Time evolution of energy eigenkets (assume case (1): H is t-indep.)

Assume $\{|a\rangle\}$ is a complete basis of kets so that

$$H|a\rangle = E_a|a\rangle.$$

The time-evolution operator $\mathcal{U}(t,t_0)$ is

$$\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)} = \sum_a |a\rangle e^{-\frac{i}{\hbar}E_a(t-t_0)}\langle a|.$$

If $|\alpha, t_0{=}0\rangle = \sum C_a(0)\,|a\rangle$,

then $|\alpha, t_0{=}0; t\rangle = \sum C_a(t)\,|a\rangle$

where $C_a(t) = e^{-\frac{i}{\hbar}E_a t}\,C_a(0)$.

Note: only phases change under time-development, probability $|C_a(t)|^2$ of being in state $|a\rangle$ is unchanged.

Useful to find CSCO $A_1, \ldots A_k$ so that
$[A_1, H] = [A_2, H] = \cdots = [A_k, H] = 0$

so can find a basis $|a_1, \ldots, a_k\rangle$ of H eigenkets.

Heisenberg equation of motion

(A possibly t-dependent)

$$\frac{d}{dt} A_{(H)}(t) = \frac{\partial \mathcal{U}^+}{\partial t} A_{(S)} \mathcal{U} + \mathcal{U}^+ A_{(S)} \frac{\partial \mathcal{U}}{\partial t} + \mathcal{U}^+ \frac{\partial A_{(S)}}{\partial t} \mathcal{U}$$

$$= \frac{i}{\hbar} \mathcal{U}^+ H \underbrace{(\mathcal{U}\mathcal{U}^+)}_{\mathbb{1}} A_{(S)} \mathcal{U} - \frac{i}{\hbar} \mathcal{U}^+ A_{(S)} (\mathcal{U}\mathcal{U}^+) H \mathcal{U} + \mathcal{U}^+ \frac{\partial A_S}{\partial t} \mathcal{U}$$

if case (1) or (2), $\mathcal{U}^+ H \mathcal{U} = H$, so $H_{(H)} = H$,

$$\boxed{\frac{d}{dt} A_{(H)}(t) = \frac{1}{i\hbar} \left[A_{(H)}(t), H \right] + \overbrace{\dot{A}_{(H)}}^{\mathcal{U}^+ \frac{\partial A_{(S)}}{\partial t} \mathcal{U}}}$$

Vanishes if $A_{(S)}$ is t-independent.

Interaction picture

Sometimes useful to use a "split picture"

Consider $H = H_0 + V(t)$

H_0: time-independent; $V(t)$: time dependent

Interaction picture: remove H_0 evolution from state, as in Heisenberg.

$$|\alpha\rangle_{(H)} = e^{\frac{i}{\hbar} H t} |\alpha, t\rangle_{(S)}$$

$$|\alpha\rangle_{(I)} = e^{\frac{i}{\hbar} H_0 t} |\alpha, t\rangle_{(S)}$$

$$A_{(H)} = e^{\frac{i}{\hbar} H t} A_{(S)} e^{-\frac{i}{\hbar} H t}$$

$$A_{(I)} = e^{\frac{i}{\hbar} H_0 t} A_{(S)} e^{-\frac{i}{\hbar} H_0 t}$$

Equation of motion in interaction picture

$$i\hbar \frac{\partial}{\partial t} | \alpha, t\rangle_{(I)} = -H_0 e^{\frac{i}{\hbar}H_0 t} |\alpha,t\rangle_{(S)} + e^{\frac{i}{\hbar}H_0 t} (H_0+V) |\alpha,t\rangle_{(S)}$$

$$= \underbrace{e^{\frac{i}{\hbar}H_0 t} V e^{-\frac{i}{\hbar}H_0 t}}_{V_I} \underbrace{e^{\frac{i}{\hbar}H_0 t} |\alpha,t\rangle_{(S)}}_{|\alpha,t\rangle_{(I)}}$$

$$= V_I |\alpha,t\rangle_{(I)}.$$

So $\boxed{i\hbar \frac{\partial}{\partial t} |\alpha,t\rangle_{(I)} = V_I |\alpha,t\rangle_{(I)}}$ evolves with V.

$$\boxed{\frac{dA_{(I)}}{dt} = \frac{1}{i\hbar}[A_{(I)}, H_0] + \dot{A}_{(I)}}$$

evolves with H.

