PATH INTEGRAL FORMULATION OF QUANTUM MECHANICS

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The way we have set up Q.M. is the conventional one, which draws on the HAMILTONIAN APPROACH to classical mechanics. This is quite evident in, say, the IVth postulate

classical Hamiltonian $\mathcal{H}(x,p)$

$$H = \mathcal{H}(x \to X,\ p \to P)$$

Q.M.

HAMILTON EQUATIONS

$$\begin{cases} \dot{x} = \dfrac{\partial \mathcal{H}}{\partial p} \\ \dot{p} = -\dfrac{\partial \mathcal{H}}{\partial x} \end{cases} \qquad \mathcal{H} = T + V = \frac{p^2}{2m} + V(x) \longrightarrow \dot{p} = -\frac{\partial V}{\partial x} \Rightarrow \{ m\ddot{x} = F \}$$

"NEWTON"

GIVEN $x(0)$, $\dot{x}(0)$ INITIAL DATA

INTEGRATE !

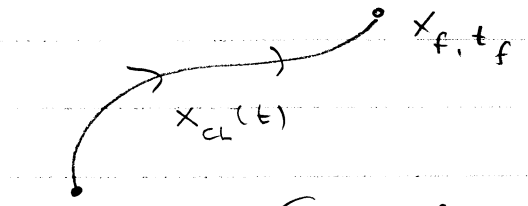
TRAJECTORY

"LOCAL APPROACH": prescribes what the particle will do in the next infinitesimal time interval. To get the trajectory, sum (integrate!) all the infinitesimal (LOCAL) steps!

$t = 0 : x(0), \dot{x}(0)$

ALTERNATIVE FORMULATION OF CLASSICAL MECHANICS

LAGRANGIAN FORMALISM



Given (x_i, t_i) and (x_f, t_f), what is the trajectory $x_{cl}(t)$?

"GLOBAL APPROACH"

Tries to determine at one stroke the full trajectory $x_{cl}(t)$, given the input data (x_i, t_i) and (x_f, t_f).

How does it do it ?

Three-step recipe :

LAGRANGIAN = Legendre transform of the HAMILTONIAN

I. Define $\mathcal{L} = T - V$, $\mathcal{L} = \mathcal{L}(x, \dot{x}, \cancel{t})$

II. For each path $x(t)$ connecting (x_i, t_i) and (x_f, t_f), calculate the ACTION

FUNCTIONAL

$$\rightarrow S[x(t)] = \int_{t_i}^{t_f} \mathcal{L}(x, \dot{x})\, dt$$

III. THE (CLASSICAL) PATH IS THE ONE WHERE S IS A MINIMUM (OR IT IS AN EXTREMUM)

"PRINCIPLE OF LEAST ACTION"

Lagrangian formalism	Hamiltonian formalism
The state of a system with n degrees of freedom is described by n coordinates $(q_1, \ldots, q_n)$ and n velocities $(\dot{q}_1, \ldots, \dot{q}_n)$, or in a more compact notation by $(q, \dot{q})$.	(1) The state of a system with n degrees of freedom is described by n coordinates and n momenta $(q_1, \ldots, q_n; p_1, \ldots, p_n)$ or, more succinctly, by (q, p).
The state of the system may be represented by a point moving with a definite velocity in an *n-dimensional configuration space.*	(2) The state of the system may be represented by a point in a *2n-dimensional phase space*, with coordinates $(q_1, \ldots, q_n; p_1, \ldots, p_n)$.
The n coordinates evolve according to n second-order equations.	(3) The $2n$ coordinates and momenta obey $2n$ first-order equations.
For a given $\mathscr{L}$, several trajectories may pass through a given point in configuration space depending on $\dot{q}$.	(4) For a given $\mathscr{H}$ only one trajectory passes through a given point in phase space.

In 1933 Dirac published a paper in *Physikalische Zeitschrift der Sowjetunion* on "The Lagrangian in Quantum Mechanics." He begins by saying:

"Quantum mechanics was built up on a foundation of analogy with the Hamiltonian theory of classical mechanics. This is because the classical notion of canonical coordinates and momenta was found to be one with a very simple quantum analogue....

