PHY 742 Quantum Mechanics II
1-1:50 PM MWF Olin 103

Plan for Lecture 10

Path integral approach to quantum analysis
Ref: Chapter 11 A-C of Professor Carlson's text

1. Some background/motivation
2. Review of classical action
3. Quantum action for a free particle
4. Path integral vs Schrödinger formulation of QM
5. Examples

Course schedule for Spring 2022

(Preliminary schedule -- subject to frequent adjustment.)

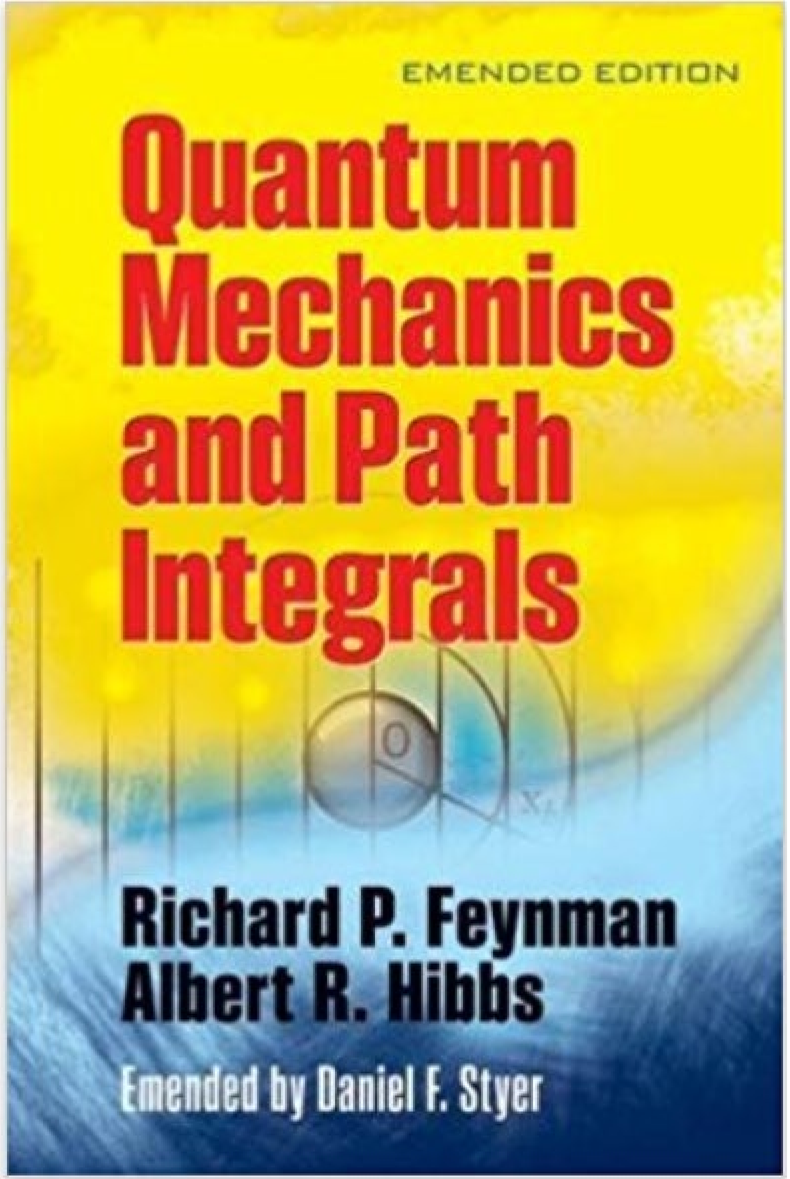
	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/10/2022	Chap. 12	Approximate solutions for stationary states -- The variational approach	#1	01/14/2022
2	Wed: 01/12/2022	Chap. 12 C	Approximate solutions for stationary states -- Perturbation theory	#2	01/19/2022
3	Fri: 01/14/2022	Chap. 12 D	Approximate solutions for stationary states -- Degenerate perturbation theory	#3	01/21/2022
	Mon: 01/17/2022		MLK Holiday -- no class		
4	Wed: 01/19/2022	Chap. 12 C & D	Approximate solutions for stationary states -- Additional tricks	#4	01/24/2022
5	Fri: 01/21/2022	Chap. 13	Examples of of the use of perturbation theory	#5	01/26/2022
6	Mon: 01/24/2022	Chap. 13 & 12 B	Hyperfine perturbation and also the WKB approximation	#6	01/28/2022
7	Wed: 01/26/2022	Chap. 14	Scattering theory		
8	Fri: 01/28/2022	Chap. 14	Scattering theory	#7	02/04/2022
9	Mon: 01/31/2022	Chap. 14	Scattering theory	#8	02/07/2022
	Wed: 02/02/2022	No class	Fire caution		
	Fri: 02/04/2022	No class	Fire caution		
10	Mon: 02/07/2022	Chap. 11 (A-C)	Time evolution and Feynman path integrals	#9	02/09/2022
11	Wed: 02/09/2022	Chap. 11 (A-C)	Time evolution and Feynman path integrals		

