2. Time evolution (Quantum dynamics)

2.1 Time evolution & the Schrödinger equation

Time in QM is a parameter ($|\psi(t)\rangle \in \mathcal{H}$),
not an observable like X.

Note: SR relates x, t; restored in relativistic QFT, where x is no longer an observable.

Question: how does a state $|\psi(t)\rangle$ evolve in time?

Postulate (Schrödinger eqn.)

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

Write ~~In~~ terms of time-evolution operator $\mathcal{U}(t, t_0)$;

If state at time t_0, $|\alpha, t_0\rangle \in \mathcal{H}$
becomes at time t $|\alpha, t_0; t\rangle \in \mathcal{H}$,

write $|\alpha, t_0; t\rangle = \mathcal{U}(t, t_0) |\alpha, t_0\rangle$.

Properties of $\mathcal{U}(t, t_0)$:

i) Unitary - conserves probability, norm

$$\boxed{\mathcal{U}^{+}(t, t_0)\, \mathcal{U}(t, t_0) = \mathbb{1}}$$

$$\langle \alpha, t_0; t | \alpha, t_0; t\rangle = \langle \alpha, t_0 | \mathcal{U}^{+}(t, t_0)\, \mathcal{U}(t, t_0) | \alpha, t_0\rangle$$
$$= \langle \alpha, t_0 | \alpha, t_0\rangle .$$

ii) composition law

$$\boxed{\mathcal{U}(t,t_1)\,\mathcal{U}(t_1,t_0) = \mathcal{U}(t,t_0)}$$

$$|\alpha,t_0;t\rangle = \mathcal{U}(t,t_1)\,|\alpha,t_0;t_1\rangle$$

$$= \mathcal{U}(t,t_1)\,\mathcal{U}(t_1,t_0)\,|\alpha,t_0\rangle.$$
$$= \mathcal{U}(t,t_0)\,|\alpha,t_0\rangle$$

iii) identity at $t=t_0$

$$\boxed{\lim_{t\to t_0}\mathcal{U}(t,t_0) = \mathbb{1}} \quad \text{since } \lim_{t\to t_0}|\alpha,t_0;t\rangle = |\alpha,t_0\rangle.$$

Properties i) — iii) satisfied when infinitesimal form is

$$\mathcal{U}(t_0+dt,\,t_0) = 1 - \frac{iH(t_0)dt}{\hbar}$$

(equivalent to Schrödinger.)

Appearance of $\hbar$ — needed on dimensional grounds.
— discuss further in context of classical – quantum correspondence

Schrödinger for $\mathcal{U}(t,t_0)$

$$\boxed{i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0) = H(t)\,\mathcal{U}(t,t_0)} \qquad (*)$$

$$i\hbar\frac{\partial}{\partial t}|\alpha,t_0;t\rangle = i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0)\,|\alpha,t_0\rangle$$

$$= H(t)\,\mathcal{U}(t,t_0)\,|\alpha,t_0\rangle$$

$$= H(t)\,|\alpha,t_0;t\rangle$$

Solutions of (*).

1) Time-independent $H(t) = H$

$$\lim_{N\to\infty}\left[1 - \frac{i}{\hbar} H \frac{(t-t_0)}{N}\right]^N = e^{-\frac{iH}{\hbar}(t-t_0)}$$

so

$$\boxed{\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}}$$

(can easily verify solves $i\hbar \frac{d}{dt}\mathcal{U}(t,t_0) = H\,\mathcal{U}(t,t_0)$).

2) Time-dependent, but $[H(t), H(t')] = 0$.

(Ex: particle in magnetic field, constant direction, vary'ing strength
$H = \frac{p^2}{2m} + B(t) S_z$)

similar solution but now

$$\boxed{\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'}}$$

verify: $i\hbar\frac{d}{dt}\mathcal{U}(t,t_0) = \frac{d}{dt}\left[\int_{t_0}^{t} H(t')dt'\right]\mathcal{U}(t,t_0)$

$= H(t)\,\mathcal{U}(t,t_0)$

3) Time-dependent $H(t)$, $[H(t), H(t')] \neq \emptyset$.

(Ex: particle in B field, direction changes in time.)

Solve iteratively

$$\int_{t_0}^{t} dt' \left[\frac{d}{dt'} \mathcal{U}(t', t_0) \right] = -\frac{i}{\hbar} \int_{t_0}^{t} dt' \, H(t') \, \mathcal{U}(t', t_0)$$

$$\Rightarrow \quad \mathcal{U}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, H(t') \, \mathcal{U}(t', t_0)$$

defines $\mathcal{U}(t,t_0)$ in terms of $\mathcal{U}(t',t_0)$, $t' \leq t$.

iterating:

$$\mathcal{U}(t,t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, H(t')$$

$$+ \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt^{(1)} \int_{t_0}^{t^{(1)}} dt^{(2)} \, H(t^{(1)}) H(t^{(2)}) \, \mathcal{U}(t^{(2)}, t_0)$$

$$\vdots$$

$$= 1 + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n \, H(t_1) \cdots H(t_n)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n T\left(\int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n \, H(t_1) H(t_2) \cdots H(t_n) \right)$$

(<u>Dyson series</u>)

where T is time-ordering operator - orders following ops so time goes up to left.

can write answer in compact form

$$\boxed{\mathcal{U}(t,t_0) = T\left[e^{-\frac{i}{\hbar} \int_{t_0}^{t} dt' \, H(t')} \right]}$$

(looks same as (2), but T carries extra info above)

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.

2.2 Schrödinger, Heisenberg, & interaction pictures

Previous discussion used Schrödinger picture:
$|\alpha, t_0; t\rangle \in \mathcal{H}$ evolves in time, operators fixed.

