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

Plan for Lecture 19

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

1. **Review of path integral formulation and example for free particle**
2. **Role of classical trajectory**
3. **Examples**

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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**

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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				

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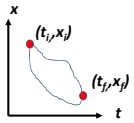
Feynman's idea

Probability of quantum system to evolve from $(t_i, x_i) \leftrightarrow (t_f, x_f)$

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



$$S(i,f) = \int_{t_i}^{t_f} L(x,\dot{x},t)dt \qquad L(x,\dot{x},t) = \frac{1}{2}m\dot{x}^2 - V(x)$$

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For free particle, $V(x) = 0$:

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

General formula for evaluating path integral using $(N-1)$ intermediate points:

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

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

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Relationship of path integral to time evolution of probability amplitude:

$\Psi(x_f,t_f) = \int dx_i K(x_f,t_f,x_i,t_i)\Psi(x_i,t_i)$

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

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

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

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

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

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

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Relationship of path integral to time evolution of probability amplitude:

Considering intermediate kernels

$$K(x_f,t_f,x_i,t_i)=\int dx_{N-1}K(x_f,t_f,x_{N-1},t_{N-1})\int dx_{N-2}K(x_{N-1},t_{N-1},x_{N-2},t_{N-2})...\int dx_1K(x_1,t_1,x_i,t_i)$$

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

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

Result consistent with path formulation given previously for same N intervals:

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

In both cases, the accuracy of the evaluation converges as $N\to\infty$.

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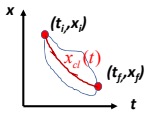
Role of the "classical" trajectory



$$S(i,f)=\int_{t_i}^{t_f}L(x,\dot{x},t)dt \qquad L(x,\dot{x},t)=\frac{1}{2}m\dot{x}^2-V(x)$$

Classical trajectory:

$\delta S=0$ Euler-Lagrange equation: $\frac{\partial L}{\partial x}-\frac{d}{dt}\frac{\partial L}{\partial \dot{x}}=0$

$x_{cl}(t)$ is a solution to the Euler-Lagrange equation

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Role of the "classical" trajectory -- continued

$$S_{cl}(i,f)=\int_{t_i}^{t_f}L(x_{cl},\dot{x}_{cl},t)dt \qquad L(x,\dot{x},t)=\frac{1}{2}m\dot{x}^2-V(x)$$

Example of a free particle --

$$L(x,\dot{x},t)=\frac{1}{2}m\dot{x}^2 \qquad x_{cl}(t)=x_i+\frac{x_f-x_i}{t_f-t_i}(t-t_i)$$

$$L(x_{cl},\dot{x}_{cl},t)=\frac{1}{2}m\left(\frac{x_f-x_i}{t_f-t_i}\right)^2 \quad \text{(constant)}$$

$$S_{cl}(i,f)=\frac{1}{2}m\frac{(x_f-x_i)^2}{t_f-t_i}$$

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Role of the "classical" trajectory -- example of free particle -- continued

Applying Feynman's idea

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

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

For this case, suggest that $K(i,f) \approx K_{cl}(i,f) \propto \exp(iS_{cl}(i,f)/\hbar)$

For this case, $S_{cl}(i,f) = \frac{1}{2} m \frac{(x_f - x_i)^2}{t_f - t_i} \Rightarrow K_{cl}(i,f) = C \exp\left(\frac{im}{2\hbar} \frac{(x_f - x_i)^2}{t_f - t_i}\right)$

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

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Recap – For free particle, classical path gives exact result!

$$K_{cl}(i,f) = C \exp\left(\frac{im}{2\hbar} \frac{(x_f - x_i)^2}{t_f - t_i}\right)$$

For $C = \left(\frac{m}{2\pi i\hbar(t_f - t_i)}\right)^{1/2}$ $K_{cl}(i,f) = K_{\text{Path Integral}}(i,f)$

More generally, when can we expect: $K(i,f) \approx K_{cl}(i,f) = C\exp(iS_{cl}(i,f)/\hbar)$?

