B) Quantization & Hamiltonian Mechanics

In principle, all quantum systems (not including gravity) described by Standard model (Quantum field theory)

Sometimes we want to "guess" underlying quantum system, given classical description: Quantization

Often, can be done by taking $\{\cdot, \cdot\} \longrightarrow [\cdot, \cdot]$ through

$$\{f, g\} = h \quad \Rightarrow \quad [F, G] = i\hbar H$$

For example, $\{x, p\} = 1 \quad \rightarrow \quad [X, P] = i\hbar \mathbb{1}$.

This program can encounter ambiguities due to Operator ordering problems.

Ex: $xp \neq px$, so how to quantize xp operator?

Can use Hermiticity as guideline

$\rightarrow \frac{1}{2}(xp + px)$ is Hermitian.

But this doesn't always work. Generally, need to try various possibilities.

$\left[\text{Ex. } x^2p^2 \xrightarrow{?} \frac{1}{2}[x^2p^2 + p^2x^2] = xp^2x \quad - \hbar^2\right]$

This trial & error process led to many correct QM models.

Quantization takes Hamiltonian EOM

$$\frac{d}{dt} q = \{q, H\}$$

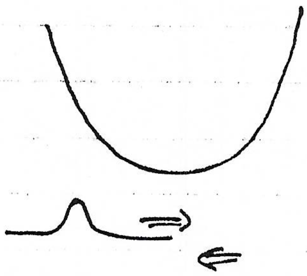
to Heisenberg EOM $\quad i\hbar \frac{d}{dt} A = [A, H]$

(This is why Ehrenfest works.)

Classical picture emerges from QM in limit $\hbar \to 0$.

Wavefunction "close to" eigenstate of all relevant classical operators

Particularly nice example: coherent states of SHO.
Retain shape, act like classical states



slosh back & forth.

c) WKB approximation

Quasi-classical approximation

$$\psi = \sqrt{\rho}\, e^{iS/\hbar}$$

Expand $\quad i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V(x)\psi = E\psi \quad$ in $\hbar$,

$O(1)$ terms:

$$-\frac{\partial S}{\partial t} = V + \frac{1}{2m}|\nabla S|^2 = H(\vec{q}, \nabla S, t)$$

(Hamilton-Jacobi eqn: satisfied by H. principal fn)
[another approach to classical mech - see eg wikipedia]

Look at a stationary state in 1D

$$\frac{1}{2m}(S')^2 = E - V$$

$$\Rightarrow \quad S(x) = \pm\int\sqrt{2m(E-V)}\,dx'$$

$$= \pm\int p\,dx \qquad\qquad p = \sqrt{2m(E-V)}$$

$O(\hbar)$ terms:

$$\frac{\partial \rho}{\partial t} = -\frac{1}{m}\frac{\partial}{\partial x}\left(\rho\frac{\partial S}{\partial x}\right) = 0 \qquad \text{(continuity eqn)}$$

$$= -\frac{1}{m}\frac{\partial}{\partial x}\left[\rho\sqrt{2m(E-V)}\right]$$

$$\Rightarrow \quad \rho = \frac{\text{const}}{\sqrt{2m(E-V)}} = \frac{C}{\sqrt{p}}$$

(physical interp: time spent in region w/ mom. p $\sim 1/p$ - agrees w/ classical intuition)

So for a stationary bound state

$$\psi(x) = \frac{C_1}{\sqrt{p}} e^{\frac{i}{\hbar}\int p\,dx} + \frac{C_2}{\sqrt{p}} e^{-\frac{i}{\hbar}\int p\,dx}$$

$$p = \sqrt{2m(E-V)}$$

This is <u>WKB approximation</u>

Valid when $\hbar S'' \ll (S')^2$

$$\Leftrightarrow \quad \left|\frac{d}{dx}\left(\frac{\hbar}{S'}\right)\right| \ll 1$$

$$\frac{d}{dx}\left(\frac{\hbar}{\sqrt{2m(E-V)}}\right) = \frac{2m\hbar\, V'(x)}{2(2m(E-V))^{3/2}}$$