Two ways to view expectation values:

Schrödinger:

$$\langle A\rangle = \langle \alpha, t | A | \alpha, t\rangle = \overbrace{\langle \alpha, 0| \mathcal{U}^\dagger(t,0)}^{\langle\alpha,t|_{(S)}}\ \overbrace{A}^{A_{(S)}}\ \overbrace{\mathcal{U}(t,0)|\alpha,0\rangle}^{|\alpha,t\rangle_{(S)}}$$

Heisenberg

$$\underbrace{\langle \alpha, 0|}_{\langle\alpha|_{(H)}}\ \underbrace{\mathcal{U}^\dagger(t,0)\, A\, \mathcal{U}(t,0)}_{A_{(H)}}\ \underbrace{|\alpha,0\rangle}_{|\alpha\rangle_{(H)}}$$

Heisenberg picture: operators evolve in time, state fixed

Same physics - different formalism.

Convention: set equal at $t=0$

$$|\alpha, 0\rangle_{(S)} = |\alpha\rangle_{(H)} \qquad A_{(H)}(0) = A_{(S)}$$

then

$$|\alpha, t\rangle_{(S)} = \mathcal{U}(t,t_0)\,|\alpha\rangle_{(H)} \qquad A_H(t) = \mathcal{U}^\dagger(t,0)\, A_{(S)}\, \mathcal{U}(t,0)$$

If H time-independent,

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

Heisenberg equation of motion ~~At time-independent~~ (A possibly t-dependent)

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

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

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

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

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 $\qquad V(t)$: time dependent

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

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

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

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

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

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

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

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

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

don't change in time.

Heisenberg:

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

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

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

<u>Base kets change in time in H. picture</u> (Eigenvalues unchanged)

Two interpretations:

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

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

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

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?

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")

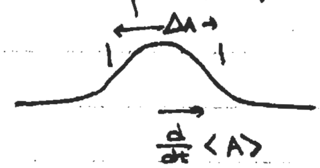
Generally, $\quad |\alpha\rangle = \sum c_a |a\rangle$

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

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

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

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



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

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

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.

<u>Interpretation of wavefunction</u> ("probability fluid")

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

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

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

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

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

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

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

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

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

"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

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

<u>Physical significance of phase</u>

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

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

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

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

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

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 principle 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 $V(\vec{x})$

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

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

Use Heisenberg equation 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)

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: $\quad Xp \neq pX,\quad$ so how to quantize Xp operator?

Can use Hermiticity as guideline

$$\rightarrow \tfrac{1}{2}(xp + px) \quad \text{is Hermitian.}$$

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

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

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

Quantization takes Hamiltonian EOM

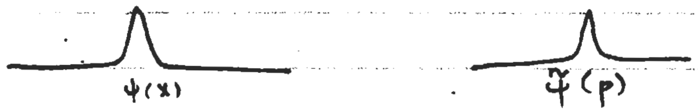
$$\frac{d}{dt} q = \{q, H\}$$

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

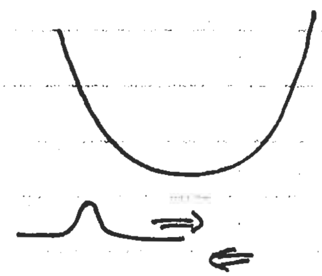
(This is why Ehrenfest works.)

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.

[⇒ C1) WKB]

C2) Propagators & path integrals

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

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

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.o.

[convention: $K_{ret}(x,t;x',t_0) = 0$ if ~~$t \geq t_0$~~ $t < t_0$]

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 $\Delta x \to$ large ∇S, consistent w/ large p.]

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 $\hbar$.

$\mathcal{O}(1)$ terms:

$$-\frac{\partial S}{\partial t} = V + \frac{1}{2m}|\nabla S|^2$$

(Hamilton-Jacobi eqn: satisfied by H. principal fn.)

Look at a stationary state in 1D

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

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

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

$\mathcal{O}(\hbar)$ terms:

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

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

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

(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 WKB approximation

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

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

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

so condition for validity is

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

distance over which V changes appreciably.

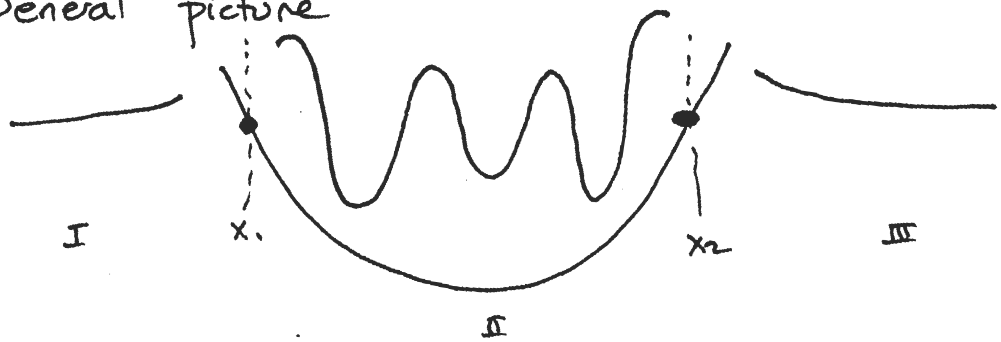
WKB valid in short wavelength limit.
not near $E = V(x)$ (classical turning points)

Still valid when $E < V(x)$ though

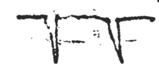
$$\psi(x) = \frac{c_\pm}{\sqrt{2m(V-E)}} e^{\pm\frac{1}{\hbar}\int\sqrt{2m(V-E)}}$$

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

General picture



know ψ in regions I, II, III,
must match behaviour @ 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 $$\Phi(x) \sim \int_0^\infty \cos\left(ux + \tfrac{1}{3}u^3\right) du \sim \begin{array}{ll} J_{\pm 1/3}\left(\tfrac{2}{3}|x|^{3/2}\right) & \text{II} \\ K_{1/3}\left(\tfrac{2}{3}x^{3/2}\right) & \text{III} \end{array}$$

using asymptotic behaviour, match to ψ in regions II, III

Clearer approach: analytic continuation in x plane, away from x

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

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

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

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

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

(analytic cont. in UHP)

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

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

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

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

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

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

[like Bohr-Sommerfeld except ½]

WKB approximation for bound state energies.