Summary:

	State	Operator
Schrödinger	evolves w/ H	const.
Heisenberg	constant	evolves w/ H
Interaction	evolves w/ $V_{(I)}$	evolves w/ H_0

Will return to this picture for time-dependent pert. thy.

Base kets & transition amplitudes

Schrödinger : State ket $|\psi(t)\rangle$ changes
Heisenberg : " " $|\psi\rangle$ doesn't change.

Schrödinger eqn: $i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_{(S)} = H |\psi(t)\rangle_{(S)}$ $\qquad |\psi(t)\rangle = \mathcal{U}(t,t_0)|\psi(t_0)\rangle$

Heisenberg eqn: $\frac{dA(t)}{dt} = \frac{1}{i\hbar}[A_{(H)}, H] + \dot{A}_{(H)}$ $\qquad A_H(t) = \mathcal{U}^\dagger(t,t_0) A_{(H)}(t_0)\, \mathcal{U}(t,t_0)$

Given a (time independent) operator A,
$(\dot{A} = 0)$

in Schrödinger picture ~~AP~~ states $|a'\rangle$ satisfying

$$A|a'\rangle = a'|a'\rangle$$

don't change in time.

Heisenberg:

$$A_H(t) = \mathcal{U}^\dagger A(0)\, \mathcal{U}$$

$$A_H(\mathcal{U}^\dagger|a'\rangle) = \mathcal{U}^\dagger A(0)|a'\rangle = a'(\mathcal{U}^\dagger|a'\rangle)$$

so $\quad |a',t\rangle_{(H)} = \mathcal{U}^\dagger|a'\rangle$

Base kets change in time in H. picture (Eigenvalues unchanged)

Two interpretations:

$$C_{a'} = \underbrace{\overbrace{\langle a'|}^{S:\ \text{base}}\ \mathcal{U}}_{H\ \ \text{base}}\ \overbrace{\mathcal{U}\,\underbrace{|\alpha, t=0\rangle}_{\text{state}}}^{\text{state}}$$

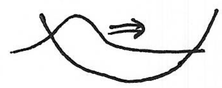
Transition amplitude if $A = a'$ at time $t = 0$, what is prob. $B = b'$ at time t

$$\Big|\underbrace{\overbrace{\langle b'|}^{S:\ \text{base}}\ \mathcal{U}(t,0)}_{H:\ \text{base}}\ \overbrace{\mathcal{U}(t,0)\,\underbrace{|a'\rangle}_{\text{state}}}^{\text{state}}\Big|^2$$

Energy – time uncertainty relation

Unlike x, t is not an operator, so no direct analog of $\Delta x \, \Delta p \geq \hbar/2$ $\quad (\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \hbar^2/4)$

Q: how rapidly does a state change form?



e.g. coherent state

Define $\quad C(t) = \langle \alpha | \mathcal{U}(t, t_0) | \alpha \rangle$

(Don't confuse w/ $C(t)$ from prob. 15 in bk)

If $|\alpha\rangle$ an eigenvector of H, $\quad |C(t)| = 1, \ \forall t.$
("stationary state")

Generally, $\quad |\alpha\rangle = \sum c_a |a\rangle$

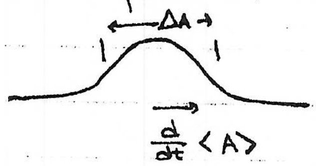
$$C(t) = \sum |c_a|^2 e^{-\frac{iE_a t}{\hbar}}$$

as t increases, generically $C(t)$ decreases.

(through $[A,H]$: not $\dot{A} = 0$)

Imagine measuring an observable A which changes in time
- use as clock (i.e., position of particle, hands of clock, ..)

