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Introduction to Feynman path integrals

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github.com/gertingold/feynman-intro

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Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

1 Motivation
2 Propagator
3 Derivation of path integral
4 Particle on a ring
5 Particle in a box
6 Harmonic oscillator

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

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1 Motivation

2 Propagator

3 Derivation of path integral

4 Particle on a ring

5 Particle in a box

6 Harmonic oscillator

Classical mechanics: Hamilton vs. Lagrange

Hamilton formalism	**Lagrange formalism**
Hamiltonian $H(q,p)$	Lagrangian $L(q,\dot{q})$
Poisson bracket $\{q,p\}=1$	action $S=\int \mathrm{d}t\, L(q,\dot{q})$
equations of motion	equation of motion from
$\dot{q}=\{q,H\}, \dot{p}=\{p,H\}$	Hamilton's principle $\delta S=0$
$\Vert$	$\Vert$
canonical quantization	?
$[\hat{q},\hat{p}]=\mathrm{i}\hbar$	$\Downarrow$
$\Downarrow$	
Heisenberg, Schrödinger, …(1925)	Dirac (1933), Feynman (1948)
Schrödinger equation	Path integral formulation of quantum mechanics
$\hat{H}\vert\Psi\rangle=\mathrm{i}\hbar\frac{\partial}{\partial t}\vert\Psi\rangle$	

Why base quantum mechanics on Lagrange formalism?

path integral formulation of quantum mechanics …

- …can provide an alternative view on physical problems
- …does without operators
  for fermionic fields, Grassmann variables are used
- …is very well suited for relativistic field theories

  action $S = \int \mathrm{d}^4 x \, \mathcal{L}(\phi, \partial_\mu \phi)$ is a Minkowski scalar

  Hamiltonian density $\mathcal{H}(\phi, \pi)$ corresponds to the $0 - 0$ component of the energy-momentum tensor
- …is very well suited to consider the semiclassical limit $S \gg \hbar$

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

1 Motivation

2 Propagator

3 Derivation of path integral

4 Particle on a ring

5 Particle in a box

6 Harmonic oscillator

Propagator

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

time evolution of a state

$$|\Psi(t)\rangle = U(t)|\Psi(0)\rangle \quad \text{with} \quad U(t) = \exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)$$

in position representation

$$\langle q_\mathrm{f}|\Psi(t)\rangle = \int \mathrm{d}q_\mathrm{i}\langle q_\mathrm{f}|U(t)|q_\mathrm{i}\rangle\langle q_\mathrm{i}|\Psi(0)\rangle$$

$$\Psi(q_\mathrm{f}, t) = \int \mathrm{d}q_\mathrm{i} K(q_\mathrm{f}, q_\mathrm{i}, t)\Psi(q_\mathrm{i}, 0)$$

$\Rightarrow$ propagator $K(q_\mathrm{f}, q_\mathrm{i}, t) = \langle q_\mathrm{f}|U(t)|q_\mathrm{i}\rangle$

Propagator of a free particle

Hamiltonian of the free particle $H = \frac{p^2}{2m}$

propagator of the free particle

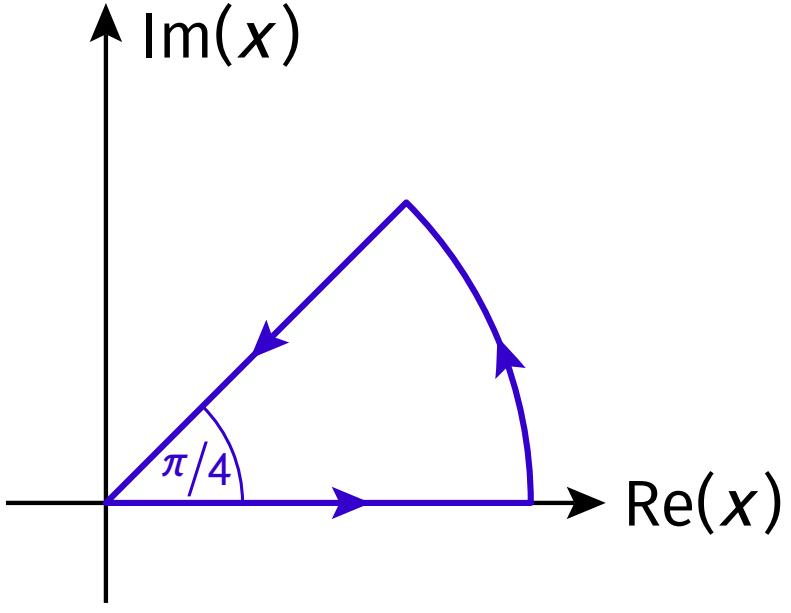
$$
\begin{aligned}
K(q_\mathrm{f}, q_\mathrm{i}, t) &= \langle q_\mathrm{f} | \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H t} | q_\mathrm{i} \rangle \\
&= \int_{-\infty}^{+\infty} \mathrm{d}p \langle q_\mathrm{f} | p \rangle \langle p | q_\mathrm{i} \rangle \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} \frac{p^2}{2m} t} \\
&= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \mathrm{d}p \exp\left[-\frac{\mathrm{i}}{\hbar} \left(\frac{p^2}{2m} t - (q_\mathrm{f} - q_\mathrm{i}) p \right) \right] \\
&= \frac{1}{2\pi\hbar} \exp\left(\frac{\mathrm{i}}{\hbar} \frac{m(q_\mathrm{f} - q_\mathrm{i})^2}{2t} \right) \int_{-\infty}^{+\infty} \mathrm{d}p \exp\left(-\frac{\mathrm{i}}{\hbar} \frac{t}{2m} p^2 \right)
\end{aligned}
$$

Digression: Fresnel integral

$$\int_0^\infty \mathrm{d}x\, \mathrm{e}^{\mathrm{i}\alpha x^2} = \mathrm{e}^{\mathrm{i}\pi/4} \int_0^\infty \mathrm{d}u\, \mathrm{e}^{-\alpha u^2}$$

$$= \frac{1}{2}\sqrt{\frac{\mathrm{i}\pi}{\alpha}}$$

$$\Rightarrow \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}\alpha x^2} = \sqrt{\frac{\pi}{\mathrm{i}\alpha}}$$



Propagator of a free particle and relation to classical properties

propagator

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \langle q_\mathrm{f}| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H t} |q_\mathrm{i}\rangle = \sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \exp\left(\frac{\mathrm{i}}{\hbar}\frac{m(q_\mathrm{f}-q_\mathrm{i})^2}{2t}\right)$$

classical motion from position q_i to q_f in time t:

- classical path $\quad q(s) = q_\mathrm{i} + (q_\mathrm{f} - q_\mathrm{i})\dfrac{s}{t}$
- classical action $\quad S_\mathrm{cl} = \int_0^t \mathrm{d}s \dfrac{m}{2}\dot{q}^2 = \dfrac{m(q_\mathrm{f}-q_\mathrm{i})^2}{2t}$

propagator of free particle in terms of classical properties

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \sqrt{-\frac{1}{2\pi \mathrm{i}\hbar}\frac{\partial^2 S_{cl}}{\partial q_\mathrm{i}\partial q_\mathrm{f}}} \exp\left(\frac{\mathrm{i}}{\hbar} S_\mathrm{cl}\right)$$