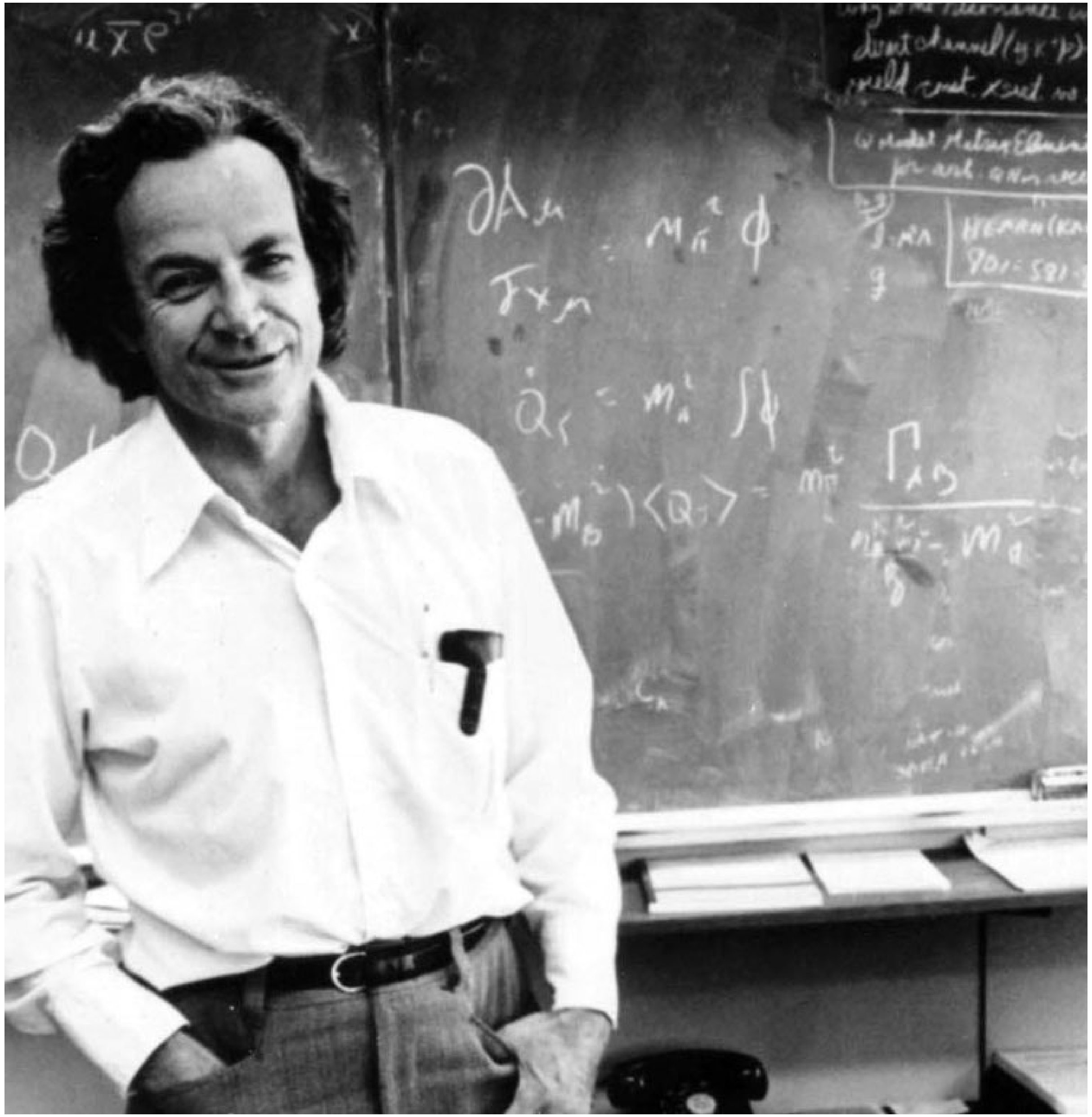
PHY 742 -- Assignment #9

Febrary 04, 2022

Read Chapter 11 (A-C) in **Carlson's** textbook.

1. Carry out the intermediate steps to verify the result for propagator given in Eq. 11.11 of your textbook.





Dover reprinted version of classic text.

From: https://www.britannica.com/biography/Richard-Feynman

Richard Feynman, in full **Richard Phillips Feynman**, (born May 11, 1918, New York, New York, U.S.—died February 15, 1988, Los Angeles, California), American theoretical physicist who was widely regarded as the most brilliant, influential, and iconoclastic figure in his field in the post-World War II era.

Undergraduate project – Feynman-Hellman theorem

AUGUST 15, 1939 PHYSICAL REVIEW VOLUME 56

Forces in Molecules

R. P. FEYNMAN
Massachusetts Institute of Technology, Cambridge, Massachusetts

(Received June 22, 1939)

Formulas have been developed to calculate the forces in a molecular system directly, rather than indirectly through the agency of energy. This permits an independent calculation of the slope of the curves of energy *vs.* position of the nuclei, and may thus increase the accuracy, or decrease the labor involved in the calculation of these curves. The force on a nucleus in an atomic system is shown to be just the classical electrostatic force that would be exerted on this nucleus by other nuclei and by the electrons' charge distribution. Qualitative implications of this are discussed.

Ph. D. Thesis of R. P. Feynman –

"Principle of least action in Quantum Mechanics", Princeton 1942.

REVIEWS OF

MODERN PHYSICS

VOLUME 20, NUMBER 2 APRIL, 1948

Space-Time Approach to Non-Relativistic Quantum Mechanics

R. P. FEYNMAN

Cornell University, Ithaca, New York

