Lectures 1-3

The two projects of Physics 142

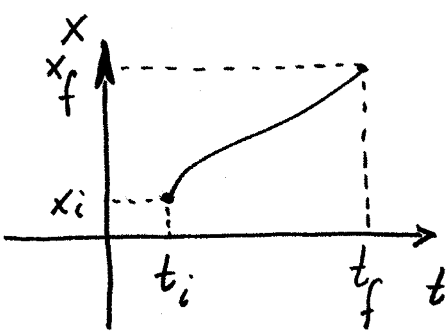
We will study computational method to do

I The Feynman Path Integral

II Quantum Monte Carlo

Feynman Path Integral

Elevates Action Principle to quantum theory



particle moving in one dimension

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

classical action

$$L = K - V$$

$$K = \frac{1}{2} m \dot{x}^2$$

$$V(x) = \begin{cases} 0 & \text{free particle} \\ \frac{1}{2} m \omega^2 x^2 & \text{oscillator} \\ \vdots & \end{cases}$$

$\delta S = 0$ Action Principle (fixed initial and final config)

Classical physics selects physical trajectory

Equivalent to Newton equation in mechanics

$$\delta S = \int_{t_i}^{t_f} \left[L(x+\delta x, \dot{x}+\delta\dot{x}) - L(x,\dot{x}) \right] dt$$

$$\delta S = \int_{t_i}^{t_f} \left(\frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial \dot{x}}\delta\dot{x} \right) dt =$$

partial integration

$$= \int_{t_i}^{t_f} \left(\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} \right) \delta x \, dt = 0$$

for arbitrary δx

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

$$\frac{\partial L}{\partial \dot{x}} = m\dot{x}$$

$$\frac{\partial L}{\partial x} = -\frac{\partial V}{\partial x}$$

$$m\ddot{x} = -\frac{\partial V}{\partial x}$$ Newton eq.

$$S_{cl} = \frac{m}{2}\frac{(x_f - x_i)^2}{t_f - t_i}$$ along classical path for free particle

In quantum mechanics:

$$K(x_f, t_f; x_i, t_i) = \langle x_f | e^{-\frac{i}{\hbar} H (t_f - t_i)} | x_i \rangle$$

probability amplitude
fundamental object

at $t = t_i$ particle is prepared at x_i
probability amplitude (complex) that particle will be found at $x = x_f$ at time $t = t_f$

$$H = K + V$$

$$\langle \psi_f | e^{-\frac{i}{\hbar} H (t_f - t_i)} | \psi_i \rangle = \int dy \int dx \; \psi_f^*(y) K(y, t_f; x, t_i) \psi_i(x)$$

at $t = t_i$ $|\psi_i\rangle$ general initial state

at $t = t_f$ $|\psi_f\rangle$ final state at $t = t_f$

$$e^{-\frac{i}{\hbar} H t} = 1 - \frac{i}{\hbar} H t - \frac{1}{2} \frac{1}{\hbar^2} H^2 t^2 + \cdots$$

Taylor expansion

If we know K we solved the problem

Feynman Path Integral determines (defines) K

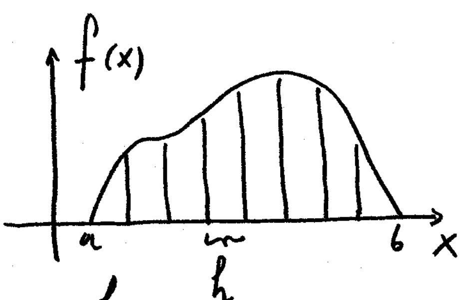
$$K(x_f, t_f; x_i, t_i) = \sum_{\text{all paths}} e^{\frac{i}{\hbar} S(\text{path})}$$

Quantum Action Principle (Feynman path integral)

naturally contains classical limit!

How to define sum over all paths?

Analogy with Riemann integral:



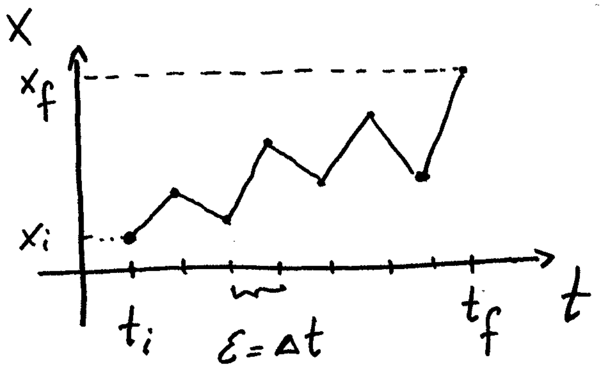
$$\int_a^b f(x)\,dx = \lim_{\substack{h \to 0 \\ N \to \infty}} \left(h \sum_{i=1}^{N} f(x_i) \right)$$