Now there is an alternative formulation for classical dynamics, provided by the Lagrangian. This requires one to work in terms of coordinates and velocities instead of coordinates and momenta. The two formulations are, of course, closely related, but there are reasons for believing that the Lagrangian one is the more fundamental.

In the first place the Lagrangian method allows one to collect together all the equations of motion and express them as the stationary property of a certain action function. (This action function is just the time integral of the Lagrangian.) There is no corresponding action principle in terms of the coordinates and momenta of the Hamiltonian theory. [This is not true, but it doesn't matter.] Secondly the Lagrangian method can easily be expressed relativistically, on account of the action function being a relativistic invariant; while the Hamiltonian method is essentially nonrelativistic in form, since it marks out a particular time variable....

For these reasons it would seem desirable to take up the question of what corresponds in the quantum theory to the Lagrangian method of the classical theory."

IN 1933 PAUL DIRAC WROTE A PAPER ...

... EXPANDING ON IDEAS HE HAD ALREADY DISCUSSED IN HIS BOOK ON QUANTUM MECHANICS

THE BOOK ON Q.M.!

The Principles of Quantum Mechanics

FOURTH EDITION

P. A. M. DIRAC

THIS GOT FEYNMAN STARTED AS HE READS DIRAC'S BOOK (AS A STUDENT AT PRINCETON IN THE 1940s)

Path integral formulation of q. m.

Dirac 1933, **Feynman 1949**

Central object in quantum mechanics = the propagator $U(t)$

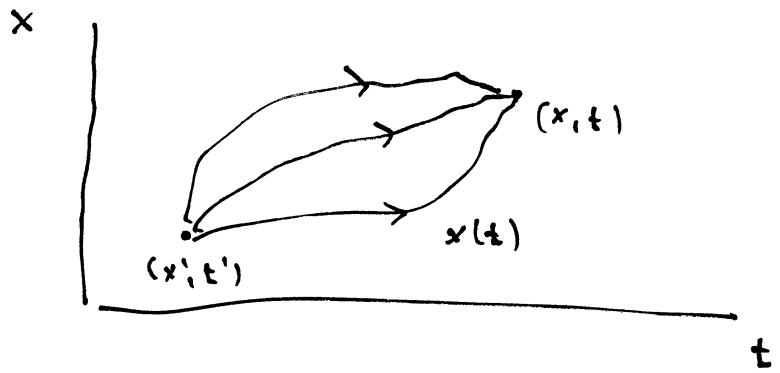
$$U(t)\,|\psi(0)\rangle = |\psi(t)\rangle$$

Feynman:

For a single particle in 1D, to find $U(x,t;x',t') = \langle x|U(t-t')|x'\rangle$

do the following:

(i) Draw all paths in the x-t plane connecting (x',t') and (x,t)



(ii) Find the action S[x(t)] for each path x(t)

Then,

(iii) $U(x,t;x',t') = A \sum_{\text{ALL PATHS}} e^{iS[x(t)]/\hbar}$

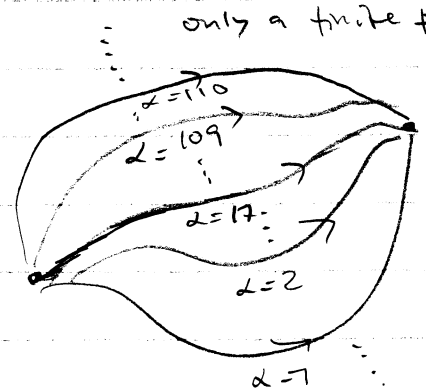
↑ normalization factor

Every path gets the same weight?!

How do we recover the classical path?

$$\sum_{\text{ALL PATHS}} \ldots = \sum_{\alpha} \underbrace{e^{iS[x_\alpha(t)]/\hbar}}_{Z_\alpha}$$

↑ let's pretend we have only a finite # of paths



Z_α ← Why "Z_α"? Change metric!