Non-relativistic quantum mechanics is formulated here in a different way. It is, however, mathematically equivalent to the familiar formulation. In quantum mechanics the probability of an event which can happen in several different ways is the absolute square of a sum of complex contributions, one from each alternative way. The probability that a particle will be found to have a path $x(t)$ lying somewhere within a region of space time is the square of a sum of contributions, one from each path in the region. The contribution from a single path is postulated to be an exponential whose (imaginary) phase is the classical action (in units of $\hbar$) for the path in question. The total contribution from all paths reaching x, t from the past is the wave function $\psi(x, t)$. This is shown to satisfy Schroedinger's equation. The relation to matrix and operator algebra is discussed. Applications are indicated, in particular to eliminate the coordinates of the field oscillators from the equations of quantum electrodynamics.

PHYSICAL REVIEW VOLUME 97, NUMBER 3 FEBRUARY 1, 1955

Slow Electrons in a Polar Crystal

R. P. Feynman
California Institute of Technology, Pasadena, California
(Received October 19, 1954)

A variational principle is developed for the lowest energy of a system described by a path integral. It is applied to the problem of the interaction of an electron with a polarizable lattice, as idealized by Fröhlich. The motion of the electron, after the phonons of the lattice field are eliminated, is described as a path integral. The variational method applied to this gives an energy for all values of the coupling constant. It is at least as accurate as previously known results. The effective mass of the electron is also calculated, but the accuracy here is difficult to judge.