We introduce the discretization of paths:

$$N\varepsilon = t_f - t_{init}$$

$$\varepsilon = t_{k+1} - t_k \qquad t_0 = t_i \qquad t_N = t_f$$

$$x_0 = x_i \qquad x_N = x_f$$



$$A = \left(\frac{2\pi i \hbar \varepsilon}{m} \right)^{\frac{1}{2}}$$

$$K(f,i) = \lim_{\varepsilon \to 0} \frac{1}{A} \iint \cdots e^{\frac{i}{\hbar} S[f,i]} \frac{dx_1}{A} \frac{dx_2}{A} \cdots \frac{dx_{N-1}}{A}$$

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

along zig-zag paths

$$\ddot{x} = \frac{1}{\varepsilon^2} \left(x_{k+1} - 2x_k + x_{k-1} \right)$$

acceleration (discretized)

$$K(x_f, t_f; x_i, t_i) = \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S}$$

path integral

$$\hbar = \frac{h}{2\pi} = 1.0546 \times 10^{-34}\ Js = 6.5822 \times 10^{-22}\ MeVs$$

$\frac{S}{\hbar}$ is the phase of path

they are added in amplitude in $K(f,i)$

in microscopic quantum motion $S \lesssim \hbar$

all paths contribute
(quantum regime)

Consider electron moving over distance

$$x_f - x_i = 0.1 \times 10^{-8}\ cm$$

$$t_f - t_i = \frac{0.1 \times 10^{-8}\ cm}{0.3 \times 10^{10}\ \frac{cm}{s}} = 3 \times 10^{-19} s$$

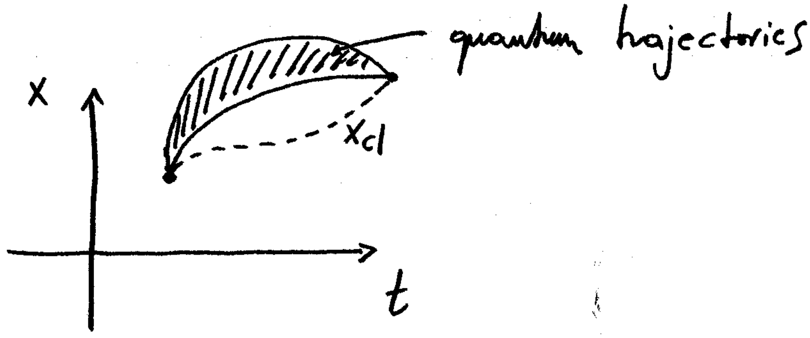
typical distance between two points inside atom

$v = 0.1\ c$ nonrelativistic

$$S = \frac{1}{2} \underbrace{0.5 \frac{MeV}{c^2}}_{m_e} \times (0.01 c^2) \times 0.3 \times 10^{-18} s = 7 \times 10^{-22}\ MeVs$$

$$\sim \hbar$$

$\frac{\delta S}{\hbar}$ phase is slowly changing in quantum motion over spread of path bundle, nonclassical trajectories all contribute.

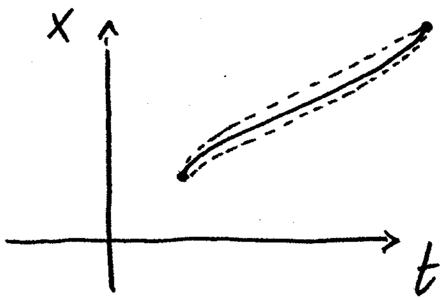


<u>Macroscopic body</u> (classical limit)

$$m = 1\ gr \qquad (\, m_e = 9.1 \times 10^{-28}\ gr \,)$$

$$v = \frac{1}{10} c \qquad S \sim 10^{17}\ MeVs \sim 10^{40}\ \hbar$$

$$l = 1\ cm$$



only very narrow band around classical path contributes

virtual quantum paths far from classical one cancel due to rapid phase variation

Feynman Path Integral Project

1. Harmonic Oscillator

    to learn the method

    path integral

    connection with statistical physics

    Monte Carlo

2. Monte Carlo Methods

    Random Numbers

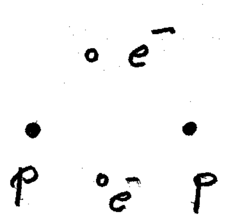
    Metropolis MC (Ising model)

    Path Integral MC

    Diffusion MC

    Hybrid Overrelaxation

3. Hydrogen Molecule



ground state energy

ground state wf