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

Plan for Lecture 18

Path integral approach to quantum analysis
Ref: Chapter 11C 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**

1

Topics for Quantum Mechanics II

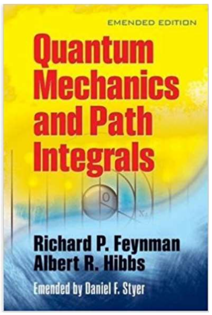
Single particle analysis
- Single particle interacting with electromagnetic fields – EC Chap. 9
- Scattering of a particle from a spherical potential – EC Chap. 14
- More time independent perturbation methods – EC Chap. 12, 13
- Single electron states of a multi-well potential ➔ molecules and solids – EC Chap. 2,6
- Time dependent perturbation methods – EC Chap. 15
- Relativistic effects and the Dirac Equation – EC Chap. 16
- Path integral formalism (Feynman) – EC Chap. 11.C

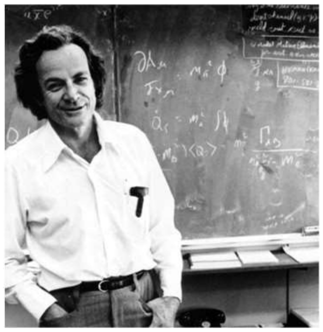
Multiple particle analysis
- Quantization of the electromagnetic fields – EC Chap. 17
- Photons and atoms – EC Chap. 18
- Multi particle systems; Bose and Fermi particles – EC Chap. 10
- Multi electron atoms and materials
  - Hartree-Fock approximation
  - Density functional approximation

2

11	Fri: 02/07/2020	Chap. 15	Time-dependent perturbations	#11	02/14/2020
12	Mon: 02/10/2020	Chap. 15	Time-dependent perturbations	#12	02/14/2020
13	Wed: 02/12/2020	Chap. 15	Time-dependent perturbations	#13	02/17/2020
14	Fri: 02/14/2020	Chap. 16	The Dirac equation		
15	Mon: 02/17/2020	Chap. 16	The Dirac equation	#14	02/19/2020
16	Wed: 02/19/2020	Chap. 16	The Dirac equation	#15	02/21/2020
17	Fri: 02/21/2020	Chap. 16	The Dirac equation	#16	02/24/2020
18	Mon: 02/24/2020	Chap. 11C	Path integral formalism		
19	Wed: 02/26/2020	Chap. 11C	Path integral formalism		
20	Fri: 02/28/2020		Review		
	Mon: 03/02/2020	No class	*APS March Meeting*	Take Home Exam	
	Wed: 03/04/2020	No class	*APS March Meeting*	Take Home Exam	
	Fri: 03/06/2020	No class	*APS March Meeting*	Take Home Exam	
	Mon: 03/09/2020	No class	*Spring Break*		
	Wed: 03/11/2020	No class	*Spring Break*		
	Fri: 03/13/2020	No class	*Spring Break*		
21	Mon: 03/16/2020				

3





Dover reprinted version of classic text.

4

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.

5

Ph. D. Thesis of R. P. Feynman –
"Principle of least action in Quantum Mechanics", Princeton 1942.

6

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.

7

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

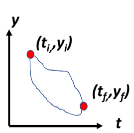
California Institute of Technology, Pasadena, California 91109

(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

8

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

Potential energy

In our example:

$$L\left(\left\{y(t),\frac{dy}{dt}\right\},t\right) \equiv T - U = \frac{1}{2}m\left(\frac{dy}{dt}\right)^2 - mgy$$

Euler-Lagrange relations:

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

Hamilton's principle states:

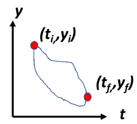
$$S \equiv \int_{t_i}^{t_f} L\left(\left\{y(t),\frac{dy}{dt}\right\},t\right)dt \quad \text{is minimized for physical } y(t)$$

9

Feynman's idea

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

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



10

Digression – Recall the time evolution of a free quantum particle
(See Chapter 11 B of your textbook)

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

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

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

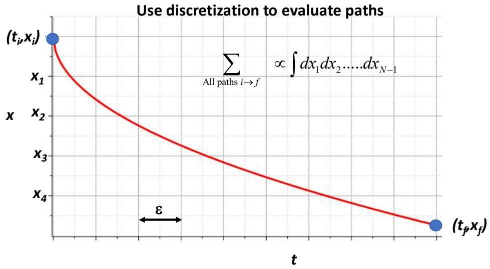
For $H(x,t) = H(x) = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}$

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

11

Application of Feynman's path integral idea to the free particle in one dimension

Use discretization to evaluate paths



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

12

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

2/24/2020 PHY 742 -- Spring 2020 -- Lecture 18 13

13

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

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

2/24/2020 PHY 742 -- Spring 2020 -- Lecture 18 14

14

Application of Feynman's path integral -- continued

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

$$= \left(3A^2\right)^{-1/2}\exp\left(\frac{im}{2\hbar\epsilon(3)}\left(x_3 - x_0\right)^2\right)$$

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

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

2/24/2020 PHY 742 -- Spring 2020 -- Lecture 18 15

15

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 $x_N - x_0 = x_f - x_i$

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

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

Previous results for free particle kernel:

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

16

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

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

17

Feynman's path integral

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

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?

18

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

2/24/2020 PHY 742 -- Spring 2020 -- Lecture 18 19

19

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 $u = x' - x$

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

2/24/2020 PHY 742 -- Spring 2020 -- Lecture 18 20

20

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:

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

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

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

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

2/24/2020 PHY 742 -- Spring 2020 -- Lecture 18 21

21

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:

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

22