PHYSICAL REVIEW B VOLUME 1, NUMBER 10 15 MAY 1970

Velocity Acquired by an Electron in a Finite Electric Field in a Polar Crystal

K. K. Thornber*† and Richard P. Feynman
California Institute of Technology, Pasadena, California 91109
(Received 24 November 1969)

The expectation value of the steady-state velocity acquired by an electron interacting with the longitudinal, optical phonons of a polar crystal in a finite electric field is analyzed quantum mechanically for arbitrary coupling strength, field strength, and temperature. The rate of loss of momentum by an electron

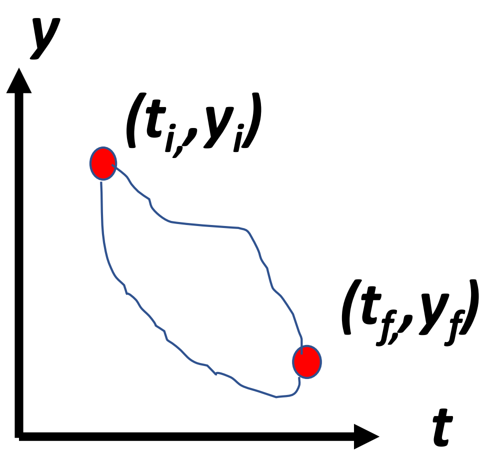
Review of classical Lagrangian mechanics:

Now consider the Lagrangian defined to be :

$$L\left(\left\{y(t),\frac{dy}{dt}\right\},t\right) \equiv T - U$$

Kinetic energy (T)

Potential energy (U)



Hamilton's principle states:

$$S \equiv \int_{t_i}^{t_f} L\left(\left\{y(t),\frac{dy}{dt}\right\},t\right)dt \quad \text{is minimized for physical } y(t)$$

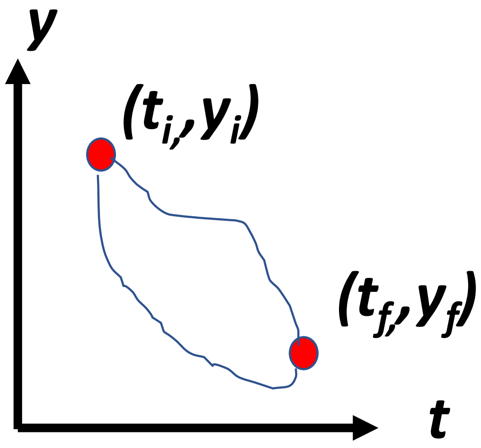
Euler-Lagrange relations:

$$\frac{\partial L}{\partial y} - \frac{d}{dt}\frac{\partial L}{\partial \dot{y}} = 0$$

Feynman's idea

Probability of quantum system to evolve from $\left(t_i, y_i\right) \leftrightarrow \left(t_f, y_f\right)$

$$K(i,f) \propto \sum_{\text{All paths } i \to f} \exp(iS(t_i,t_f)/\hbar)$$



In classical mechanics, the action is optimized for the physical path.

In Feynman's notion of path integrals, the probability amplitude is obtained from constructive interference of all possible actions.

In order to develop Feynman's idea, we need to think about the time evolution of quantum systems. Ref. 11 A & B in Professor Carlson's text

Schrödinger Equation: $$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=H(\mathbf{r},t)\Psi(\mathbf{r},t)$$

For the case that the Hamiltonian is time independent:

$H(\mathbf{r},t)=H(\mathbf{r}),$ the partial differential equation is separable in time and the solutions may take the form

$\Psi(\mathbf{r},t)\rightarrow\phi_n(\mathbf{r})e^{-iE_nt/\hbar}$ if $H(\mathbf{r})\phi_n(\mathbf{r})=E_n\phi_n(\mathbf{r})$.