so condition for validity is

$$\lambda\!\!\!^{-} = \frac{\hbar}{p} \ll \frac{2(E-V)}{V'}$$

distance over which V changes appreciabl

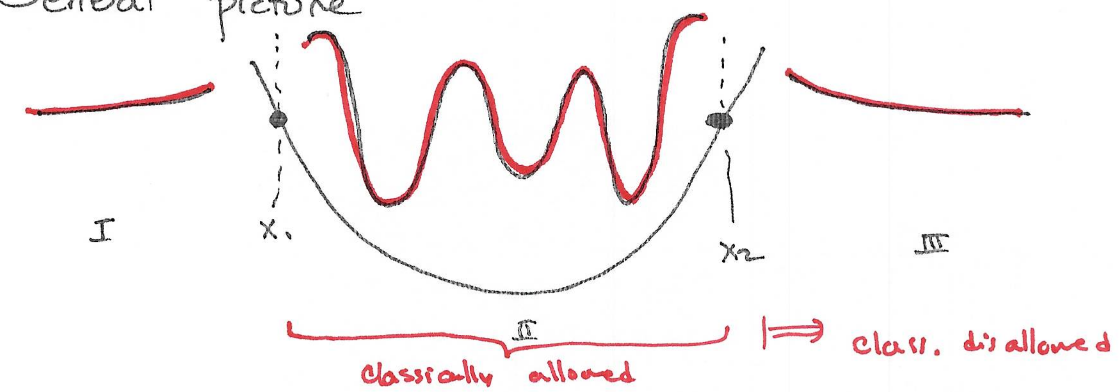
WKB valid in short wavelength limit,
<u>not</u> near $E = V(x)$ (classical turning points)

<u>Still</u> valid when $E < V(x)$ though

$$\psi(x) = \frac{C_\pm}{\sqrt[4]{2m(V-E)}} e^{\pm\frac{1}{\hbar}\int\sqrt{2m(V-E)}}$$

[only one term is valid – take exponential damping for bd. state]

General picture



know ψ in regions I, II, III,
must match behavior @ x_1, x_2

(like exact solution in  potential or

Region II:
$$\psi = \frac{C_1}{p^{1/2}} e^{\frac{i}{\hbar}\int_{x_2}^{x} p\,dx'} + \frac{C_2}{p^{1/2}} e^{-\frac{i}{\hbar}\int_{x_2}^{x} p\,dx'}$$

III:
$$\psi = \frac{C}{|p|^{1/2}} e^{-\frac{1}{\hbar}\int_{x_2}^{x} |p|\,dx'}$$

One approach: use exact solution near X_2: $V(x) \sim E + F(x-x_2)$

Airy functions $\Phi(x) \sim \int_0^\infty \cos(ux + \frac{1}{3}u^3)\,du \sim J_{\pm 1/3}\left(\frac{2}{3}|x|^{3/2}\right)$ II
$K_{1/3}\left(\frac{2}{3}x^{3/2}\right)$ III

using asymptotic behavior, match to ψ in regions II, III.

Clearer approach: analytic continuation in x plane, away from $x = x_2$

$$\psi^{(III)} = \frac{C}{\sqrt[4]{2mF(x-x_2)}} e^{-\frac{1}{\hbar}\int_{x_2}^{x}\sqrt{2mF(x'-x_2)}dx'}$$

$$= \frac{C}{\sqrt[4]{2mF(x-x_2)}} e^{-\frac{2}{3\hbar}\sqrt{2mF}(x-x_2)^{3/2}}$$

(defined for $x > x_2$)

say $x = x_2 + \hat{\rho}e^{i\phi} \Rightarrow (x-x_2)^{3/2} = \hat{\rho}^{3/2}e^{\frac{3}{2}i\phi}$

if $x = x_2 - \hat{\rho}$, take $\phi = \pi$, $(x-x_2)^{3/2} = \hat{\rho}^{3/2}(-i)$

so $\psi^{(III)} \longrightarrow \frac{Ce^{-i\pi/4}}{(2mF(x_2-x))^{1/4}} e^{\frac{2i}{3\hbar}\sqrt{2mF}(x_2-x)^{3/2}}$

(analytic cont. in UHP)

matches with C_2 term in $\psi^{(II)}$,

$$C_2 = Ce^{-i\pi/4}$$

similarly $C_1 = Ce^{i\pi/4}$ (analytic cont. in LHP)

so $$\psi^{(II)} = \frac{C}{(2mF(x_2-x))^{1/4}}\cos\left[-\frac{1}{\hbar}\int_x^{x_2}\sqrt{2mF(x_2-x')}\,dx' + \frac{\pi}{4}\right]$$

when

$$\psi^{(III)} = \frac{C}{(2mF(x-x_2))^{1/4}} e^{-\frac{1}{\hbar}\int_{x_2}^{x}\sqrt{2mF(x'-x_2)}dx'}$$

Using II/III & I/II overlaps,

$$\psi^{\text{inside}} = \frac{C}{(E-V)^{1/4}} \cos\left[-\frac{1}{\hbar}\int_x^{x_2} \sqrt{2m(E-V(x'))}\, dx' + \frac{\pi}{4}\right]$$

$$= \frac{C}{(E-V)^{1/4}} \cos\left[\frac{1}{\hbar}\int_{x_1}^{x} \sqrt{2m(E-V(x'))}\, dx' - \frac{\pi}{4}\right]$$

but wavefunction is unique, so

$$\boxed{\int_{x_1}^{x_2} dx' \sqrt{2m(E-V(x'))} = \left(n+\frac{1}{2}\right)\pi\hbar}$$

[like Bohr Sommerfeld ~~except~~ except ½]

WKB approximation for bound state energies.