Improves as $n \to \infty$, since $\lambda \to 0$

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

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

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

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

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

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

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 $t_0 < \tilde{t} < t$]

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

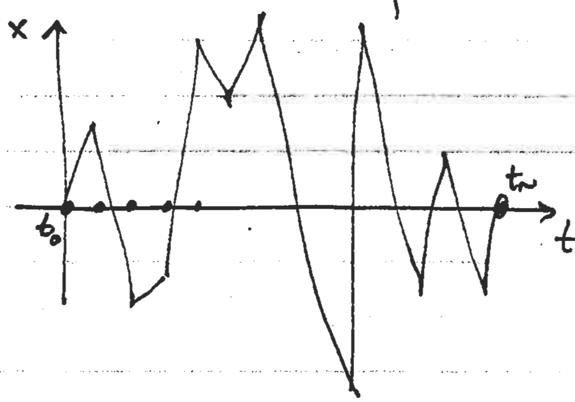
Break $t - t_0$ into N equal time intervals

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

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

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

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

$$= \int \prod_{k=1}^{N-1} dx_k \, \langle x_N | e^{-\frac{i\varepsilon}{\hbar} H} | x_{N-1} \rangle \langle x_{N-1} | e^{-\frac{i\varepsilon}{\hbar} H} | x_{N-2} \rangle \cdots \langle x_1 | e^{-\frac{i\varepsilon}{\hbar} H} | x_0 \rangle$$

$[\varepsilon = \Delta t]$

Note: easy to include t-dependent H, time ordering works out automatically but will ignore for clarity.

write

$$\langle x_k | e^{-\frac{i\varepsilon}{\hbar} H(p,x)} | x_{k-1} \rangle = \int dp_k \, \langle x_k | p_k \rangle \langle p_k | e^{-\frac{i\varepsilon}{\hbar} H(p,x)} | x_{k-1} \rangle$$

Introduce notation: <u>Normal ordering.</u>

$\mathcal{O}(p,x)$ is a normal-ordered operator if p's on left, x's on right.
[often use NO notation for a^+, a's]

Ex. $H = \frac{p^2}{2m} + V(x)$ is normal ordered.

Write $:\mathcal{O}(p,x):$ for normal-ordered form of $\mathcal{O}$.

Ex. $xp = px + i\hbar = :xp: + i\hbar$

$\cancel{:xp: = px + i\hbar = xp - i\hbar}$

[normal ordering introduces commutators]

Ex: $H = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{x})\right)^2$ [particle in EM field]

$$H = \frac{1}{2m}\left(\vec{p}^{\,2} - \frac{e}{c}[\vec{p}\cdot\vec{A}(x) + \vec{A}(x)\cdot\vec{p}] + \frac{e^2}{c^2}\vec{A}^2(x)\right)$$

$$= \; :H: \; - \frac{ie}{c}\vec{\nabla}\cdot\vec{A}(x)$$

would like $e^{-\frac{i\varepsilon}{\hbar}H(p,x)}$ to be normal ordered.

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

$$e^{-\frac{i\varepsilon}{\hbar}H(p,x)} = 1 - \frac{i\varepsilon}{\hbar}\left[\frac{p^2}{2m} + V(x)\right]$$
$$- \frac{\varepsilon^2}{2\hbar^2}\left[\left(\frac{p^2}{2m}\right)^2 + \frac{p^2}{2m}V(x) + V(x)\frac{p^2}{2m} + V(x)^2\right]$$

$$= :e^{-\frac{i\varepsilon}{\hbar}H(p,x)}: \underbrace{- \frac{\varepsilon^2}{2\hbar^2}\left[V(x), \frac{p^2}{2m}\right]}_{-\frac{\varepsilon^2}{4m}\left[2\frac{i}{\hbar}V'(x)p - V''(x)\right]}$$

Generally, if $H(p,x)$ is normal-ordered,

$$e^{-\frac{i\varepsilon}{\hbar}H(p,x)} = :e^{-\frac{i\varepsilon}{\hbar}H(p,x)}: + \mathcal{O}(\varepsilon^2).$$

as $\Delta t \to 0$, replace $e^{-\frac{i\varepsilon}{\hbar}H(p,x)} \longrightarrow :e^{-\frac{i\varepsilon}{\hbar}H(p,x)}:$

so
$$\int dp_k \langle x_k | p_k \rangle \langle p_k | e^{-\frac{i\varepsilon}{\hbar}H(p,x)} | x_{k-1} \rangle$$

becomes

$$\int dp_k \left(\frac{1}{2\pi\hbar}\right) e^{\frac{i}{\hbar}p_k(x_k - x_{k-1}) - \frac{i\varepsilon}{\hbar}H(p_k, x_{k-1})} + \mathcal{O}(\varepsilon^2)$$

so
$$K(x_N, t_N; x_0, t_0) \approx \int \left(\prod_{k=1}^{N-1} dx \prod_{k=1}^{N} \frac{dp_k}{2\pi\hbar}\right) e^{\sum_{k=1}^{N}\left[\frac{i}{\hbar}p_k(x_k - x_{k-1}) - \frac{i\varepsilon}{\hbar}H(p_k, x_{k-1})\right]}$$