The eigenstates $\phi_n(\mathbf{r})\rightarrow\left|\phi_n\right\rangle$ form a complete set of basis functions such that $\sum_n\left|\phi_n\right\rangle\left\langle\phi_n\right|=1.$

Now consider the time evolution operator -- $U(t,t_0)$

$$|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle. \qquad (11.1)$$

$$U(t_0,t_0) = 1, \qquad (11.2a)$$

$$U^\dagger(t,t_0)U(t,t_0) = 1, \qquad (11.2b)$$

$$U(t_2,t_1)U(t_1,t_0) = U(t_2,t_0). \qquad (11.2c)$$

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

➔ $$i\hbar\frac{\partial}{\partial t}U(t,t_0)|\Psi(t_0)\rangle = HU(t,t_0)|\Psi(t_0)\rangle,$$

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = HU(t,t_0). \qquad (11.3)$$

From these properties, we can conclude that for a time independent *H(r):*

$$U(t,t_0) = \exp\left[-iH(t-t_0)/\hbar\right]. \qquad (11.4)$$

This can be evaluated in terms of the eigenstates:

$$U(t,t_0) = \sum_n \exp\left[-iH(t-t_0)/\hbar\right]|\phi_n\rangle\langle\phi_n|, = \sum_n |\phi_n\rangle e^{-iE_n(t-t_0)/\hbar}\langle\phi_n|. \qquad (11.5)$$

Now consider the example where *H(*r*)* represents the Hamiltonian of a free particle – for simplicity, we will take assume the motion is only in the x direction

$$H(\mathbf{r}) = H(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \qquad |\phi_n\rangle \Rightarrow \frac{e^{ikx}}{\sqrt{2\pi}}$$

$$\langle x,t|U(t,t_0)|x_0,t_0\rangle \equiv K(x,t,x_0,t_0) =$$

$$\sum_n |\phi_n\rangle e^{-iE_n(t-t_0)/\hbar}\langle\phi_n| = \frac{1}{2\pi}\int dk\ e^{-ik(x-x_0)-i(\hbar k^2/2m)(t-t_0)}$$

$$K(x,t;x_0,t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\exp\left[\frac{im(x-x_0)^2}{2\hbar(t-t_0)}\right]. \qquad (11.11)$$

Summary -- the time evolution of a free quantum particle

Time dependent Schrödinger equation: $$i\hbar \frac{\partial\Psi(x,t)}{\partial t} = H(x,t)\Psi(x,t)$$