Can measure $\quad \Delta T = \dfrac{\Delta A}{\frac{d}{dt}\langle A \rangle}$



$$\frac{d}{dt}\langle A \rangle = \frac{1}{i\hbar}\langle [A, H] \rangle$$

$$\langle \Delta A^2 \rangle \langle \Delta H^2 \rangle \geq \frac{1}{4} |\langle [A, H] \rangle|^2 = \frac{\hbar^2}{4} \left| \frac{d}{dt}\langle A \rangle \right|^2$$

So $\quad \dfrac{\langle \Delta A^2 \rangle}{\left|\frac{d}{dt}\langle A \rangle\right|^2} \langle \Delta H^2 \rangle \geq \hbar^2/4$

$$\boxed{\Delta T \, \Delta E \geq \hbar/2}$$

$\Delta E = \langle \Delta H^2 \rangle^{1/2}$

$\Delta T = \left(\langle \Delta A^2 \rangle \Big/ \left|\frac{d}{dt}\langle A \rangle\right|^2 \right)^{1/2}.$

Basic idea: if energy width is small, form of state ~~particle~~ takes a long time to change.

Interpretation of wavefunction ("probability fluid")

Start with Schrödinger picture for particle in 3D potential $\quad i\hbar \frac{\partial}{\partial t}\psi(\vec{x},t) = H\,\psi(\vec{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x},t) + V(\vec{x})\,\psi(\vec{x},t)$

Think about $\rho(x) = |\psi(x,t)|^2$ as probability density

[probability ($\vec{x} \in R) = \int_R |\psi(\vec{x}',t)|^2\, d^3x'$ $\quad R$]

Compute $\frac{\partial \rho}{\partial t}$ for $\rho(\vec{x},t)$ in 3D

$$\frac{\partial \rho}{\partial t} = \psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi$$

$$\left.\begin{aligned} \frac{\partial \psi}{\partial t} &= i\frac{\hbar}{2m}\nabla^2\psi - \frac{iV}{\hbar}\psi \\ \frac{\partial \psi^*}{\partial t} &= -\frac{i\hbar}{2m}\nabla^2\psi^* + \frac{iV}{\hbar}\psi^* \end{aligned}\right\} \text{cancel, since } V \text{ real}$$

$$\Rightarrow \frac{\partial \rho}{\partial t} = -\frac{i\hbar}{2m}\left[(\nabla^2\psi^*)\psi - \psi^*(\nabla^2\psi)\right]$$

$$= -\frac{i\hbar}{2m}\vec{\nabla}\cdot\left[(\vec{\nabla}\psi^*)\psi - \psi^*(\vec{\nabla}\psi)\right]$$

$$= -\vec{\nabla}\cdot\underbrace{\left[\frac{\hbar}{m}\mathrm{Im}(\psi^*\vec{\nabla}\psi)\right]}_{\vec{j}(\vec{x},t)}$$

"probability flux"

so $\boxed{\partial\rho/\partial t = -\vec{\nabla}\cdot\vec{j}(\vec{x},t)}$

continuity equation

$\vec{j}$ has natural interpretation as flux vector for probability.

$$\left(\frac{d}{dt}\int_V \rho\, dV = -\int_{\partial V}\vec{j}\cdot d\vec{A}\right)$$

$\vec{J}$ related to momentum

$$\int d^3\bar{x}\ j(\vec{x},t) = \frac{1}{m}\int \psi^*(\vec{x},t)\,(-i\hbar\vec{\nabla})\,\psi(\vec{x},t)$$

$$= \frac{1}{m}\langle\psi(t)|\ \vec{p}\ |\psi(t)\rangle$$

<u>Physical significance of phase</u>

write $\psi(\vec{x},t) = \sqrt{\rho(\vec{x},t)}\ e^{\frac{iS(\vec{x},t)}{\hbar}}$ ← phase

↑ amplitude

$$\psi^*\vec{\nabla}\psi = \frac{1}{2}\vec{\nabla}\rho + \frac{i}{\hbar}\rho\vec{\nabla}S$$

so $\vec{j}(\vec{x},t) = \frac{1}{m}\rho(\vec{x},t)\,\vec{\nabla}S(\bar{x},t)$

So: rate of variation of S controls flow of probability.
Faster phase variation ⟶ more prob. flow