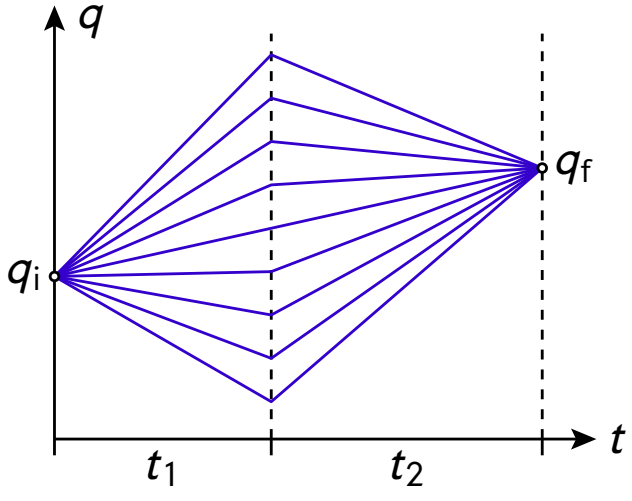
Combining two propagators

semigroup property

$$K(q_\mathrm{f}, q_\mathrm{i}, t_2 + t_1) = \langle q_\mathrm{f}| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H t_2} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H t_1} |q_\mathrm{i}\rangle$$

$$= \int_{-\infty}^{+\infty} \mathrm{d}q' \langle q_\mathrm{f}| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H t_2} |q'\rangle\langle q'| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H t_1} |q_\mathrm{i}\rangle$$

$$= \int_{-\infty}^{+\infty} \mathrm{d}q' K(q_\mathrm{f}, q', t_2) K(q', q_\mathrm{i}, t_1)$$



Exercise 1: Check the semigroup property for the propagator of a free particle.

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

1 Motivation

2 Propagator

3 Derivation of path integral

4 Particle on a ring

5 Particle in a box

6 Harmonic oscillator

Strategy for the derivation of the Feynman path integral

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Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

basic steps:

- use semigroup property to split the propagator into a large number of short-time propagators
- use the Baker-Campbell-Hausdorff formula to separate kinetic and potential contributions to the Hamiltonian in the time-evolution operator

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

application to a short-time propagator with operators T and V representing kinetic and potential energy, respectively

$$\exp\left(-\frac{\mathrm{i}}{\hbar}(T+V)\Delta t\right) = \exp\left(-\frac{\mathrm{i}}{\hbar}V\Delta t\right)\exp\left(-\frac{\mathrm{i}}{\hbar}T\Delta t\right)\exp\left(-\frac{\mathrm{i}}{\hbar^2}X\Delta t^2\right)$$

$$X = \frac{\mathrm{i}}{2}[V,T] - \frac{1}{6\hbar}\Big([V,[V,T]] - 2[T,[T,V]]\Big)\Delta t + \ldots$$

for $\Delta t \longrightarrow 0$, the last factor may be neglected

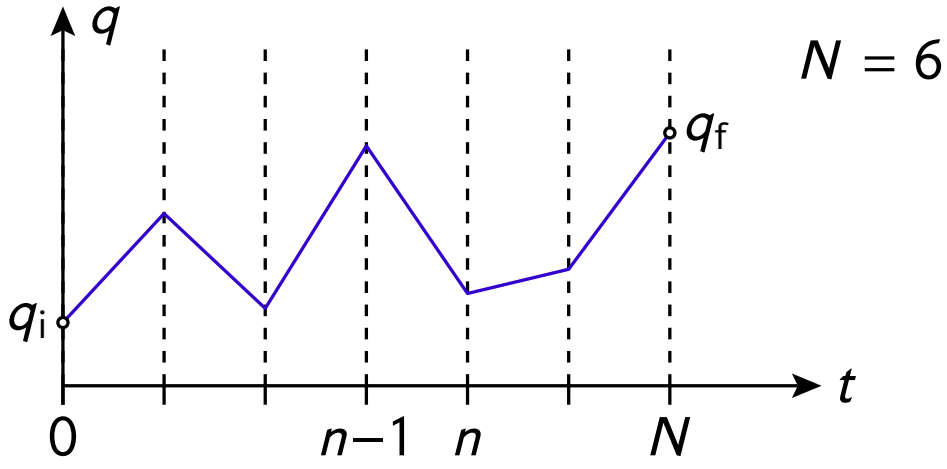
$\Longrightarrow$ Lie-Trotter formula

$$\exp\left(-\frac{\mathrm{i}}{\hbar}(T+V)t\right) = \lim_{N\to\infty}\left[\exp\left(-\frac{\mathrm{i}}{\hbar}V\frac{t}{N}\right)\exp\left(-\frac{\mathrm{i}}{\hbar}T\frac{t}{N}\right)\right]^N$$

Splitting the propagator I

propagator $\Delta t = \frac{t}{N} \quad q_0 = q_\mathrm{i} \quad q_N = q_\mathrm{f}$

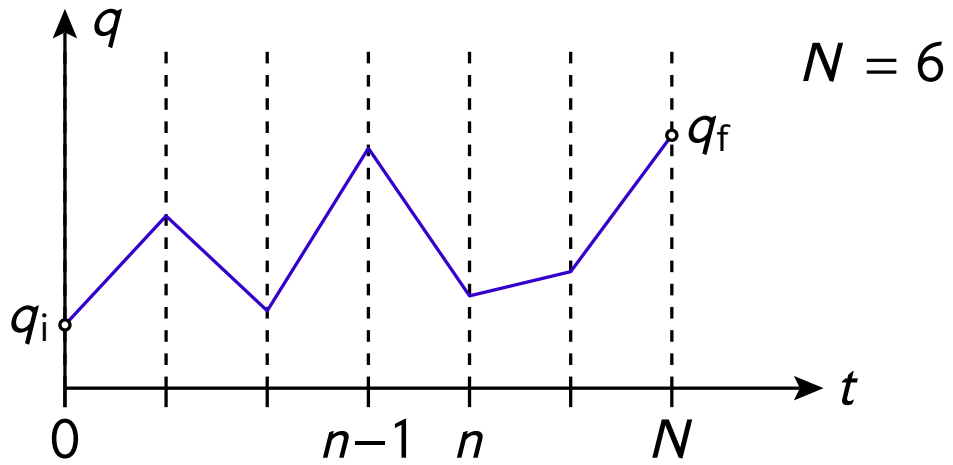
$$\langle q_\mathrm{f}|U(t)|q_\mathrm{i}\rangle = \int_{-\infty}^{+\infty} \left(\prod_{n=1}^{N-1} \mathrm{d}q_n\right) \langle q_\mathrm{f}|\cdots|q_n\rangle \underbrace{\langle q_n|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V\Delta t}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}T\Delta t}|q_{n-1}\rangle}_{\sqrt{\frac{m}{2\pi\mathrm{i}\hbar\Delta t}}\exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{m(q_n-q_{n-1})^2}{2\Delta t}-V(q_n)\Delta t\right)\right]} \langle q_{n-1}|\cdots|q_\mathrm{i}\rangle$$