Improves as $n \to \infty$. since $\cancel{\hbar} \to 0$

10/26/20 2.25

D) Path integral: alternative formulation of QM

Correlation function, e.g. $\langle x(t_2)\, x(t_1) \rangle$ [see HW 6]

Ham picture: $= \langle \psi(t_2) | \, x(t_2)\, e^{-\frac{i}{\hbar} H (t_2 - t_1)}\, x(t_1)\, | \psi(t_1) \rangle$

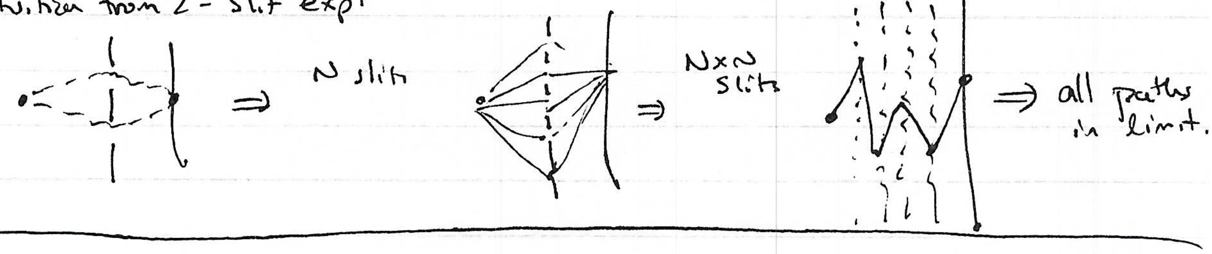
final state — initial state

PI picture $= \int \mathcal{D}[x(t)]\, e^{iS[x(t)]}\, x(t_2)\, x(t_1)$

action

path integral over all $x(t)$ given i,f BC's.
– ∞-dim $\int$! Definition requires care

Claim: pictures equivalent
- Useful technique, part. in QFT
- intuition from 2-slit expt



Propagators

Recall time-development

$$|\psi_a(t)\rangle = \sum_{a'} C_{a'}(t)\, |a'\rangle$$

$$C_{a'}(t) = e^{-\frac{i}{\hbar} E_{a'} (t - t_0)}\, C_{a'}(t_0)$$

For particle in 1D / 3D

If ~~$\langle x|a'\rangle$~~ $\langle x | a' \rangle = u_{a'}(x)$,

$$\psi(x,t) = \sum_{a'} e^{-\frac{i}{\hbar} E_{a'} (t - t_0)}\, C_{a'}(t_0)\, u_{a'}(x).$$

Can rewrite in terms of <u>propagator</u>

$$\psi(x,t) = \int dx' \, K(x,t;x',t_0)\, \psi(x',t_0)$$

where

$$K(x,t;x',t_0) = \langle x | \mathcal{U}(t,t_0) | x' \rangle$$

$$= \sum_{a'} \langle x | a' \rangle e^{-\frac{i}{\hbar} E_{a'}(t-t_0)} \langle a' | x' \rangle$$

[often use <u>retarded</u> propagator $K_{ret} = K\,\theta(t-t_0)$ s.t. $K_{ret}(x,t;x',t_0) = 0$ if $t < t_0$]

K is <u>Green's function</u> for Schrödinger equation

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - V(x) \right] K(x,t;x',t_0) = 0,$$

$$\lim_{t \to t_0} K(x,t;x',t_0) = \delta^3(x-x')$$

for K_{ret}: $\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - V(x) \right] K_{ret}(x,t;x',t_0) = i\hbar\,\delta^3(x-x')\,\delta(t-t_0)$

Think of K_{ret} as solution to Schrödinger with a δ-function source.
K is solution to " w/ no source, $= \delta(x-x')$ @ $t = t_0$