$t \to -i\tau$

$S \to$ "$\mathcal{H}$" (quantum fluctuations; thermal fluctuations)

$\hbar \to kT$

⇓

PARTITION FUNCTION IN STATISTICAL PHYSICS

!

QUANTUM PHYSICS AND STATISTICAL PHYSICS HAVE A COMMON MATHEMATICAL STRUCTURE

POWERFUL TOOL TO SOLVE PROBLEMS!

$x_{cl}(t) = x_{17}(t)$

$\alpha = 17 \to$ Classical path

$\delta S_{17} = \delta S[x_{17}(x)] = 0$ since $S_{classical}$ at extremum

⇓

Z_α's with α close to 17 add constructively

⇒ large contribution to the sum

⇓

$U(t)$ dominated by paths near $\alpha = 17$

The classical path is important not because it contributes a lot by itself, but because paths in its vicinity contribute coherently ("constructive phase interference")

cont'd on p. 6

How far must we deviate from the classical path before destructive interference sets in ?

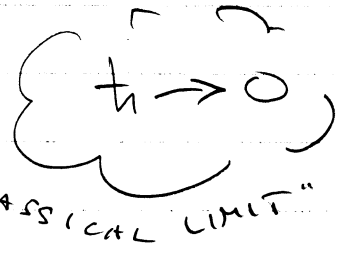
ROUGH ESTIMATE : Coherence is lost when the phase differs from the stationary value $S[x_{CL}(t)]$ by $\sim \pi$

"$S_{CLASSICAL}$"

$\Downarrow$

THE ACTION FOR THE COHERENCE PATHS MUST BE WITHIN $\sim \pi$th OF $S_{CLASSICAL}$

$\Downarrow$



$\Rightarrow$ CLASSICAL PATH SINGLED OUT

$\sim 6.6 \times 10^{-34}$ Js which is pretty close to zero on macroscopic scales

Comment : Since $\hbar$ is already pretty small on the scale of macroscopic "everyday life" phenomena, no wonder that it took so long time before Q.M. was discovered !

NEXT, let's test Feynman's recipe for a simple case

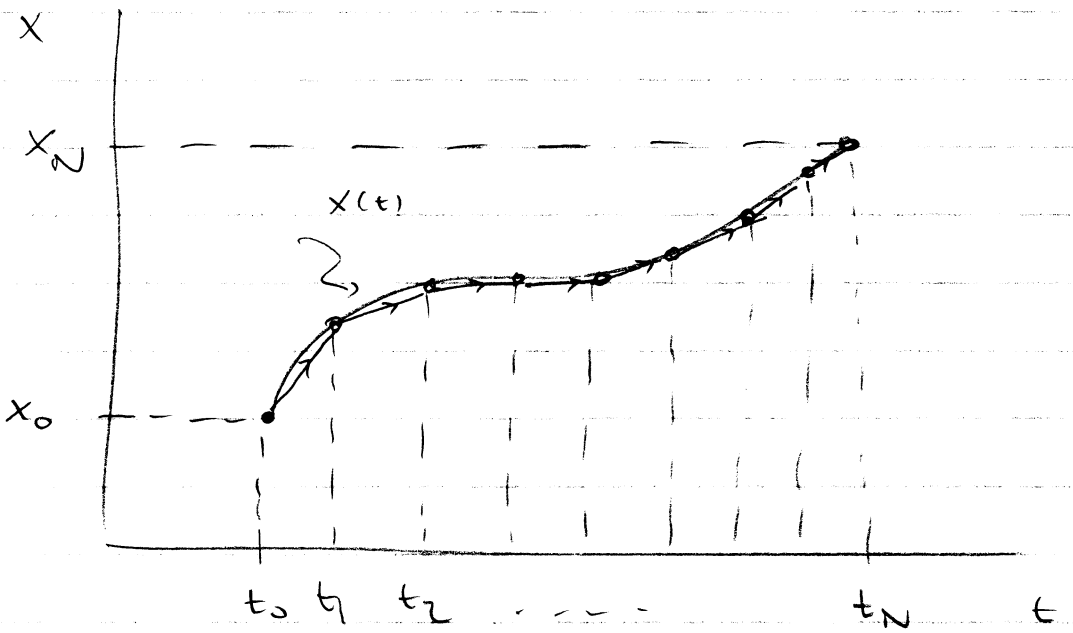
PATH INTEGRAL REPRESENTATION OF THE FREE-PARTICLE PROPAGATOR

$$U(x_N, t_N; x_0, t_0) = \sum_{\text{ALL PATHS}} \ldots \longrightarrow \int_{x_0}^{x_N} e^{iS[x(t)]/\hbar}\, \mathcal{D}[x(t)]$$