Replacing $\frac{x_k - x_{k-1}}{\varepsilon} \longrightarrow \dot{x}$

$$\sum_k \varepsilon f_k \longrightarrow \int dt\, f(t)$$

$$\left(\prod_{k=1}^{N-1} dx_k\right)\left(\prod_{k=1}^{N} \frac{dp_k}{2\pi\hbar}\right) \longrightarrow \mathcal{D}[x(t)]\,\mathcal{D}[p(t)]$$

[Functional measure defined by limit]

gives phase space form of path integral:

$$\boxed{K(x_N, t_N; x_0, t_0) = \int \mathcal{D}[x(t)]\mathcal{D}[p(t)]\, e^{\frac{i}{\hbar}\int dt\left[p(t)\dot{x}(t) - H(p(t), x(t))\right]}}\ .$$

Lagrangian form of PI

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

$$\frac{1}{2\pi\hbar}\int dp_k\, e^{\frac{i}{\hbar}p_k(x_k - x_{k-1}) - \frac{i\varepsilon}{\hbar}H(p_k, x_{k-1})}$$

$$= \frac{1}{2\pi\hbar}\int dp_k\, e^{\frac{-i\varepsilon}{2m\hbar}\left[\left(p_k - \frac{m}{\varepsilon}(x_k - x_{k-1})\right)^2 - \frac{m^2}{\varepsilon^2}(x_k - x_{k-1})^2\right] - \frac{i\varepsilon}{\hbar}V(x_{k-1})}$$

$\int e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}$

$$= \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\, e^{+\frac{im}{2\hbar\varepsilon}(x_k - x_{k-1})^2 - \frac{i\varepsilon}{\hbar}V(x_{k-1})}$$

so

$$K(x,t;x_0,t_0) \approx \underbrace{\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2}\int\prod_{k=1}^{N-1} dx_k}_{\mathcal{D}[x(t)]}\, e^{\sum_{k=0}^{N}\, -\frac{i\varepsilon}{\hbar}V(x_{k-1}) + \frac{im}{2\hbar\varepsilon}(x_k - x_{k-1})^2}$$

$$K(x,t;x_0,t_0) = \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar}\int dt\left[\frac{1}{2}m\dot{x}(t)^2 - V(x)\right]}$$

$$= \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar}\int dt\, \mathcal{L}(x(t),\dot{x}(t))}$$

$$= \boxed{\int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar}S[x(t)]}}\,.$$

Check formalism: Calculate free particle prop explicitly

Choose $N = 2^A$ for simplicity

Calc. $$K_N = \left(\frac{mN}{2\pi i\hbar t}\right)^{N/2}\int \prod_{k=1}^{N-1} dx_k\, e^{\sum_k \frac{imN}{2\hbar t}(x_k - x_{k-1})^2}$$

Exponent is $$\frac{imN}{2\hbar t}\Big[x_0^2 + 2x_1^2 + 2x_2^2 + \dots + 2x_{N-1}^2 + x_N^2$$
$$-2x_0x_1 - 2x_1x_2 \cdots - 2x_{N-1}x_N\Big]$$

Do odd integrals first

$\int \prod_{n=1}^{N/2} dx_{2n}$

$$K_N = \prod_{\substack{k\ \mathrm{odd}\\ k=1}}^{N-1}\left[\left(\frac{m2^A}{2\pi i\hbar t}\right)\int \underset{(k\ \mathrm{odd})}{dx_k}\, e^{\frac{im2^A}{2\hbar t}\underbrace{\left(2x_k^2 + x_{k-1}^2 + x_{k+1}^2 - 2x_k(x_{k-1}+x_{k+1})\right)}_{\left[2\{x_k - \frac{1}{2}(x_{k-1}+x_{k+1})\}^2 + \frac{1}{2}x_{k-1}^2 + \frac{1}{2}x_{k+1}^2 - x_{k-1}x_{k+1}\right]}}\right.$$

$$= \left(\frac{m2^{A-1}}{2\pi i\hbar t}\right)^{2^{A-2}}\int \prod_{n=1}^{2^{A-1}-1} dx_{2n}\, e^{\sum_n^{2^{A-1}} \frac{im2^{A-1}}{2\hbar t}(x_{2n} - x_{2n-2})^2}$$

$$= K_{N/2}\,.$$

So by induction,

$$K_N = K_1 = \sqrt{\frac{m}{2\pi i\hbar t}}\, e^{\frac{im}{2\hbar t}(X_N - X_0)^2}$$

$$= K(X_N, t;\, X_0, 0)$$ as promized [Exactly].

Feynman path integral approach:

- Alternative formulation of quantum theories.
- Requires classical action $S[x(t)]$ as starting point.
- Requires definition of measure $\mathcal{D}[x(t)]$
- Not practical for most QM calculations
- Highly useful in formulating quantum field theory ("Feynman diagrams")
- Avoids conceptual problems of Hamiltonian formalism of QM.

→ Not a "realist" approach: no $|\psi(t)\rangle$, can replace by correlation function $\int e^{iS/\hbar}\, \mathcal{O}(t_2)\mathcal{O}(t_1)$

→ Thus, no collapse of wavefunction.

Stationary phase

Given a function $g(x)$, so $\frac{dg}{dx}(x_c) = 0$ at a unique $x = x_c$.

consider $\int dx\, e^{\frac{i}{\varepsilon} g(x)}$, ε small.

$$g(x) = g(x_c) + \frac{1}{2} g''(x_c)(x - x_c)^2 + \frac{1}{6} g'''(x_c)(x - x_c)^3 + \dots$$

$$\int dx\, e^{\frac{i}{\varepsilon} g(x)} = e^{\frac{i}{\varepsilon} g(x_c)} \sqrt{\frac{2\pi i \varepsilon}{g''(x_c)}} \left[1 + O(\varepsilon^2) \right]$$

Integral dominated by part near x_c.