Splitting the propagator II

$$\langle q_\mathrm{f}|U(t)|q_\mathrm{i}\rangle = \sqrt{\frac{m}{2\pi \mathrm{i}\hbar\Delta t}} \int_{-\infty}^{+\infty} \prod_{n=1}^{N-1} \left(\sqrt{\frac{m}{2\pi \mathrm{i}\hbar\Delta t}} \mathrm{d}q_n \right)$$

$$\times \exp\left[\frac{\mathrm{i}}{\hbar} \sum_{n=1}^{N} \left(\frac{m}{2} \left(\frac{q_n - q_{n-1}}{\Delta t} \right)^2 - V(q_n) \right) \Delta t \right]$$



let us now take the continuum limit $N \longrightarrow \infty$

Action

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$$\lim_{N\to\infty} \sum_{n=1}^{N} \left(\frac{m}{2} \left(\frac{q_n - q_{n-1}}{\Delta t} \right)^2 - V(q_n) \right) \Delta t = \int_0^t \mathrm{d}s \left(\frac{m}{2} \dot{q}(s)^2 - V(q) \right)$$

in the exponent of the propagator, we find the action functional

$$S[q] = \int_0^t \mathrm{d}s \left(\frac{m}{2} \dot{q}(s)^2 - V\big(q(s)\big) \right)$$

which takes a function $q(s)$ and returns a number S

$\Rightarrow$ we have obtained a connection between the Lagrange formalism of classical mechanics and the quantum mechanical propagator

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

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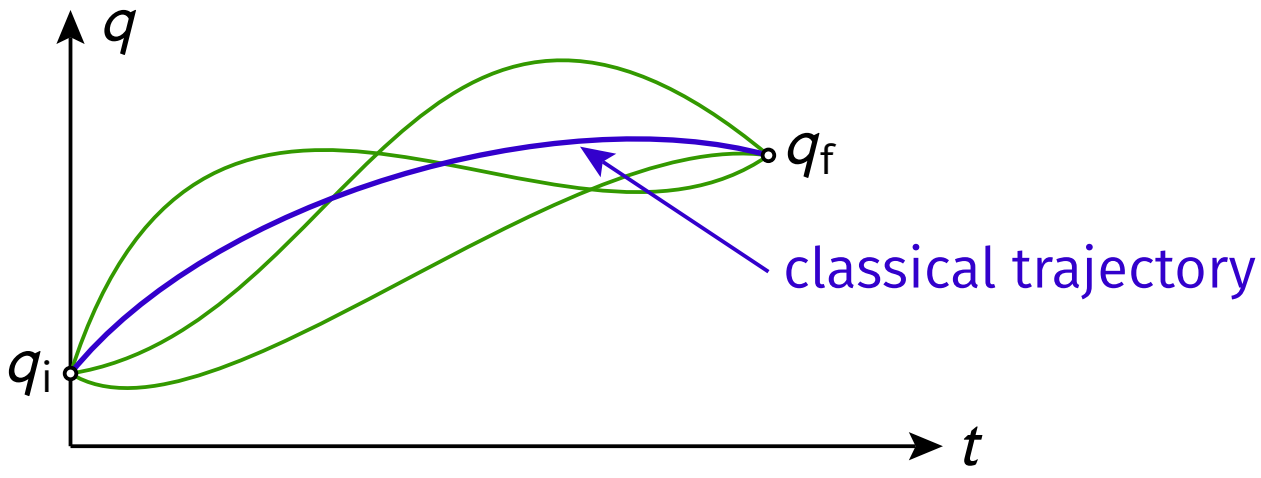
Harmonic oscillator

propagator as functional integral (Feynman path integral)

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \int_{q(0)=q_\mathrm{i}}^{q(t)=q_\mathrm{f}} \mathcal{D}q \, exp\left(\frac{\mathrm{i}}{\hbar} S[q]\right)$$

the integral runs over all trajectories $q(s)$ satisfying the boundary conditions $q(0) = q_\mathrm{i}$ and $q(t) = q_\mathrm{f}$



Evaluation of a Feynman path integral

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

- evaluate discretized version as an N-dimensional integral

  for linear systems, the following relation is useful:

$$\int_{-\infty}^{+\infty} \mathrm{d}x^N \exp\left(-\mathbf{x}^\mathsf{T}\mathbf{A}\mathbf{x}\right) = \sqrt{\frac{\pi^N}{\det(\mathbf{A})}}$$

- expansion in a complete set of functions

  $\longrightarrow$ see our later discussion of the harmonic oscillator

Exercise 2: Evaluate the Feynman path integral for the free particle by means of discretization. Why is the result independent of N?

Introduction to Feynman path integrals

Motivation

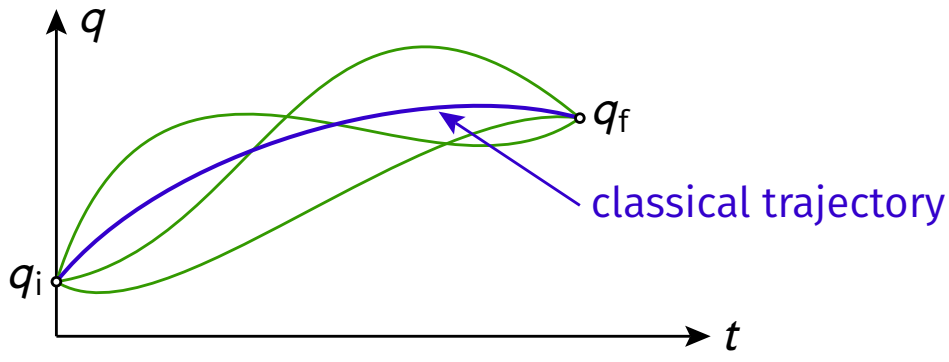
Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator



- All trajectories connecting initial to final point in the given time contribute to the propagator.
- Almost all of these trajectories are not solutions of the corresponding classical equation of motion.
- Each trajectory contributes with a phase factor depending on the action associated with the trajectory, cf. double slit.
- The nonclassical trajectories can be viewed as contributions of quantum fluctuations.

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

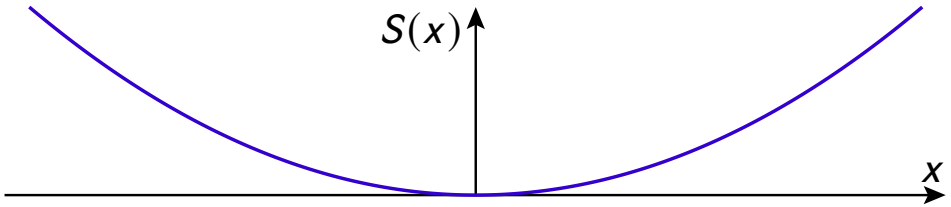
Particle in a box

Harmonic oscillator

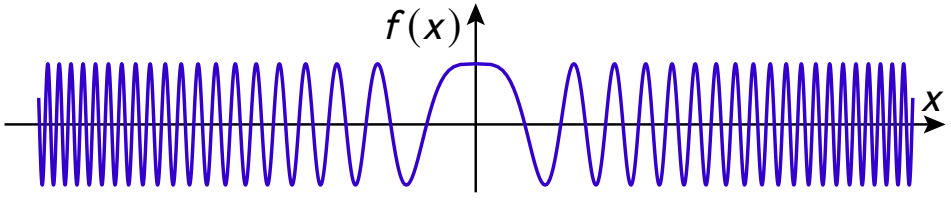
Conventional integral as an analogy:

$S(x) = x^2$

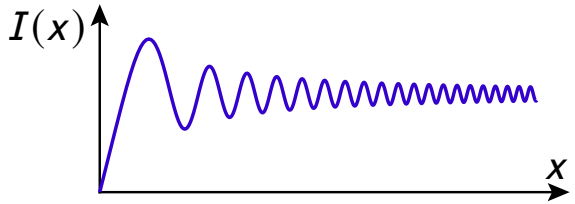
$x = 0$ corresponds to classical trajectory



$f(x) = \cos(S(x))$



$I(x) = \int_{-x}^{x} \mathrm{d}u \cos(S(u))$



The dominant contributions come from stationary points of the action and fluctuations around it.