Ex. stationary bound state: $\psi(\vec{x},t)$ has constant phase
(can choose real @ $t=0$)
⟶ no flow of probability

Ex. Plane wave $\psi(\vec{x},t) \sim e^{\frac{ipx}{\hbar} - \frac{iEt}{\hbar}}$

$$\vec{\nabla}S = \vec{p}$$

So $\frac{1}{m}\vec{\nabla}S$ is like velocity "$\vec{v}$"

$$\frac{\partial\rho}{\partial t} \sim \vec{\nabla}(\rho\,\text{"}\vec{v}\text{"}).$$

Suggestive, like fluid mechanics. Gives intuition, but not to be taken literally.

2.3 Connections between Classical & Quantum Mechanics

Review of Classical physics

3 Approaches:

A) Newton

EoM: $F = ma$

Ex. 1D SHO with potential $V(x) = \frac{1}{2} m\omega^2 x^2$

$$m\ddot{x} = -\frac{d}{dx} V(x) = -m\omega^2 x \qquad \left[= -kx, \ \omega = \sqrt{k/m}\right]$$

B) Hamiltonian

Phase space (x's & p's) with Poisson bracket

$$\{x^i, p_j\} = \delta^i{}_j \quad \text{(locally)}$$

Ham. function H

EoM: $\dot{q} = \{q, H\}$

Ex. SHO $\quad H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

$$\dot{x} = \{x, H\} = p/m$$
$$\dot{p} = \{p, H\} = -m\omega^2 x^2$$

c) Lagrangian (principle of least action)

Start with Lagrangian $\mathcal{L}(x^i, \dot{x}^i)$
[Related to Hamiltonian through $H = p_i \dot{x}^i - \mathcal{L}$]

Define Action $S[x(t)]$ as functional on space of paths

$$S = \int dt\, \mathcal{L}(x^i, \dot{x}^i)$$

Classical trajectory extremizes S

$\delta S = 0 \Rightarrow$ Euler - Lagrange equations

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}^i} - \frac{\partial \mathcal{L}}{\partial x^i} = 0$$

Ex. SHO

$$\mathcal{L} = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2$$

$$\frac{d}{dt} m\dot{x} + m\omega^2 x = 0$$

$$\Rightarrow \quad m\ddot{x} = -m\omega^2 x .$$

S Related to Hamilton's priciple function (as in WKB) through

$$S[x, t; x_0, t_0] = S[x_{class}(t)]$$

$$= \int_{t_0}^{t} dt\, \mathcal{L}(x^i, \dot{x}^i)$$ along classical trajectory from $t_0, x_0 \to x, \ldots$

Relating Classical & Quantum mechanics

A) Ehrenfest

Consider a particle in a 3D potential $V(\vec{x})$

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

$$= -\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{x})$$

Use Heisenberg equations to write $\langle \frac{d\vec{x}}{dt} \rangle$, $\langle \frac{d^2\vec{x}}{dt^2} \rangle$

$$\frac{d\vec{x}}{dt} = \frac{1}{i\hbar}[\vec{x}, H] = \frac{\vec{P}}{m}$$

so $\langle \frac{d\vec{x}}{dt} \rangle = \frac{1}{m}\langle \vec{p} \rangle$

$$\frac{d^2\vec{x}}{dt} = \frac{1}{i\hbar}\left[\frac{\vec{P}}{m}, V(x)\right] = -\frac{1}{m}\vec{\nabla}V(x).$$

So $\boxed{m\frac{d^2}{dt^2}\langle \vec{x} \rangle = \frac{d}{dt}\langle \vec{p} \rangle = -\langle \vec{\nabla} V(x) \rangle}$

Ehrenfest's theorem

Classical EOM emerges – note: no $\hbar$!

Generally, for any system described by classical physics, classical description can be derived from QM starting point.

Not all systems have classical limits (eg. 2-state system)