Similarly, $\int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]}$

dominated by x_{class} where $\frac{\delta S}{\delta x}[x_{class}] = 0$.

$$\text{so } K(x,t;x_0,t_0) \cong e^{iS[x_{class}(t)]/\hbar}$$

$$\cong e^{iS(x,t;x_0,t_0)/\hbar}$$

For free particle, $S(x,t;x_0,t_0) = \frac{m(x-x_0)^2}{2(t-t_0)}$,

so this is exactly right.

2.4 Quantum particles in potentials and EM fields

Potentials

In Classical & Quantum mech, shifing potential by overall constant

$$V \to V + V_0$$

has no effect on measurable quantities

Classical: EOM all involve derivatives of V

Newtonian: $F = m - \nabla V$
Hamiltonian: $\{p, V(x)\}$ involves $\partial V / \partial x$
Lagrangian: S shifts by $\int V_0(t)\,dt$, no effect on δS.

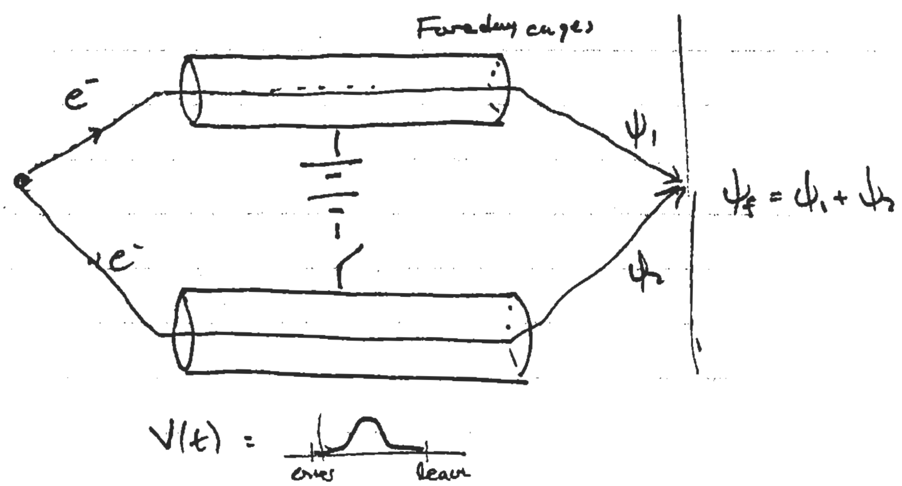
Quantum: $H \to H + V_0 \Rightarrow$

$$|\psi(t)\rangle \Rightarrow e^{-\frac{i}{\hbar}\int V_0 dt} |\psi(t)\rangle$$

Overall phase $e^{i\theta}$ not observable.

since in expansion $|\psi\rangle = \sum c_a |a\rangle$,
just changes $c_a \Rightarrow e^{i\theta} c_a$.

Changing potential in one region is observable



without V, by superposition

$$\psi_f = \psi_1 + \psi_2$$

with V, $\quad \psi_f = \left(e^{-\frac{i}{\hbar}\int V(t)\,dt}\,\psi_1 + \psi_2\right)$

gives phase difference, changes interference pattern.

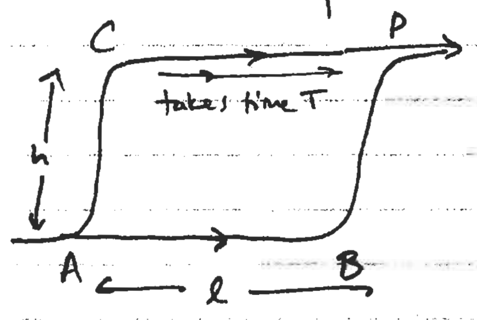
No effect in classical limit $\hbar \to 0$.

Note: no fields introduced in region with particles (!)
[this is a variation of Aharanov - Bohm]

<u>Example</u>: Gravity Induced quantum interference

- No quantum theory of gravity
- Hard to see quantum effects where gravity is relevant (Gravity $\sim 10^{-39}\times$ as strong as EM forces (e N vs e p⁺))

Possible to see quantum effect through phase difference

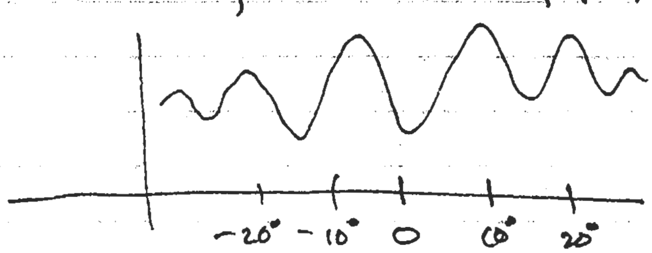


paths ABD vs. ACD:

$$\delta V = mgh$$

Phase difference: $e^{\frac{i}{\hbar} mghT}$

Interference seen using neutrons following loops rotated @ angle δ from horizontal



Colella, Overhauser, Werner
1975

Particles in EM fields

Recall Electromagnetism:

Fields $F_{\mu\nu} = \partial_{[\mu} A_{\nu]} = \partial_\mu A_\nu - \partial_\nu A_\mu$.

A_μ is 4-vector potential, $A_\mu = (-\phi, \vec{A})$

$(x^\mu = (ct, \vec{x}))$

$$F_{0i} = -F_{i0} = -E_i \qquad (i = 1,2,3)$$

$$F_{ij} = \varepsilon_{ijk} B^k$$

(Einstein summation convention)

or

$$E_i = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \frac{\partial \phi}{\partial x^i}$$

$$B^i = \varepsilon^{ijk}\partial_j A_k$$

<u>Gauge invariance</u>: $A_\mu \to A_\mu + \partial_\mu \Lambda$

leaves $F_{\mu\nu}$, thence E & B unchanged.