Formal integral solution: $$\Psi(x,t) = \int dx'\, K(x,x',t)\Psi(x',0)$$

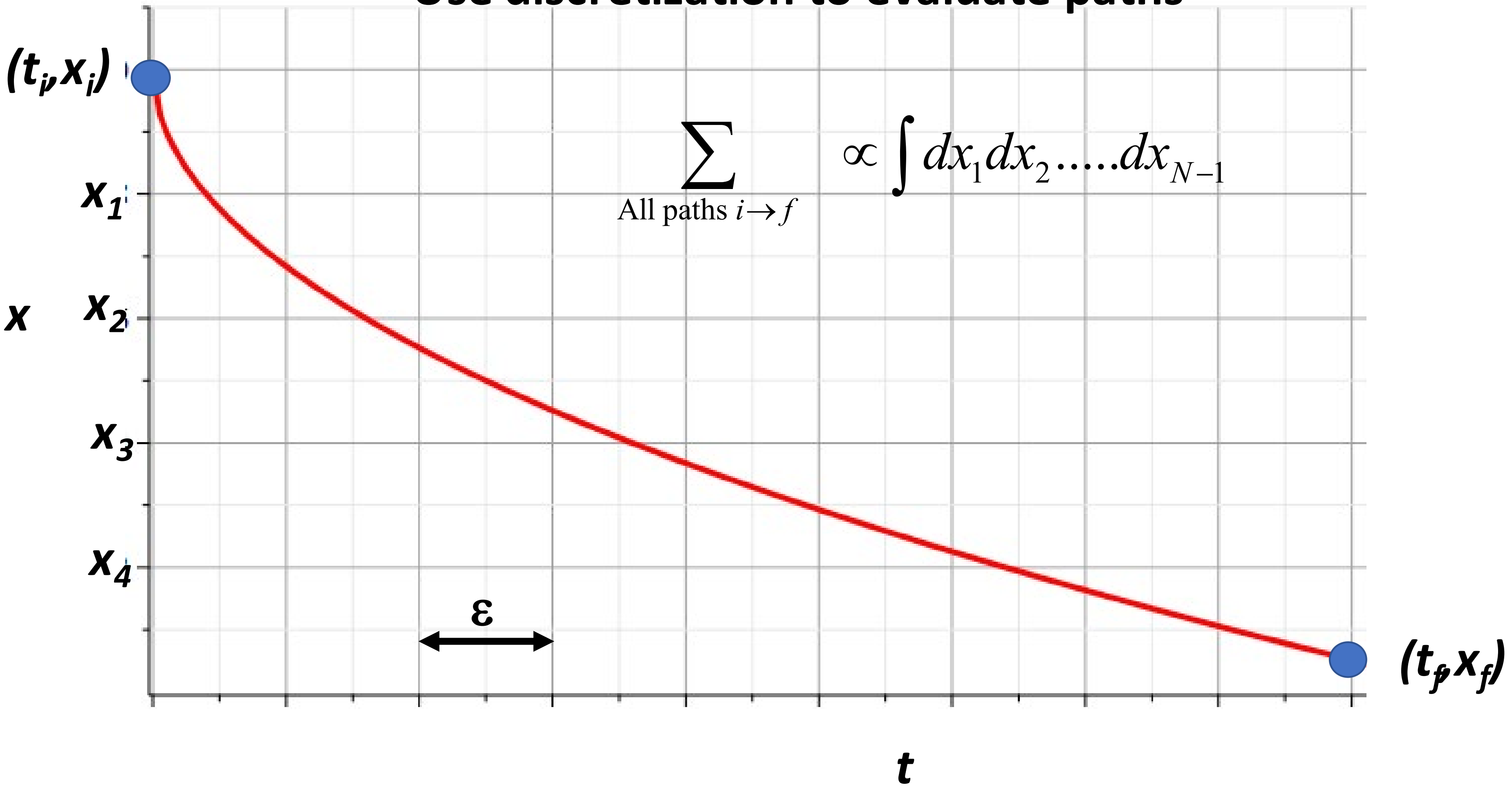
where: $$\left(i\hbar\frac{\partial}{\partial t} - H(x,t) \right) K(x,x',t) = \delta(x-x')$$

For $$H(x,t) = H(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$K(x,x',t) = \left(\frac{m}{2\pi i\hbar t} \right)^{1/2} \exp\left(-\frac{m(x-x')^2}{2i\hbar t} \right)$$

Application of Feynman's path integral idea to the free particle in one dimension -- need scheme to evaluate all possible paths --

Use discretization to evaluate paths



$$\sum_{\text{All paths } i \to f} \propto \int dx_1 dx_2 .....dx_{N-1}$$

Application of Feynman's path integral -- continued

Discretization over time: $\frac{t_f - t_i}{N} \equiv \epsilon$

Discretization over position; $N-1$ variable positions $x_1, x_2, \ldots x_{N-1}$

$$S(i,f) = \int_{t_i}^{t_f} L(x,\dot{x},t)\,dt$$

In this case, $L(x,\dot{x},t) = \frac{m}{2}\dot{x}^2$

We can approximate $\dot{x} \approx \frac{x_n - x_{n-1}}{\epsilon}$ where $x_0 \equiv x_i$ and $x_N \equiv x_f$

For any given choice of path: $S_P(i,f) \approx \exp\left(\frac{im}{2\hbar\epsilon}\sum_{n=1}^{N}\left(x_n - x_{n-1}\right)^2\right)$

Application of Feynman's path integral -- continued

For any given choice of path: $$S_P(i,f) \approx \exp\left(\frac{im}{2\hbar\epsilon}\sum_{n=1}^{N}\left(x_n - x_{n-1}\right)^2\right)$$

In order to perform path integral, need to consider all values of the interior points $x_1, x_2, \ldots x_{N-1}$

For example $$I_1(x_2) \equiv \int_{-\infty}^{\infty} dx_1 \exp\left(\frac{im}{2\hbar\epsilon}\left(\left(x_1 - x_0\right)^2 + \left(x_2 - x_1\right)^2\right)\right)$$

$$= \left(2A\right)^{-1/2} \exp\left(\frac{im}{2\hbar\epsilon(2)}\left(x_2 - x_0\right)^2\right) \quad \text{where } A \equiv \frac{m}{2\pi i\hbar\epsilon}$$

