picture is very useful for classical oscillators. We will see it's analoge now in the quantum theory

Quantized SHO

To look at the Quantum theory we let x and p become operators

$$x \to \hat{x} \qquad p \to \hat{p} \quad \text{with} \quad [\hat{x}, \hat{p}] = i\hbar$$

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

The new constant $\hbar$ provides a scale for the action from we obtain a natural scale for energy

$$E_c = \hbar\omega$$

$$\Rightarrow P_c = \sqrt{2m\hbar\omega} \qquad X_c = \sqrt{\frac{2\hbar}{m\omega}}$$

Let $\hat{\underline{X}} = \frac{\hat{x}}{x_c} \qquad \hat{\underline{P}} \equiv \frac{\hat{p}}{p_c}$

$$[\hat{\underline{X}}, \hat{\underline{P}}] = \frac{1}{x_c p_c} [\hat{x}, \hat{p}] = \frac{i\hbar}{2\hbar} = \frac{i}{2}$$

$$\hat{H} = \hbar\omega (\hat{\underline{X}}^2 + \hat{\underline{P}}^2)$$

Now let $\hat{a} \equiv \hat{\underline{X}} + i\hat{\underline{P}}$ (non-Hermitian operator)

$$\hat{a}^\dagger = \hat{\underline{X}} - i\hat{\underline{P}}$$

(Quantum analog of α and α^*)

$$[\hat{a}, \hat{a}^\dagger] = [\hat{X} + i\hat{P}, \hat{X} - i\hat{P}]$$

$$= -i \underbrace{[\hat{X}, \hat{P}]}_{i/2} + i \underbrace{[\hat{P}, \hat{X}]}_{-i/2}$$

$$\Rightarrow \boxed{[\hat{a}, \hat{a}^\dagger] = 1}$$ "canonical commutation relation"

Let's express the Hamiltonian, $\hat{X}$, $\hat{P}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$

$$\hat{X} = \frac{\hat{a} + \hat{a}^\dagger}{2} \qquad \hat{P} = \frac{\hat{a} - \hat{a}^\dagger}{2i}$$

$$\Rightarrow \hat{X}^2 = \frac{1}{4}\left(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger\right)$$

$$\hat{P}^2 = \frac{1}{4}\left(-\hat{a}^2 - \hat{a}^{\dagger 2} + \hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger\right)$$

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

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

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

This is a form that is one of the most familiar in quantum mechanics

The "Number operator"

Let $\hat{N} \equiv \hat{a}^{+}\hat{a}$ (Quantum analog of $\alpha^{*}\alpha$)

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

$\Rightarrow$ Eigenvectors of $\hat{N}$ are the energy eigenvectors (stationary state)

Commutation relations:

$$[\hat{N}, \hat{a}] = [\hat{a}^{+}\hat{a}, \hat{a}] = \hat{a}^{+}\underbrace{[\hat{a}, \hat{a}]}_{=0} + \underbrace{[\hat{a}^{+}, \hat{a}]}_{=-1}\hat{a}$$

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

$$\therefore \boxed{\begin{aligned}[\hat{N}, \hat{a}] &= -\hat{a} \\ [\hat{N}, \hat{a}^{+}] &= +\hat{a}^{+}\end{aligned}}$$

(We will use these to find the energy eigenvalues algebraically)

Other properties of the number operator

$\hat{N}$ is Hermitian

(Aside $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$)

$\Rightarrow \hat{N}^\dagger = (\hat{a}^\dagger \hat{a})^\dagger = \hat{a}^\dagger (\hat{a}^\dagger)^\dagger = \hat{a}^\dagger \hat{a} = \hat{N}$

$\Rightarrow \hat{N}$ has real eigenvalues and orthogonal (if non degenerate) eigenvectors

$$\hat{N}|\lambda\rangle = \lambda|\lambda\rangle$$

$\uparrow$ real #

The eigenvalues are <u>positive</u> (non-negative)

Proof: Consider an arbitrary state

$$\langle\psi|\hat{N}|\psi\rangle = \langle\psi|\hat{a}^\dagger\hat{a}|\psi\rangle = \langle\phi|\phi\rangle$$

$$= \|\phi\|^2 \geq 0 \quad \text{where } |\phi\rangle = \hat{a}|\psi\rangle$$

$\Rightarrow \hat{N}$ is a "positive operator"

$\Rightarrow$ It's eigenvalues are <u>non-negative</u>

(see Homework)

$\Rightarrow$ Eigenvalues of $\hat{H} \geq \frac{\hbar\omega}{2}$ (zero point)