FINISH START

"INTEGRATE OVER ALL PATHS CONNECTING x_0 AND x_N (IN THE TIME INTERVAL t_0 TO t_N)"

First, discretize each path:



Then, given a discretized path, we discretize the corresponding ACTION

FREE PARTICLE $\Leftrightarrow \mathcal{L} = T - \cancel{V} = T = \frac{1}{2}m\dot{x}^2$

$$S[x(t)] = \int_{t_0}^{t_N} \mathcal{L}(x(t), \dot{x}(t))\, dt = \int_{t_0}^{t_N} \frac{1}{2}m\dot{x}^2\, dt$$

$$\xrightarrow{\text{DISCRETIZATION}} \sum_{i=0}^{N-1} \frac{1}{2}m\left(\frac{x_{i+1} - x_i}{\varepsilon}\right)^2 \varepsilon \quad , (dt \to \Delta t \equiv \varepsilon)$$

$$x_i = x(t_i)$$

Then,

$$U(x_N, t_N; x_0, t_0) = \int_{x_0}^{x_N} e^{iS[x(t)]/\hbar} \mathcal{D}[x(t)]$$

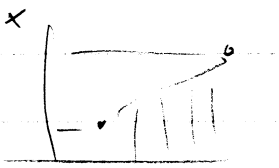
$$= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} A \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\frac{m}{2}\sum_{j=0}^{N-1}\frac{(x_{j+1}-x_j)^2}{\varepsilon}\right] \times$$

$\uparrow$ normalization constant

$$\times\, dx_1 \cdots dx_{N-1}$$

IMPORTANT!

Look at the picture on the previous page to understand how the integral over all paths get approximated by a multiple integral over coordinates



Introduce $y_j \equiv \left(\frac{m}{2\hbar\varepsilon}\right)^{1/2} x_j$

$$U(x_N, t_N; x_0, t_0) = A\left(\frac{2\hbar\varepsilon}{m}\right)^{(N-1)/2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\left[i\sum_{j=0}^{N-1}(y_{j+1}-y_j)^2\right] \times$$

$$\times\, dy_1 dy_2 \cdots dy_{N-1}$$

GAUSSIAN OF THIS FORM

$$\int_{-\infty}^{\infty} e^{-ax^2+\beta x}\,dx = e^{\beta^2/4a}\left(\frac{\pi}{a}\right)^{1/2}$$

Start doing the y_1-integral:

$$\int_{-\infty}^{\infty} \exp\left\{ i\left[(y_2-y_1)^2+(y_1-y_0)^2\right]\right\} dy_1 = \left(\frac{i\pi}{2}\right)^{1/2} e^{-(y_2-y_0)^2/2i}$$

THIS IS TRIVIAL.

Repeat for $y_2, y_3, \cdots, y_{N-1}$

At the end of the day, choosing $A = \left[\frac{2\pi\hbar\varepsilon i}{m}\right]^{-N/2}$

$$U(x_N, t_N; x_0, t_0) = \left(\frac{m}{2\pi\hbar i N\varepsilon}\right)^{1/2} \exp\left(\frac{im(x_N-x_0)^2}{2\hbar N\varepsilon}\right)$$

IT WORKS!

This is the free-particle propagator we saw in Tuesday's lecture!

(Take $N\to\infty$, $\varepsilon\to 0$, $N\varepsilon = t_N - t_0$)

Now, what about bringing in a potential to do a slightly more severe test of Feynman's recipe?!

Let me sketch how that works...

BLACKBOARD...

DIRAC FEYNMAN

... SOME YEARS LATER