Feynman showed that the classical trajectory approximation is valid for all Lagrangians which depend on its variables up through quadratic order.

Form for Lagrangians for which $K(i,f) = K_{cl}(i,f)$

$$L(x, \dot{x}; t) = A(t) + B(t)x + C(t)\dot{x} + D(t)\dot{x}^2 + E(t)x^2 + F(t)x\dot{x}$$

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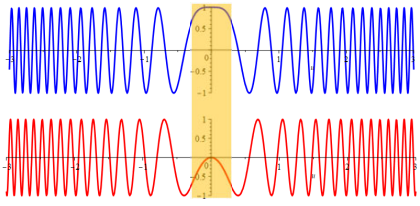
Importance of classical trajectory in analysis of path integrals

Consider free particle case in a small increment of time: ϵ

Define a deviation from the classical trajectory $u(t) = x_{cl}(t) - x(t)$

Action: $S \approx \frac{mu^2}{2\epsilon}$ Kernel: $K \approx C \exp\left(\frac{imu^2}{2\hbar\epsilon}\right)$



$\Re\left(\exp\left(\frac{imu^2}{2\hbar\epsilon}\right)\right)$

$\Im\left(\exp\left(\frac{imu^2}{2\hbar\epsilon}\right)\right)$

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Kernel for the one-dimensional harmonic oscillator

This is a case for the classical analysis: $K(i,f) \approx K_{cl}(i,f) = C\exp(iS_{cl}(i,f)/\hbar)$

$$L(x,\dot{x};t) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2$$

Classical trajectory: $x(t) = A\sin(\omega t + \phi)$

with $x_i = A\sin(\omega t_i + \phi)$ and $x_f = A\sin(\omega t_f + \phi)$ $\quad T \equiv t_f - t_i$

$$L(x_{cl}(t)) = \frac{m\omega^2 A^2}{2}\left(\cos^2(\omega t + \phi) - \sin^2(\omega t + \phi)\right) = \frac{m\omega^2 A^2}{2}\cos\left(2(\omega t + \phi)\right)$$

$$S_{cl} = \frac{m\omega^2 A^2}{2}\left(\frac{\sin\left(2(\omega t_f + \phi)\right) - \sin\left(2(\omega t_i + \phi)\right)}{2\omega}\right) = \frac{m\omega A^2}{4}\left(\sin\left(2(\omega t_f + \phi)\right) - \sin\left(2(\omega t_i + \phi)\right)\right)$$

$$= \frac{m\omega}{2\sin(\omega T)}\left(\left(x_i^2 + x_f^2\right)\cos(\omega T) - 2x_i x_f\right) \qquad \text{(Feynman magic)}$$

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Kernel for the one-dimensional harmonic oscillator -- continued

$$K(i,f) = K_{cl}(i,f) = C\exp(iS_{cl}(i,f)/\hbar)$$

$$S_{cl} = \frac{m\omega}{2\sin(\omega T)}\left(\left(x_i^2 + x_f^2\right)\cos(\omega T) - 2x_i x_f\right)$$

Determining constant C by recalling free particle result

For free particle: $K(x_i, x_f, T) = \left(\frac{m}{2\pi i\hbar T}\right)^{1/2}\exp\left(-\frac{m(x_i - x_f)^2}{2i\hbar T}\right)$

For harmonic oscillator:

$$K(x_i, x_f, T) = \left(\frac{m\omega}{2\pi i\hbar\sin(\omega T)}\right)^{1/2}\exp\left(-\frac{m\omega}{2i\hbar\sin(\omega T)}\left(\left(x_i^2 + x_f^2\right)\cos(\omega T) - 2x_i x_f\right)\right)$$

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Examples of using path integrals in research

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.