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

1 Motivation
2 Propagator
3 Derivation of path integral
4 Particle on a ring
5 Particle in a box
6 Harmonic oscillator

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

particle of mass m on a ring of radius R

Hamiltonian $H = -\frac{\hbar^2}{2mR^2}\frac{\mathrm{d}^2}{\mathrm{d}\phi^2}$

eigenfunctions with $\psi(0) = \psi(2\pi)$ and $\psi'(0) = \psi'(2\pi)$

$$\psi_\ell(\phi) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}\ell\phi} \qquad \ell = 0, \pm 1, \pm 2, \ldots$$

eigenenergies

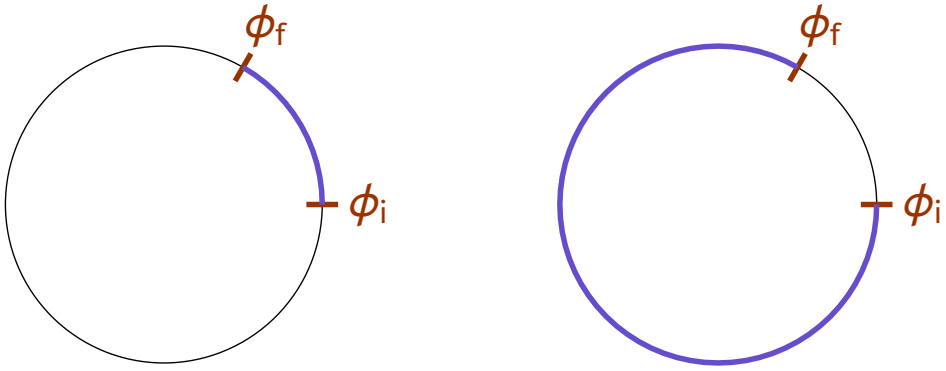
$$E_\ell = \frac{\hbar^2 \ell^2}{2mR^2}$$

propagator

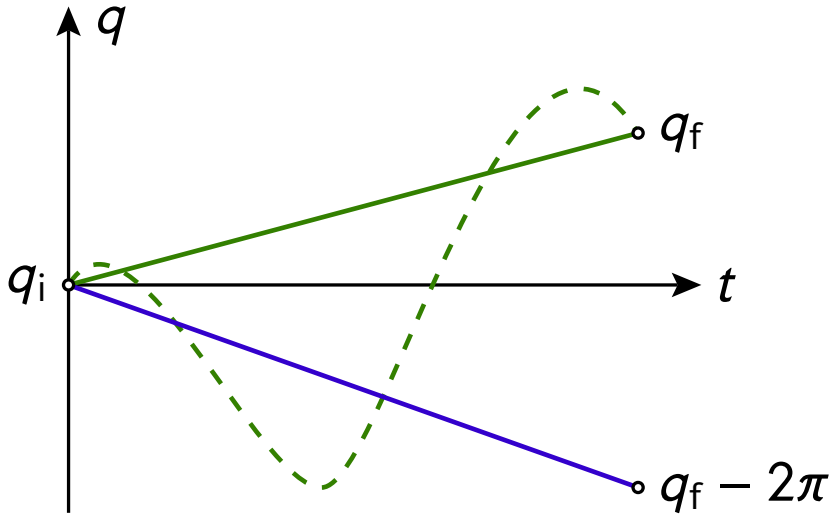
$$K(\phi_\mathrm{f}, \phi_\mathrm{i}, t) = \frac{1}{2\pi} \sum_{\ell=-\infty}^{+\infty} \exp\left(\mathrm{i}\ell(\phi_\mathrm{f} - \phi_\mathrm{i}) - \mathrm{i}\frac{\hbar\ell^2}{2mR^2} t\right)$$

More than one way

two ways to reach ϕ_f:

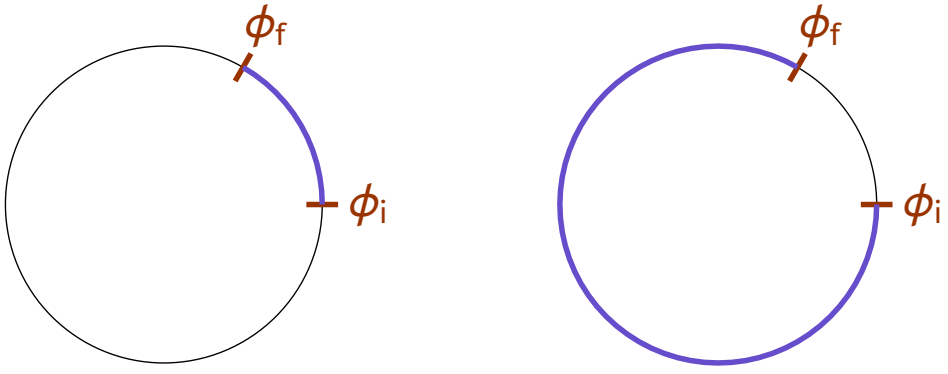


- the two paths cannot be deformed into each other



More than one way

two ways to reach ϕ_f:



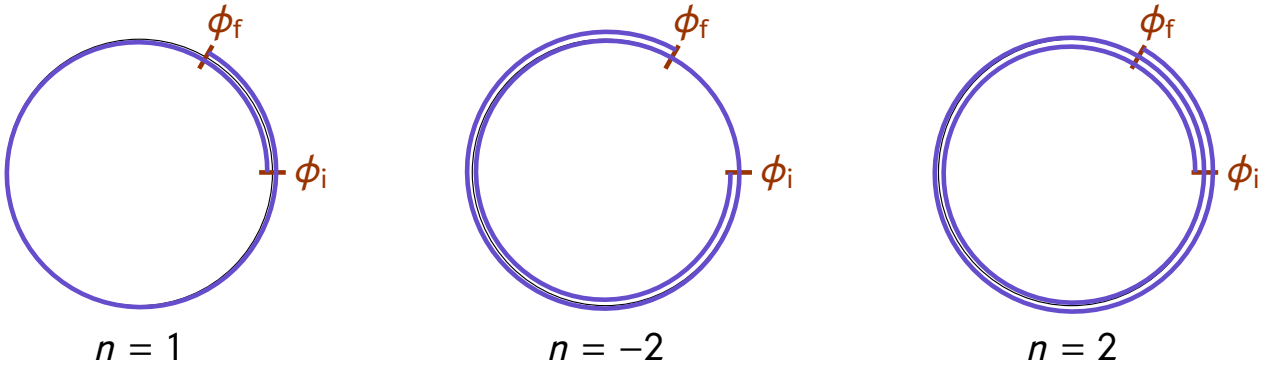
- the two paths cannot be deformed into each other
- two contributions:

$$R\sqrt{\frac{m}{2\pi i\hbar t}}\exp\left(\frac{i}{\hbar}\frac{mR^2}{2}\frac{(\phi_f-\phi_i)^2}{t}\right) \quad \text{and}$$

$$R\sqrt{\frac{m}{2\pi i\hbar t}}\exp\left(\frac{i}{\hbar}\frac{mR^2}{2}\frac{\left((\phi_f-2\pi)-\phi_i\right)^2}{t}\right)$$

but there is more …

Winding numbers and propagator



- the angles ϕ_f and $\phi_f + 2\pi n$ have to be identfied
- the propagator is a sum over all topologically distinct contributions

$$K(\phi_f, \phi_i, t) = R\sqrt{\frac{m}{2\pi i\hbar t}} \sum_{n=-\infty}^{+\infty} \exp\left(\frac{i}{\hbar}\frac{mR^2}{2}\frac{(\phi_f - \phi_i - 2\pi n)^2}{t}\right)$$