In Heisenberg language,

$$K(x,t;x'_0,t_0) = \langle x,t | x',t_0 \rangle_{(H)}$$

<u>Examples of propagator:</u>

1D free particle. $\quad H|p\rangle = \frac{p^2}{2m}|p\rangle$

$$K(x,t;x',t_0) = \int dp \, \langle x|p\rangle e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t-t_0)} \langle p|x'\rangle$$

$$= \frac{1}{2\pi\hbar} \int dp \, e^{-\frac{ip^2}{2m\hbar}(t-t_0) + \frac{ip(x-x')}{\hbar}}$$

$$= \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\; e^{\frac{im}{2\hbar}\frac{(x-x')^2}{(t-t_0)}}$$

[Phys. interp: from $\delta(x)$, so all p $\Rightarrow$ uniform in space. large $\Delta x \rightarrow$ large ∇S, p]

SHO: derive K in homework.

Properties of K:

Quantum stat. mech.

Define $G(t) = \int d^3x \; K(x,t;x,t_0)$

$$= \sum_{a'} e^{-\frac{iE_{a'}t}{\hbar}}$$

set $t = -i\hbar\beta$,

$$G(-i\hbar\beta) = Z = \sum_{a'} e^{-\beta E_{a'}}$$

(Related to QMC)

stat. mech. partition function $\beta \sim \frac{1}{T}$

Fourier transform.

Define $\tilde{G}(E) = -i\int dt \; G(t) \, e^{\frac{iEt}{\hbar}}$

$$= -i\sum_{a'} \int_0^\infty dt \; e^{\frac{i(E-E_{a'})t}{\hbar}}$$

For convergence, take $E + i\varepsilon$

$$\tilde{G}(E+i\varepsilon) = \sum_{a'} \frac{\hbar}{E - E_{a'} + i\varepsilon}$$

poles in limit $\varepsilon \to 0$ describe energy spectrum.

Density of states

$$\rho(E) = \sum_\alpha \delta(E - E_\alpha) \quad \text{for discrete spectrum.}$$

$$\pi\delta(E-E') = \lim_{\varepsilon\to 0} \frac{\varepsilon}{(E-E')^2+\varepsilon^2} = -\lim_{\varepsilon\to 0} \mathrm{Im} \frac{1}{E-E'+i\varepsilon}$$

so $$\rho_\varepsilon(E) = \frac{-1}{\pi\hbar} \mathrm{Im}\, \tilde{G}(E+i\varepsilon)$$

is regulated state density.

Path integrals

Note composition property of K:

$$K(x,t;x',t_0) = \int d\tilde{x}\; K(x,t;\tilde{x},\tilde{t})\, K(\tilde{x},\tilde{t};x',t_0)$$

[valid for K_{ret} for $t_0 < \hat{t} < t$]

(follow from $U(t,\hat{t})\,U(\hat{t},t_0) = U(t,t_0)$)

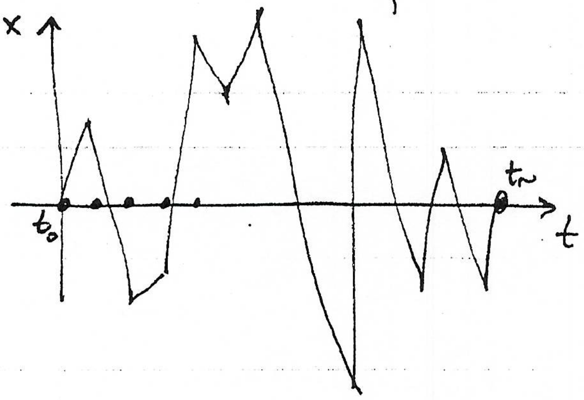
Break $t-t_0$ into N equal time intervals

$$\Delta t = \frac{t-t_0}{N}$$

$$t_k = t_0 + k\Delta t$$
$$t_N = t$$

then $$K(x_N,t_N;x_0,t_0) = \int \prod_{k=1}^{N-1} dx_k\, K(x_N,t_N;x_{N-1},t_{N-1}) \cdot K(x_{N-1},t_{N-1};x_{N-2},t_{N-2}) \cdots K(x_1,t_1;x_0,t_0)$$

so final answer includes all paths



Feynman proposed:

$$K(x'',t;x',t_0) = \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]}$$

where $\mathcal{D}[x(t)]$ is a measure on the space of paths with $x(t_0) = x'$, $x(t) = x''$.

- Clearly obeys composition rule
- Simple connection to classical physics — phases cancel except near stationary point $\delta S = 0$.

To make rigorous, must define measure on path space [Wiener measure, etc... [now used in economics/finance, etc.]]

Plan: start from definition of K.
"Derive" PI & appropriate measure,
go back & rederive K for free particle