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Examples of using path integrals in research

PHYSICAL REVIEW VOLUME 127, NUMBER 4 AUGUST 15, 1962

Mobility of Slow Electrons in a Polar Crystal

R. P. Feynman
California Institute of Technology, Pasadena, California
R. W. Hellwarth
Hughes Research Laboratories, Malibu, California
C. K. Iddings
Enrico Fermi Institute for Nuclear Studies, University of Chicago, Chicago, Illinois
and
P. M. Platzman
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received March 26, 1962)

We have obtained an approximate expression for the impedance function at all frequencies, temperatures, and coupling strengths of an electron coupled to a polar lattice (a system commonly called a polaron). The starting point for the calculation is the quantum mechanical expression for the expected current. The phonon coordinates are eliminated from this expression by well-known field-theory techniques. The resulting exact "influence functional" is then approximated by a corresponding quadratic "influence functional" which, it is hoped, imitates the real polaron. Correction terms are computed to account for the difference between the approximate impedance and the exact polaron impedance in a manner closely analogous to Feynman's treatment of the polaron self-energy. In fact, the analytic evaluation of the expression for the impedance obtained here is carried out using the approximate "influence functional" that was successfully employed in minimizing the binding (and free) energy of the polaron in earlier calculations. However, the accuracy obtained using this approximation, for the impedance calculation, is less satisfactory and its limitations are discussed. Nevertheless, beginning at intermediate coupling strengths, the approximate impedance produces a level structure of increasing complexity and narrowing resonances as the coupling strengthens. This suggests that further refinements may be fruitful. Methods for finding a better quadratic influence functional for use in our impedance expression as well as ways of improving the expression further are suggested. A comparison of our results with those of the Boltzmann equation points up interesting differences which arise from reversing the order of taking limits of zero frequency and coupling.

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Examples of using path integrals in research

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
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(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 drifting through the crystal in the applied field is expressed in a form in which the lattice coordinates (the phonons) have been eliminated exactly by path-integral methods. This expression is then evaluated by a path-integral approach similar to that used to calculate the impedance of electrons in polar crystals. We present numerical calculations of field (loss of energy per unit distance) versus velocity for three coupling strengths using the Fröhlich polaron model. In a single curve, all the expected phenomena appear, including a threshold field for producing hot electrons and a decreasing rate of energy loss with velocity for very fast electrons. Using only the experimentally measured values of the reststrahlen energy and the static and optical dielectric constants, we find an energy loss of 0.025 eV/Å for electrons near the threshold in Al_2O_3, which compares favorably with the experimental value of about 0.03 eV/Å. We conclude that optical-phonon scattering can indeed produce the high rate of energy loss that is present in tunnel-cathode structures.

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Model Hamiltonian

Phonons

$$H = \mathbf{p}^2/2m - \mathbf{F}\cdot\mathbf{x} + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + V^{-1/2} \sum_{\mathbf{k}} (C_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} + C_{\mathbf{k}}^{*} a_{\mathbf{k}}^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{x}}).$$

Electron moving in an electric field

Electron-phonon interactions

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More recent extensions --

Ab initio path integral molecular dynamics: Basic ideas

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Max-Planck-Institut für Festköperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

(Received 12 October 1995; accepted 6 December 1995)

The essential ideas underlying *ab initio* path integral molecular dynamics and its efficient numerical implementation are discussed. In this approach the nuclei are treated as quantum particles within the path integral formulation of quantum statistical mechanics. The electronic degrees of freedom are treated explicitly based on state-of-the-art electronic structure theory. This renders *ab initio* simulations of quantum systems possible without recourse to model potentials. A combined extended Lagrangian for both quantum nuclei and electrons defines a dynamical system and yields molecular dynamics trajectories that can be analyzed to obtain quantum statistical expectation values of time-independent operators. The methodology can be applied to a wide range of fields addressing problems in molecular and condensed matter chemistry and physics. © *1996 American Institute of Physics.* [S0021-9606(96)03410-2]

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