Lagrangian for charged particle in EM field is

Relativistic: $S = -m \int d\tau \sqrt{\frac{dx^\mu}{d\tau}\frac{dx_\mu}{d\tau}} + \underbrace{\frac{e}{c}\int d\tau\, A_\mu\, dx^\mu/d\tau}$

note: δ is total derivative under $\delta A_\mu = \partial_\mu \Lambda$.

Nonrelativistic: $\mathcal{L} = \frac{m}{2}\dot{x}^2 + \frac{e}{c} A_i \dot{x}^i - e\phi$

Going to Hamiltonian formalism:

<u>canonical momentum</u> $p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}^i} = m\dot{x} + \frac{e}{c}A^i$

$$\mathcal{H} = p_i \dot{x}^i - \mathcal{L}$$

$$= \frac{m}{2}\dot{x}^2 + e\phi$$

$$\boxed{\mathcal{H} = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + e\phi}$$

Classical Poisson bracket: $\{x^i, p_j\} = \delta^i{}_j$
($\underline{p \text{ canonical momentum}}$)

Quantization:

$$x^i \longrightarrow \hat{x}^i$$

$$p_j \longrightarrow \hat{p}_j = -i\hbar \frac{\partial}{\partial x^i}$$

(note: p, not $m\dot{x}$ here)

$$H \longrightarrow \frac{p^2}{2m} - \frac{e}{2mc}(A\cdot p + p\cdot A) + \frac{e^2}{2mc^2} A^2 + e\phi.$$

Ehrenfest:

$$m \frac{d^2}{dt^2}\langle \vec{x} \rangle = \frac{d}{dt}\langle \vec{p} \rangle = \frac{1}{i\hbar}\langle [\vec{p}, H] \rangle$$

$$\Rightarrow \quad m \frac{d^2}{dt^2}\langle \vec{x}\rangle = \left\langle \vec{E}e + \frac{e}{2c}\left(\frac{d\vec{x}}{dt}\times\vec{B} - \vec{B}\times\frac{d\vec{x}}{dt}\right)\right\rangle$$

(Lorentz force law)

Gauge invariance of QM

Under a gauge transform, $A_\mu \to A_\mu + \partial_\mu \Lambda$

Classically, canonical momentum $p_i = m\dot{x}^i - \frac{e}{c}A^i$ changes.
x^i, $\dot{x}^i$ remain fixed.

QM:

Schrödinger $\quad i\hbar \frac{\partial}{\partial t}\psi(\vec{x},t) = \left[\frac{1}{2m}\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 + e\phi\right]\psi(\vec{x},t)$

Take $\quad \vec{A}' = \vec{A} + \vec{\nabla}\Lambda$
$\phi' = \phi - \frac{1}{c}\frac{\partial}{\partial t}\Lambda$

Can rewrite Schrödinger

$$\left\{\left[i\hbar\frac{\partial}{\partial t} - e\phi\right] - \left[\frac{1}{2m}\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2\right]\right\}\psi(\vec{x},t) = 0.$$

Clear that $\psi'(\vec{x},t) = e^{\frac{ie}{\hbar c}\Lambda(\vec{x})}\psi(\vec{x},t)$

satisfies Schrödinger with $\phi \to \phi'$, $A \to A'$:

[illegible]

~~So~~ Since

$$\left[i\hbar\frac{\partial}{\partial t} - e\phi'\right]e^{\frac{ie}{\hbar c}\Lambda}\psi = e^{\frac{ie}{\hbar c}\Lambda}\left[i\hbar\frac{\partial}{\partial t} - e\phi\right]\psi$$

& $$\left[-i\hbar\frac{\partial}{\partial x^i} - \frac{e}{c}A'_i\right]e^{\frac{ie}{\hbar c}\Lambda}\psi = e^{\frac{ie}{\hbar c}\Lambda}\left[-i\hbar\frac{\partial}{\partial x^i} - \frac{e}{c}A_i\right]\psi.$$

So, under gauge transformations

$$\begin{aligned}\phi &\to \phi' = \phi - \frac{1}{c}\frac{\partial}{\partial t}\Lambda \\ \vec{A} &\to \vec{A}' = \vec{A} + \nabla\Lambda \\ \psi &\to \psi' = e^{\frac{ie}{\hbar c}\Lambda}\psi.\end{aligned}$$

No physical observables change, although, e.g.

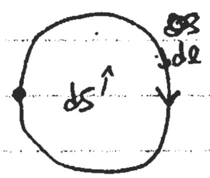
$\langle\vec{p}\rangle = \langle m\dot{\vec{x}} + \frac{e}{c}\vec{A}\rangle$ is gauge-dependent.

<u>Kinematical</u> momentum $\pi^i = m\dot{x}^i$ is gauge-independent.

Aharanov – Bohm effect

[Another quantum effect arising from fields in regions not containing QM particle].

Recall

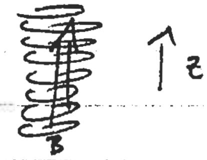


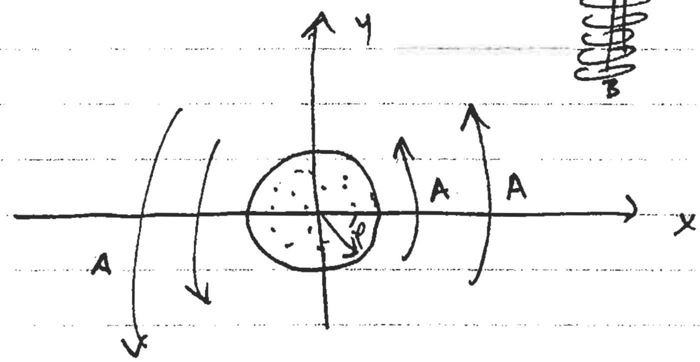
$$\int A \cdot dl = \int_{\Sigma} (\vec{\nabla} \times \vec{A}) \cdot ds$$

$$\left[\text{generally, } \int_{\Sigma} d\omega = \int_{\partial\Sigma} \omega \right]$$

for differential forms Σ p-manifold, ω (p-1) - form.