Dual representations

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

two different expressions for the propagator

winding number

$$K(\phi_\mathrm{f}, \phi_\mathrm{i}, t) = R\sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \sum_{n=-\infty}^{+\infty} \exp\left(\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2}\frac{(\phi_\mathrm{f} - \phi_\mathrm{i} - 2\pi n)^2}{t}\right)$$

angular momentum

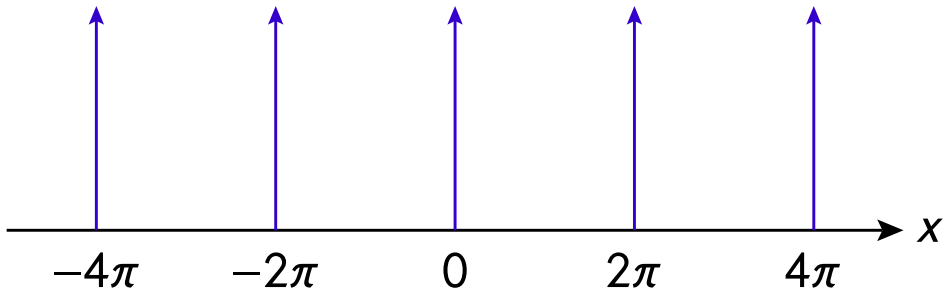
$$K(\phi_\mathrm{f}, \phi_\mathrm{i}, t) = \frac{1}{2\pi} \sum_{\ell=-\infty}^{+\infty} \exp\left(\mathrm{i}\ell(\phi_\mathrm{f} - \phi_\mathrm{i}) - \mathrm{i}\frac{\hbar\ell^2}{2mR^2}t\right)$$

compare with propagator of free particle

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{d}p}{\hbar} \exp\left(\mathrm{i}\frac{p}{\hbar}(q_\mathrm{f} - q_\mathrm{i}) - \mathrm{i}\frac{p^2}{2\hbar m}t\right)$$

A useful relation

Fourier representation of a periodic δ-comb



$$\sum_{n=-\infty}^{+\infty} \delta(x - 2\pi n) = \frac{1}{2\pi} \sum_{\ell=-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}\ell x}$$

Exercise 3: Verify this relation.

Relating the two representations

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

$$
\begin{aligned}
K(\phi_\mathrm{f}, \phi_\mathrm{i}, t) &= R\sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \sum_{n=-\infty}^{+\infty} \exp\left(\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2}\frac{(\phi_\mathrm{f}-\phi_\mathrm{i}-2\pi n)^2}{t}\right) \\
&= R\sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \int_{-\infty}^{+\infty} \mathrm{d}\phi \exp\left(\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2t}\phi^2\right) \sum_{n=-\infty}^{+\infty} \delta\big(\phi - (\phi_\mathrm{f}-\phi_\mathrm{i}-2\pi n)\big) \\
&= \frac{R}{2\pi}\sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \sum_{\ell=-\infty}^{+\infty} \exp\big(-\mathrm{i}\ell(\phi_\mathrm{f}-\phi_\mathrm{i})\big) \int_{-\infty}^{+\infty} \mathrm{d}\phi \exp\left(\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2t}\phi^2 + \mathrm{i}\ell\phi\right) \\
&= \frac{1}{2\pi} \sum_{\ell=-\infty}^{+\infty} \exp\left(\mathrm{i}\ell(\phi_\mathrm{f}-\phi_\mathrm{i}) - \mathrm{i}\frac{\hbar\ell^2}{2mR^2}t\right) \qquad \checkmark
\end{aligned}
$$

Exercise 4: Fill in the missing details.

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Motivation

Propagator

Derivation of path integral

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Particle in a box

Harmonic oscillator

1 Motivation
2 Propagator
3 Derivation of path integral
4 Particle on a ring
5 Particle in a box
6 Harmonic oscillator

Standard approach

particle of mass m in an infinitely deep potential well of width L

Hamiltonian $H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}q^2}$

eigenfunctions with $\psi(0) = \psi(L) = 0$

$$\psi_j(q) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi j}{L}q\right) \qquad j = 1, 2, 3, \ldots$$

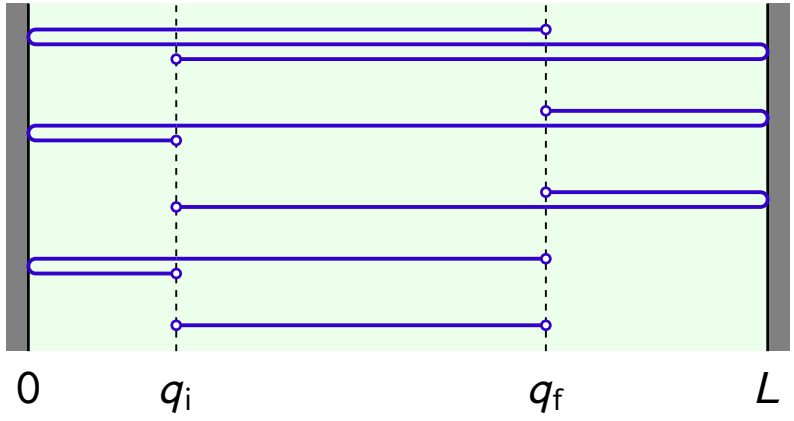
eigenenergies

$$E_j = \frac{\hbar^2\pi^2}{2mL^2}j^2$$

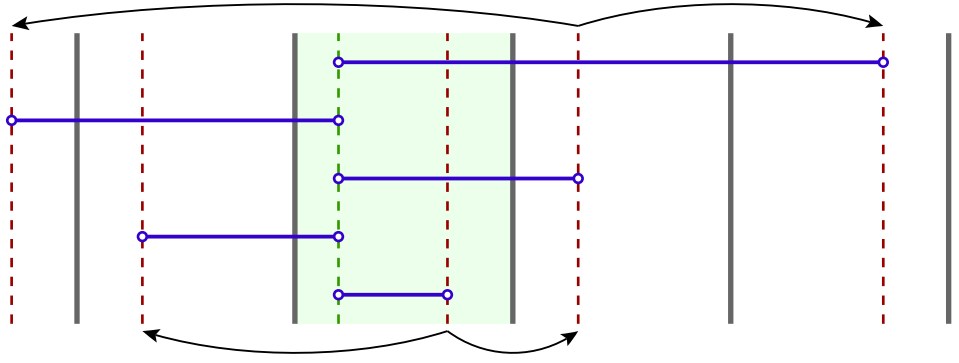
propagator

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \frac{2}{L}\sum_{j=1}^{\infty}\exp\left(-\mathrm{i}\frac{\hbar\pi^2 j^2}{2mL^2}t\right)\sin\left(\frac{\pi j}{L}q_\mathrm{f}\right)\sin\left(\frac{\pi j}{L}q_\mathrm{i}\right)$$