Application of Feynman's path integral -- continued

Continuing next:
$$I_2(x_3) \equiv \int_{-\infty}^{\infty} dx_2 I_1(x_2) \exp\left(\frac{im}{2\hbar\epsilon}(x_3 - x_2)^2\right)$$
$$= \left(3A^2\right)^{-1/2} \exp\left(\frac{im}{2\hbar\epsilon(3)}(x_3 - x_0)^2\right)$$

Continuing last:
$$I_{N-1}(x_N) \equiv \int_{-\infty}^{\infty} dx_{N-1} I_{N-2}(x_{N-1}) \exp\left(\frac{im}{2\hbar\epsilon}(x_N - x_{N-1})^2\right)$$
$$= \left(NA^{N-1}\right)^{-1/2} \exp\left(\frac{im}{2\hbar\epsilon(N)}(x_N - x_0)^2\right)$$

Application of Feynman's path integral -- continued

$$I_{N-1}(x_N) = \left(NA^{N-1}\right)^{-1/2} \exp\left(\frac{im}{2\hbar\epsilon(N)}\left(x_N - x_0\right)^2 \right)$$

Note that $t_f - t_i = N\epsilon$ and $x_N - x_0 = x_f - x_i$

$$K(i,f) \propto \sum_{\text{All paths } i\to f} \exp(iS(t_i,t_f)/\hbar) \qquad K(i,f) = C\left(NA^{N-1}\right)^{-1/2} \exp\left(\frac{im\left(x_f - x_i\right)^2}{2\hbar(t_f - t_i)} \right)$$

$$\text{where } A \equiv \frac{m}{2\pi i\hbar\epsilon}$$

Previous results for free particle kernel: $K(x,x',t) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \exp\left(-\frac{m(x-x')^2}{2i\hbar t}\right)$

$$\Rightarrow K(x_i,x_f,t_f - t_i) = \left(\frac{m}{2\pi i\hbar\left(t_f - t_i\right)}\right)^{1/2} \exp\left(-\frac{m(x_i - x_f)^2}{2i\hbar\left(t_f - t_i\right)}\right)$$

Application of Feynman's path integral – continued

Reconciling the constants --

Previous results for free particle kernel:

$$K(x_i, x_f, t_f - t_i) = \left(\frac{m}{2\pi i\hbar\left(t_f - t_i\right)}\right)^{1/2} \exp\left(-\frac{m(x_i - x_f)^2}{2i\hbar\left(t_f - t_i\right)}\right)$$

Result of integration over $N-1$ intermediate points

$$K(i,f) = C\left(NA^{N-1}\right)^{-1/2} \exp\left(\frac{im\left(x_f - x_i\right)^2}{2\hbar(t_f - t_i)}\right) \qquad \text{where } A \equiv \frac{m}{2\pi i\hbar\epsilon}$$

$$\Rightarrow C = A^{N/2}$$

General formula: $K(i,f) = \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2} \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \ldots \int_{-\infty}^{\infty} dx_{N-1} \exp(iS(t_i, t_f)/\hbar)$

Note that the accuracy of the evaluation converges as $N \to \infty$.

Feynman's path integral

General formula: $$K(i,f)=\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2\ldots\int_{-\infty}^{\infty}dx_{N-1}\exp(iS(t_i,t_f)/\hbar)$$

Note that the accuracy of the evaluation converges as $N\to\infty$.

In terms of the propagation kernel $K(x,x',t)$, the time evolution of the wavefunction is given by $\Psi(x,t)=\int dx'K(x,x',t)\Psi(x',0)$

How is the path integral formulation related to the Schrödinger equation?

How is the path integral formulation related to the Schrödinger equation?