Consider an infinite solenoid





Calculate A: $\oint 2\pi R\, A_\theta = \int B \cdot ds = \Phi_B$ for $R > \rho$

so $A_\theta = \frac{1}{2\pi R} \Phi_B$ outside solenoid!

Consider a particle moving <u>around</u> the solenoid
(impenetrable approximation)

Does B field affect interference pattern? (Yes!)

Use path integrals:

$$K(x_0,t_0;x',t') = \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]}$$

Consider paths of type ϕ:

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

$$\mathcal{L}(\dot{x},x) = \frac{m}{2}\dot{x}^2 + \frac{e}{c} A_i \dot{x}^i - \cancel{e\phi}$$

Phase coming from A:

$$e^{\frac{ie}{\hbar c}\int A_i \, dx^i/dt \, dt} = e^{\frac{ie}{\hbar c}\int_{path} A_i \, dx^i}$$

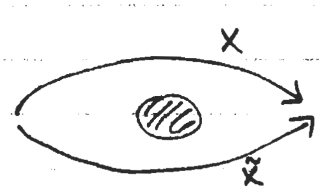
Note that $\displaystyle\int_x A_i dx^i = \int_{\tilde{x}} A_i d\tilde{x}^i$

if $x(t)$, $\tilde{x}(t)$ are topologically equivalent
(i.e., one can be deformed into the other without hitting solenoid)

Thus, <u>all</u> paths of type ϕ give a phase

$$e^{i\theta_0} = e^{\frac{ie}{\hbar c}\int_{\text{path } \phi} A_i dx^i} \quad \text{from A.}$$

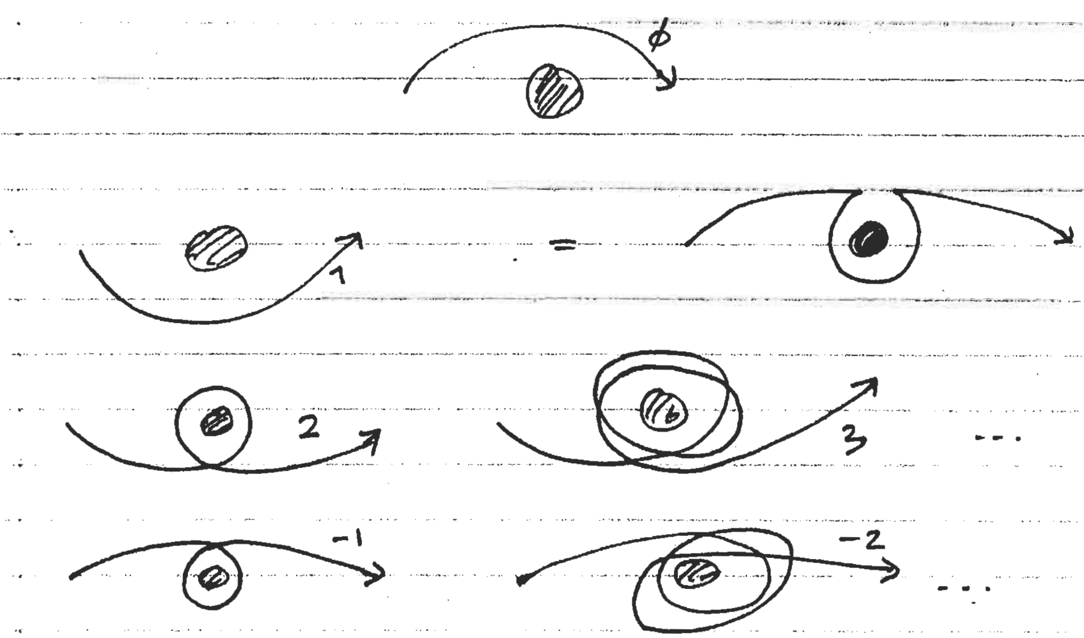
Type 1 paths:



$$\int_{\tilde{x}} A_i d\tilde{x}^i - \int_x A_i dx^i = \Phi_B$$

$$\text{so } e^{i\theta_1} = e^{i\theta_0 + \frac{ie}{\hbar c}\Phi_B}.$$

Classify topologically inequivalent paths:

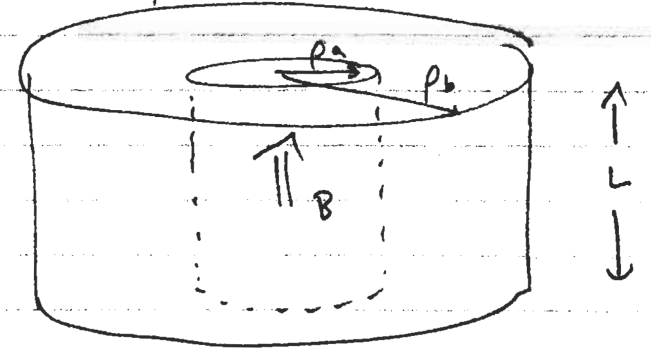


Total propagator:

$$K = \sum_{N=-\infty}^{\infty} \mathcal{D}[x_N(t)]\, e^{\frac{ie}{\hbar c}\int_0 A_i dx^i + \frac{ieN}{\hbar c}\Phi_B + \frac{i}{\hbar}\int_{x(t)} \cancel{\ } M\dot{x}^2}$$

Interference clearly affected by Φ_B.
(paths of type ϕ, 1 dominate)

Static version of problem



Flux in core, particle in region $\rho_a < r < \rho_b$.