Possible trajectories

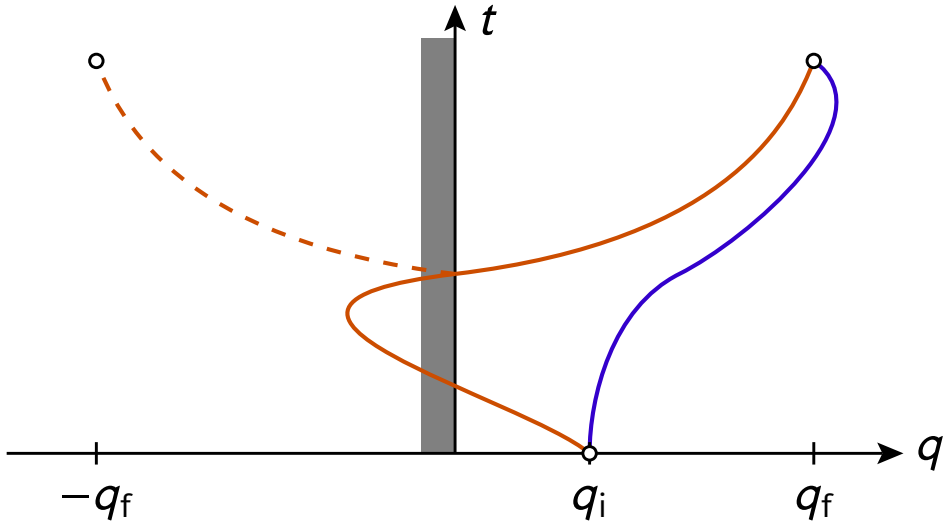


unfolding of the trajectories



- sum over propagators of a free particle
- relative phase between the various contributions?

Influence of a wall



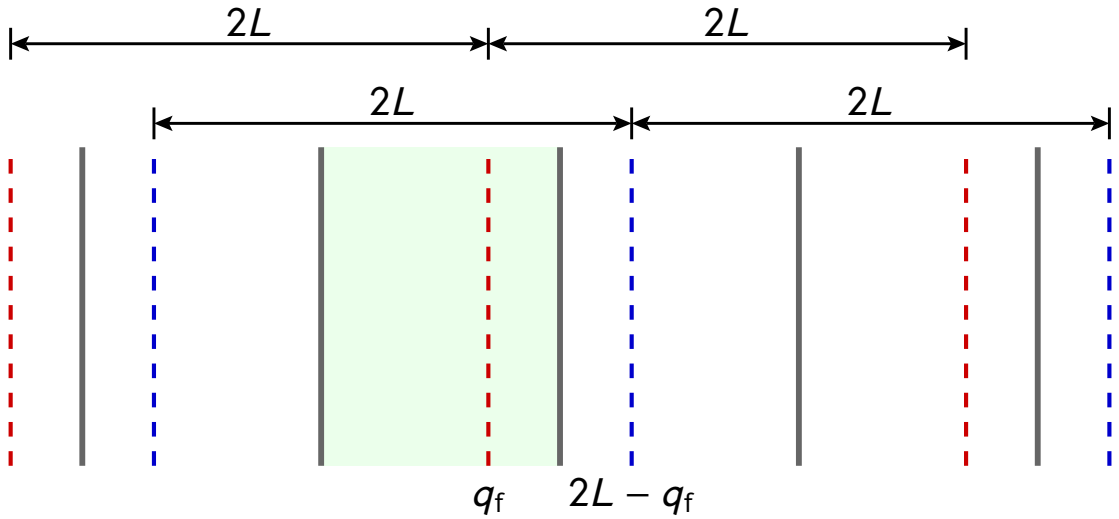
subtract the contribution of paths crossing the wall:

$$K_{\text{wall}}(q_f, q_i, t) = K_{\text{free}}(q_f, q_i, t) - K_{\text{free}}(-q_f, q_i, t)$$

- compare with method of images in electrostatics
- each reflection yields a factor -1

A. Auerbach, L. S. Schulman, J. Phys. A: Math. Gen. **30**, 5993 (1997)

Propagator for particle in a box



even number of reflections at $q = q_f + 2nL$

odd number of reflections at $q = 2nL - q_f$

propagator

$$K(q_f, q_i, t) = \sqrt{\frac{m}{2\pi i\hbar t}} \sum_{n=-\infty}^{+\infty} \left[\exp\left(\frac{i}{\hbar} \frac{m(2nL + q_f - q_i)^2}{2t} \right) - \exp\left(\frac{i}{\hbar} \frac{m(2nL - q_f - q_i)^2}{2t} \right) \right]$$

W. Janke, H. Kleinert, Lett. Nuovo Cim. **25**, 297 (1979); M. Goodman, Am. J. Phys. **49**, 843 (1981)

Two versions of the propagator

again, we have obtained two dual versions of the propagator:

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \frac{2}{L} \sum_{j=1}^{\infty} \exp\left(-\mathrm{i}\frac{\hbar\pi^2 j^2}{2mL^2} t\right) \sin\left(\frac{\pi j}{L} q_\mathrm{f}\right) \sin\left(\frac{\pi j}{L} q_\mathrm{i}\right)$$

and

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}} \sum_{n=-\infty}^{+\infty} \left[\exp\left(\frac{\mathrm{i}}{\hbar} \frac{m(2nL + q_\mathrm{f} - q_\mathrm{i})^2}{2t}\right) - \exp\left(\frac{\mathrm{i}}{\hbar} \frac{m(2nL - q_\mathrm{f} - q_\mathrm{i})^2}{2t}\right) \right]$$

Exercise 5: Show that the two representations of the propagator of a particle in a box agree. Follow the strategy which proved successful already for the particle on a ring.

Universität Augsburg University

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

1 Motivation

2 Propagator

3 Derivation of path integral

4 Particle on a ring

5 Particle in a box

6 Harmonic oscillator

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

path integral representation of the propagator of the harmonic oscillator

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \int_{q(0)=q_\mathrm{i}}^{q(t)=q_\mathrm{f}} \mathcal{D}q \exp\left[\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s \frac{m}{2}\left(\left(\frac{\mathrm{d}q}{ds}\right)^2 - \omega^2 q^2\right)\right]$$

How do we integrate over all functions satisfying the boundary conditions $q(0) = q_\mathrm{i}$ and $q(t) = q_\mathrm{f}$?

- decompose path into two contributions:
  - a path satisfying the boundary conditions
  - fluctuations around this path described by a complete set of functions vanishing at the boundaries
- integrate over the expansion coefficients of the fluctuations