Consider a small increment of time: $t_i = 0 \quad t_f = \epsilon$

$$\Psi(x,\epsilon) = \int dx' K(x,x',\epsilon)\Psi(x',0)$$

Lagrangian: $L(x,\dot{x},t) = \frac{1}{2}m\dot{x}^2 - V(x)$

Action: $S(x,x',0,\epsilon) = \int_0^\epsilon L(u,\dot{u},t)dt$ where $u(0) = x$ and $u(\epsilon) = x'$

$$S(x,x',0,\epsilon) \approx \frac{1}{2}m\left(\frac{(x'-x)^2}{\epsilon}\right) - \epsilon V\left(\frac{x'+x}{2}\right)$$

In this case: $K(x,x',\epsilon) \approx \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} \exp(iS(x,x',0,\epsilon)/\hbar).$

How is the path integral formulation related to the Schrödinger equation -- continued

$$K(x,x',\epsilon) \approx \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} \exp(iS(x,x',0,\epsilon)/\hbar).$$

$$\Psi(x,\epsilon) = \int dx' K(x,x',\epsilon)\Psi(x',0)$$

$$\approx \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} \int_{-\infty}^{\infty} dx' \Psi(x',0) \exp\left(\frac{im}{2\hbar\epsilon}(x'-x)^2\right) \exp\left(-\frac{i\epsilon}{\hbar}V\left(\frac{x'+x}{2}\right)\right)$$

Since ϵ is small, we can expand all terms about ϵ=0:

$$\frac{i\epsilon}{\hbar}V\left(\frac{x'+x}{2}\right) \approx \frac{i\epsilon}{\hbar}V(x) \qquad \exp\left(-\frac{i\epsilon}{\hbar}V\left(\frac{x'+x}{2}\right)\right) \approx 1 - \frac{i\epsilon}{\hbar}V(x)$$

Let $u = x' - x$

$$\Psi(x',0) \approx \Psi(x,0) + u\frac{\partial \Psi(x,0)}{\partial x} + \frac{1}{2}u^2 \frac{\partial^2 \Psi(x,0)}{\partial x^2}$$

How is the path integral formulation related to the Schrödinger equation -- continued

$$\Psi(x,\epsilon) = \int dx' K(x,x',\epsilon)\Psi(x',0)$$

$$\approx \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} \int_{-\infty}^{\infty} du \exp\left(\frac{imu^2}{2\hbar\epsilon}\right)\left(1-\frac{i\epsilon}{\hbar}V(x)\right)\left(\Psi(x,0)+u\frac{\partial\Psi(x,0)}{\partial x}+\frac{1}{2}u^2\frac{\partial^2\Psi(x,0)}{\partial x^2}\right)$$

Integral values:

$$\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} \int_{-\infty}^{\infty} du \exp\left(\frac{imu^2}{2\hbar\epsilon}\right) = 1 \qquad \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} \int_{-\infty}^{\infty} du\ u \exp\left(\frac{imu^2}{2\hbar\epsilon}\right) = 0$$

$$\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} \int_{-\infty}^{\infty} du\ u^2 \exp\left(\frac{imu^2}{2\hbar\epsilon}\right) = \frac{i\hbar\epsilon}{m}$$

$$\Rightarrow \Psi(x,\epsilon) = \int dx' K(x,x',\epsilon)\Psi(x',0)$$

$$\approx \left(1-\frac{i\epsilon}{\hbar}V(x)\right)\Psi(x,0) + \frac{i\hbar\epsilon}{2m}\frac{\partial^2\Psi(x,0)}{\partial x^2} + O(\epsilon^2)$$

How is the path integral formulation related to the Schrödinger equation -- continued

$$\Psi(x,\epsilon) = \int dx' K(x,x',\epsilon)\Psi(x',0)$$

$$\approx \left(1 - \frac{i\epsilon}{\hbar}V(x)\right)\Psi(x,0) + \frac{i\hbar\epsilon}{2m}\frac{\partial^2\Psi(x,0)}{\partial x^2}$$

Note that: $$\frac{\Psi(x,\epsilon) - \Psi(x,0)}{\epsilon} \approx \frac{\partial\Psi(x,t)}{\partial t}$$

So that the path integral results are consistent with:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t)$$

Summary of results –

Feynman path integral can be used to evaluate the time propagation of a quantum system based on evaluations of the action function.

Next time – some examples.