Energy levels depend on B (HW).

Magnetic Monopoles

In a source-free region, Maxwell's equations read:

{field notation} [form notation]

$$\left\{\begin{array}{l}\vec{\nabla}\cdot\vec{E}=0\\ \vec{\nabla}\times\vec{B}=\frac{1}{c}\frac{\partial}{\partial t}\vec{E}\end{array}\right\} \qquad \partial_\mu F^{\mu\nu}=0 \qquad [d^*F=0]$$

Since

$$F_{\mu\nu}=\partial_{[\mu}A_{\nu]} \qquad [F=dA]$$

$$\Downarrow$$

$$\left\{\begin{array}{l}\vec{\nabla}\cdot\vec{B}=0\\ \vec{\nabla}\times\vec{E}=-\frac{1}{c}\frac{\partial}{\partial t}\vec{B}\end{array}\right\} \quad \partial_{[\rho}F_{\mu\nu]}=\partial_{[\rho}\partial_\mu A_{\nu]}=0 \qquad [dF=ddA=0]$$

Equations are invariant under

$$\left\{\begin{array}{l}\vec{E}\longleftrightarrow-\vec{B}\\ \vec{B}\longrightarrow\vec{E}\end{array}\right\} \qquad F_{\mu\nu}\leftrightarrow\tfrac{1}{2}\varepsilon_{\mu\nu\lambda\sigma}F^{\lambda\sigma} \qquad [F\longleftrightarrow{}^*F]$$

"Maxwell duality"

Including (static) sources:

$$\vec{\nabla}\cdot\vec{E}=4\pi\rho.$$

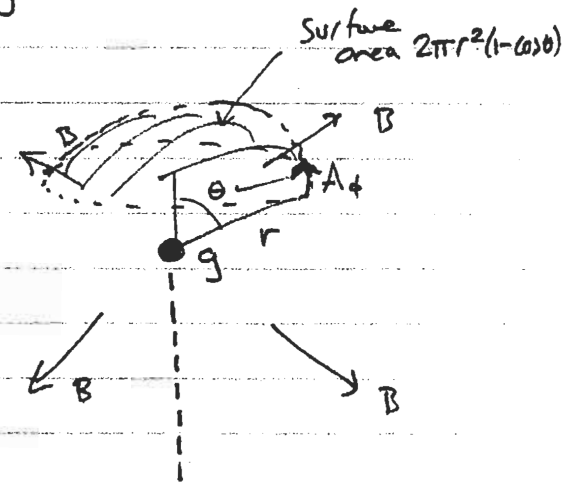
What about magnetic charge $\vec{\nabla}\cdot\vec{B}=4\pi\rho_m$?

Note: $\vec{\nabla}\cdot\vec{B}=\emptyset$ when $\vec{B}=\vec{\nabla}\times\vec{A}$ $[F=dA]$,

so need to generalize notion of vector potential, to get ρ_m.

say we have a magnetic charge g, so

$$\vec{B} = \frac{g}{r^2}\hat{r}.$$



What is $\vec{A}$?

Can try $\vec{A} = A\hat{\phi}$

$$\int \vec{A}\cdot d\vec{l} = 2\pi r \sin\theta \, A$$

$$= \frac{g}{r^2}\cdot 2\pi r^2(1-\cos\theta)$$

[Ex. show $\nabla\times\vec{A} = \vec{B}$ above]

so perhaps $\boxed{\vec{A} = \frac{g(1-\cos\theta)}{r\sin\theta}\hat{\phi}}$ (?). [valid for $\theta<\pi$]

Singular on z^- axis ("Dirac string")

$\int dA \overset{?}{=} 4\pi g$

Need to use another solution in region outside z^+:

$$\tilde{\vec{A}} = -\frac{g(1+\cos\theta)}{r\sin\theta}\hat{\phi} \qquad [\theta>0]$$

$\vec{A}, \tilde{\vec{A}}$ related by a gauge transformation on $0<\theta<\pi$.

combining local charts $\Rightarrow$ global picture

Mathematically: "Connection on a $U(1)$ fiber bundle over $\mathbb{R}^3 \setminus \{0\}$ with first Chern class 1".

Geometrically: circle over each point in space connected in topologically nontrivial fashion.

[POV useful for nonabelian gauge theories, Kaluza-Klein theories]

Classically, only $\vec{B}$ is physical, not $\vec{A}$, so "Dirac string" does not pose any obvious problems.

Quantum mechanically,

Recall $e^{\frac{ie}{\hbar c}\int_P A_\mu dx^\mu}$ enters propagator for charged particle moving along path P.

If $\oint A_\mu dx^\mu = 2\pi n \cdot \frac{\hbar c}{e}$, it is not observable.
Since position is gauge choice, this must be the case.

Thus, we have
$$4\pi g = 2\pi n \cdot \frac{\hbar c}{e},$$
so
$$g = n \cdot \frac{\hbar c}{2|e|} \cong n\left(\frac{137}{2}\right)|e|.$$

Magnetic charge is quantized in units of $\frac{\hbar c}{2|e|}$.

Turning around, assume $\exists$ magnetic monopole of charge g.

Then any electric charge is
$$e = n\frac{\hbar c}{2|g|}.$$

Can explain why proton charge $= |e|$ (known to 4×10^{-19}).

Many models of fundamental physics (GUT's, etc...) predict monopoles

No monopoles seen yet in nature [except, possibly, 1].