Path decomposition and action

$$q(s) = \bar{q}(s) + \xi(s)$$

$$\text{with} \quad q(0) = q_\mathrm{i}, q(t) = q_\mathrm{f} \quad \text{and} \quad \xi(0) = \xi(t) = 0$$

action

$$S[q] = \int_0^t \mathrm{d}s \frac{m}{2} \left[\left(\frac{\mathrm{d}q}{\mathrm{d}s} \right)^2 - \omega^2 q^2 \right]$$

$$= \int_0^t \mathrm{d}s \frac{m}{2} \left[\left(\frac{\mathrm{d}\bar{q}}{\mathrm{d}s} \right)^2 - \omega^2 \bar{q}^2 + 2 \frac{\mathrm{d}\bar{q}}{\mathrm{d}s} \frac{\mathrm{d}\xi}{\mathrm{d}s} - 2\omega^2 \bar{q}\xi + \left(\frac{\mathrm{d}\xi}{\mathrm{d}s} \right)^2 - \omega^2 \xi^2 \right]$$

integration by parts

$$= \int_0^t \mathrm{d}s \frac{m}{2} \left[\left(\frac{\mathrm{d}\bar{q}}{\mathrm{d}s} \right)^2 - \omega^2 \bar{q}^2 - 2 \left(\frac{\mathrm{d}^2\bar{q}}{\mathrm{d}s^2} + \omega^2 \bar{q} \right) \xi + \left(\frac{\mathrm{d}\xi}{\mathrm{d}s} \right)^2 - \omega^2 \xi^2 \right]$$

linear term in ξ vanishes if $\bar{q}(s)$ solves the equation of motion

Expansion around classical solution

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Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

$$q(s) = q_{\mathrm{cl}}(s) + \xi(s)$$

action

$$\begin{aligned} S[q] &= \int_0^t \mathrm{d}s \frac{m}{2} \left[\left(\frac{\mathrm{d}q_{\mathrm{cl}}}{\mathrm{d}s} \right)^2 - \omega^2 q_{\mathrm{cl}}^2 + \left(\frac{\mathrm{d}\xi}{\mathrm{d}s} \right)^2 - \omega^2 \xi^2 \right] \\ &= S_{\mathrm{cl}} + \int_0^t \mathrm{d}s \frac{m}{2} \left[\left(\frac{\mathrm{d}\xi}{\mathrm{d}s} \right)^2 - \omega^2 \xi^2 \right] \end{aligned}$$

- expansion around the classical path makes linear term in ξ disappear because $\delta S = 0$ for classical paths
- for the harmonic oscillator:
  - classical action S_{cl} contains the full dependence on q_{i} and q_{f}
  - fluctuation part is independent of q_{i} and q_{f} and only contributes to the prefactor

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

general solution of the equation of motion of the harmonic oscillator

$$q_{\mathrm{cl}}(s) = A\cos(\omega s) + B\sin(\omega s)$$

boundary conditions

$$q_{\mathrm{cl}}(0) = q_{\mathrm{i}} = A$$
$$q_{\mathrm{cl}}(t) = q_{\mathrm{f}} = A\cos(\omega t) + B\sin(\omega t)$$

classical solution satisfying the boundary conditions

$$q_{\mathrm{cl}}(s) = q_{\mathrm{i}}\cos(\omega s) + \frac{q_{\mathrm{f}} - q_{\mathrm{i}}\cos(\omega t)}{\sin(\omega t)}\sin(\omega s)$$
$$= q_{\mathrm{i}}\frac{\sin\left(\omega(t-s)\right)}{\sin(\omega t)} + q_{\mathrm{f}}\frac{\sin(\omega s)}{\sin(\omega t)}$$

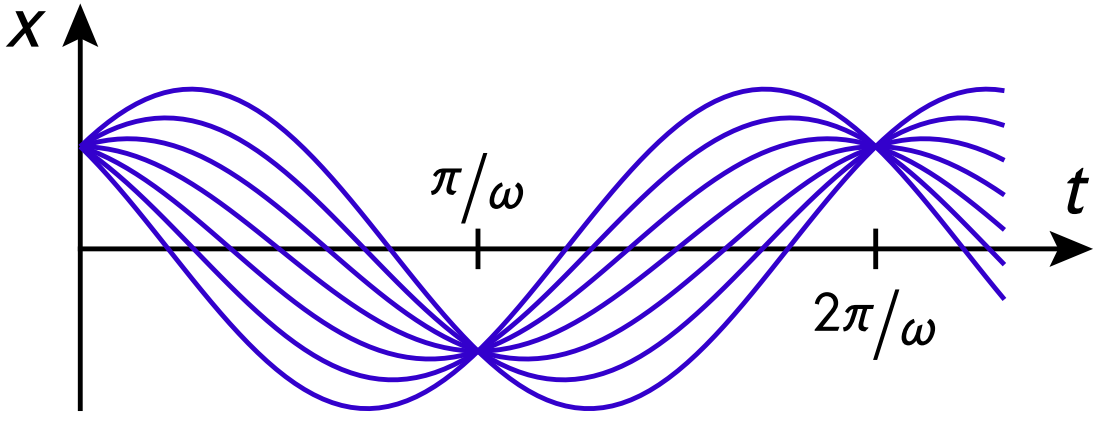
Existence of classical solution

$$q_{\mathrm{cl}}(s) = q_{\mathrm{i}} \frac{\sin\left(\omega(t-s)\right)}{\sin(\omega t)} + q_{\mathrm{f}} \frac{\sin(\omega s)}{\sin(\omega t)}$$

What happens for $t = \frac{\pi n}{\omega}$?

boundary value problems …

- …do not necessarily have a solution
- …may have more than one solution



Classical action

$$S_{\mathrm{cl}} = \int_0^t \mathrm{d}s \frac{m}{2} \left(\dot{q}_{\mathrm{cl}}^2(s) - \omega^2 q_{\mathrm{cl}}^2(s) \right)$$

integration by parts

$$= \frac{m}{2} q_{\mathrm{cl}}(s) \dot{q}_{\mathrm{cl}}(s) \Big|_0^t - \int_0^t \mathrm{d}s \frac{m}{2} q_{\mathrm{cl}}(s) \left(\ddot{q}_{\mathrm{cl}}(s) + \omega^2 q_{\mathrm{cl}}(s) \right)$$

$$= \frac{m}{2} \left(q_{\mathrm{cl}}(t) \dot{q}_{\mathrm{cl}}(t) - q_{\mathrm{cl}}(0) \dot{q}_{\mathrm{cl}}(0) \right)$$

$$\dot{q}_{\mathrm{cl}}(0) = \omega \frac{q_{\mathrm{f}} - q_{\mathrm{i}} \cos(\omega t)}{\sin(\omega t)} \qquad \dot{q}_{\mathrm{cl}}(t) = \omega \frac{q_{\mathrm{f}} \cos(\omega t) - q_{\mathrm{i}}}{\sin(\omega t)}$$

classical action of the harmonic oscillator

$$S_{\mathrm{cl}} = \frac{m\omega}{2} \frac{\left(q_{\mathrm{f}}^2 + q_{\mathrm{i}}^2 \right) \cos(\omega t) - 2 q_{\mathrm{f}} q_{\mathrm{i}}}{\sin(\omega t)}$$

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

fluctuation part of the action

$$\int_0^t \mathrm{d}s \frac{m}{2}\left(\dot{\xi}^2 - \omega^2\xi^2\right) = \underbrace{\frac{m}{2}\xi(s)\dot{\xi}(s)\Big|_0^t}_{=0} - \int_0^t \mathrm{d}s \frac{m}{2}\xi\left(\ddot{\xi} + \omega^2\xi\right)$$

$$= -\int_0^t \mathrm{d}s \frac{m}{2}\xi\left(\frac{\mathrm{d}^2}{\mathrm{d}s^2} + \omega^2\right)\xi$$

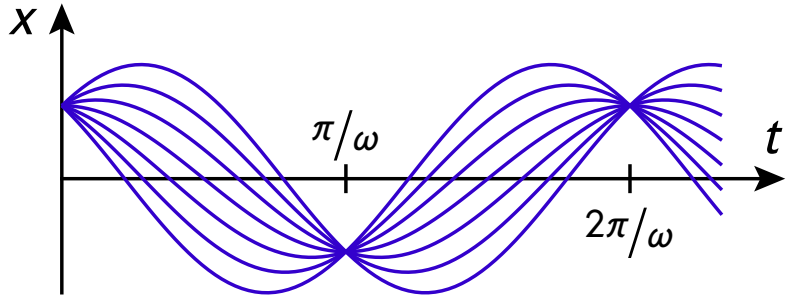
expand the fluctuations in the complete set of eigenfunctions of $\frac{\mathrm{d}^2}{\mathrm{d}s^2} + \omega^2$ vanishing at the boundaries:

$$-\left(\frac{\mathrm{d}^2}{\mathrm{d}s^2} + \omega^2\right)\xi_n(s) = \lambda_n\xi_n(s)$$

Eigenfunctions and -values

$$\xi_n(s) = \sqrt{\frac{2}{t}} \sin\left(\pi n \frac{s}{t}\right) \qquad \lambda_n = \frac{\pi^2 n^2}{t^2} - \omega^2 \qquad n = 1, 2, \ldots$$

- $0 \leq \omega t < \pi$: $\lambda_n > 0$ for all n
  classical action is a minimum
- $\omega t = \pi$: $a_1 \xi_1(s)$ is a classical solution for all amplitudes a_1



- $\pi < \omega t < 2\pi$: $\lambda_1 < 0$, $\lambda_n > 0$ for $n = 2, 3, \ldots$
  classical action is a saddle point
- ...

Total action and propagator

action

$$S[q] = S_{\mathrm{cl}} + \sum_{n=1}^{\infty} \frac{m}{2} \left(\frac{\pi^2 n^2}{t^2} - \omega^2 \right) a_n^2$$

propagator

$$K(q_{\mathrm{f}}, q_{\mathrm{i}}, t) \sim \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} \left(\prod_{n=1}^{\infty} \mathrm{d}a_n \right) \exp \left[\frac{\mathrm{i}}{\hbar} \left(S_{\mathrm{cl}} + \frac{m}{2} \sum_{n=1}^{\infty} \lambda_n a_n^2 \right) \right]$$

$$\sim \left(\prod_{n=1}^{\infty} \lambda_n \right)^{-1/2} \exp \left(\frac{\mathrm{i}}{\hbar} S_{\mathrm{cl}} \right)$$

fluctuation determinant

$$\det \left(-\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \omega^2 \right) = \prod_{n=1}^{\infty} \lambda_n$$

Prefactor

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

the prefactor unknown so far does not depend on ω
$\longrightarrow$ compare with propagator of the free particle

classical action

$$\lim_{\omega\to 0} \frac{m}{2} \underbrace{\frac{\omega}{\sin(\omega t)}}_{\to 1/t} \underbrace{\left((q_\mathrm{f}^2 + q_\mathrm{i}^2)\cos(\omega t) - 2q_\mathrm{f}q_\mathrm{i}\right)}_{\to (q_\mathrm{f}-q_\mathrm{i})^2} = \frac{m}{2}\frac{(q_\mathrm{f}-q_\mathrm{i})^2}{t} \qquad \checkmark$$

prefactor

$$\sqrt{\prod_{n=1}^{\infty} \frac{\lambda_n^{(0)}}{\lambda_n}} \sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}}$$

with

$$\lambda_n = \frac{\pi^2 n^2}{t^2} - \omega^2 \qquad \text{and} \qquad \lambda_n^{(0)} = \frac{\pi^2 n^2}{t^2}$$

Ratio of determinants

$$\prod_{n=1}^{\infty} \frac{\lambda_n}{\lambda_n^{(0)}} = \prod_{n=1}^{\infty} \left(1 - \left(\frac{\omega t}{\pi n}\right)^2\right) = \frac{\sin(\omega t)}{\omega t}$$

propagator of the harmonic oscillator

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \sqrt{\frac{m\omega}{2\pi \mathrm{i}\hbar \sin(\omega t)}} \exp\left(\mathrm{i}\frac{m\omega}{2\hbar} \frac{(q_\mathrm{f}^2 + q_\mathrm{i}^2)\cos(\omega t) - 2q_\mathrm{i}q_\mathrm{f}}{\sin(\omega t)}\right)$$

$$= \sqrt{\frac{m\omega}{2\pi\hbar|\sin(\omega t)|}} \exp\left(\mathrm{i}\frac{m\omega}{2\hbar} \frac{(q_\mathrm{f}^2 + q_\mathrm{i}^2)\cos(\omega t) - 2q_\mathrm{i}q_\mathrm{f}}{\sin(\omega t)} - \mathrm{i}\left(\frac{\pi}{4} + n\frac{\pi}{2}\right)\right)$$

n: number of zeros of the sine function crossed up to time t

This choice of the phase ensures the validity of the semigroup property, e.g.

$$K(q_\mathrm{f}, q', \tfrac{3\pi}{2\omega}) = \int_{-\infty}^{+\infty} \mathrm{d}q' K(q_\mathrm{f}, q', \tfrac{3\pi}{4\omega}) K(q', q_\mathrm{i}, \tfrac{3\pi}{4\omega})$$

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

Exercise 6: Use the Mehler formula

$$\sum_{n=0}^{\infty} \frac{H_n(x)H_n(y)}{n!}\left(\frac{z}{2}\right)^n = \frac{1}{\sqrt{1-z^2}}\exp\left(\frac{2xyz-(x^2+y^2)z^2}{1-z^2}\right)$$

to determine the propagator of the harmonic oscillator starting from its stationary wave functions and eigenenergies.

Exercise 7: Check the choice of phases in the propagator of the harmonic oscillator by combining two propagators over time intervals $3\pi/4\omega$ to a propagator over the time interval $3\pi/2\omega$ by means of the semigroup property.

Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

action

$$S[q] = \int_0^t \mathrm{d}s \left(\frac{m}{2} \dot{q}^2 - V(q) \right)$$

expansion around the classical solution: $q(s) = q_{\mathrm{cl}}(s) + \xi(s)$

$$\begin{aligned} S &= \int_0^t \mathrm{d}s \left(\frac{m}{2} (\dot{q}_{\mathrm{cl}}^2 + 2\dot{q}_{\mathrm{cl}}\dot{\xi} + \dot{\xi}^2) - V(q_{\mathrm{cl}}) - V'(q_{\mathrm{cl}})\xi - \frac{1}{2} V''(q_{\mathrm{cl}})\xi^2 + \dots \right) \\ &= S_{\mathrm{cl}} - \int_0^t \mathrm{d}s \underbrace{\left(m\ddot{q}_{\mathrm{cl}} + V'(q_{\mathrm{cl}}) \right)}_{=0} \xi - \frac{1}{2} \int_0^t \mathrm{d}s \xi \left(m \frac{\mathrm{d}^2}{\mathrm{d}s^2} + V''(q_{\mathrm{cl}}) \right) \xi + \dots \end{aligned}$$

- the quadratic contribution in the fluctuations generally depends on q_{f} and q_{i}
- it leads again to a determinant
- the expansion of ξ does not necessarily need to be done in terms of eigenfunctions

Fluctuation amplitude

- the second-order term in the fluctuations determines their typical amplitude

$$\frac{\xi^2}{\hbar} \sim 1 \quad \rightarrow \quad \xi \sim \sqrt{\hbar}$$

- the third-order term is smaller by a factor $\sqrt{\hbar}$ and can be neglected in the semiclassical limit
- however, higher-order terms can become relevant when the eigenvalue of a fluctuation mode approaches zero

  example: for a harmonic oscillator around $t = \pi/\omega$, weak anharmonicities of the potential may become relevant

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