Introduction to Feynman path integrals

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 github.com/gertingold/feynman-intro

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

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 $\delta S = 0$

$\parallel$ $\parallel$
canonical quantization $[\hat{q}, \hat{p}] = \mathrm{i}\hbar$?
$\Downarrow$ $\Downarrow$

Heisenberg, Schrödinger, ... (1925)   Dirac (1933), Feynman (1948)
Schrödinger equation
$\hat{H}|\Psi\rangle = \mathrm{i}\hbar\frac{\partial}{\partial t}|\Psi\rangle$

Path integral formulation
of quantum mechanics

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 $S \gg \hbar$

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

time evolution of a state

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

in position representation

$$\langle q_f|\Psi(t)\rangle = \int dq_i \langle q_f|U(t)|q_i\rangle\langle q_i|\Psi(0)\rangle$$

$$\Psi(q_f, t) = \int dq_i K(q_f, q_i, t)\Psi(q_i, 0)$$

$\implies$ propagator $\quad K(q_f, q_i, t) = \langle q_f|U(t)|q_i\rangle$

Introduction to
Feynman path
integrals

Motivation

Propagator

Derivation of path
integral

Particle on a ring

Particle in a box

Harmonic
oscillator

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

propagator of the free particle

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

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

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

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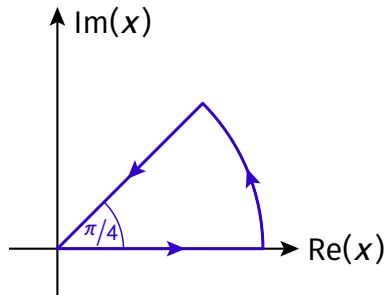
propagator

$$K(q_f, q_i, t) = \langle q_f | e^{-\frac{i}{\hbar}Ht} | q_i \rangle = \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left(\frac{i}{\hbar} \frac{m(q_f - q_i)^2}{2t} \right)$$

classical motion from position q_i to q_f in time t:

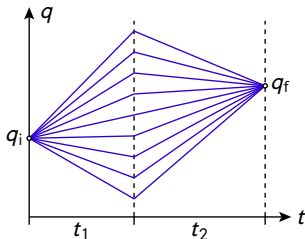- classical path $q(s) = q_i + (q_f - q_i)\dfrac{s}{t}$

- classical action $S_{cl} = \int_0^t ds \dfrac{m}{2} \dot{q}^2 = \dfrac{m(q_f - q_i)^2}{2t}$

propagator of free particle in terms of classical properties

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

semigroup property

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

$$= \int_{-\infty}^{+\infty} dq' \langle q_f | e^{-\frac{i}{\hbar} H t_2} | q' \rangle \langle q' | e^{-\frac{i}{\hbar} H t_1} | q_i \rangle$$

$$= \int_{-\infty}^{+\infty} dq' K(q_f, q', t_2) K(q', q_i, t_1)$$

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

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

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

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

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

for $\Delta t \to 0$, the last factor may be neglected
$\Rightarrow$ Lie-Trotter formula

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

propagator $\qquad \Delta t = \dfrac{t}{N} \qquad q_0 = q_\mathrm{i} \qquad q_N = q_\mathrm{f}$

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

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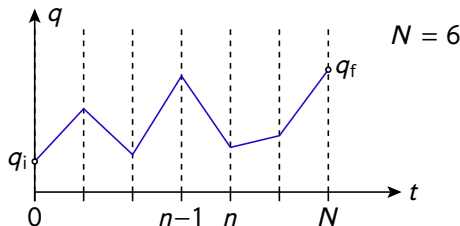
$$\langle q_{\mathrm{f}}|U(t)|q_{\mathrm{i}}\rangle = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \int_{-\infty}^{+\infty} \prod_{n=1}^{N-1}\left(\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\mathrm{d}q_n\right)$$

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

$N = 6$
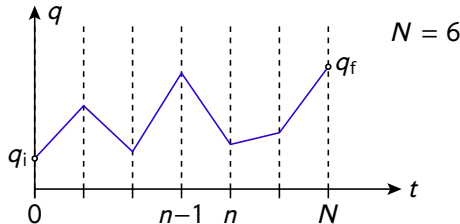
let us now take the continuum limit $N \to \infty$

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

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

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

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

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

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 $q(t) = q_\mathrm{f}$
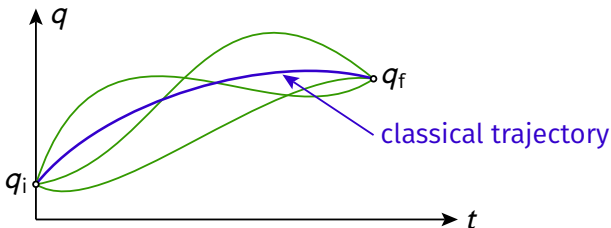
- evaluate discretized version as an N-dimensional integral
  for linear systems, the following relation is useful:

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

- expansion in a complete set of functions
  $\rightarrow$ 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?
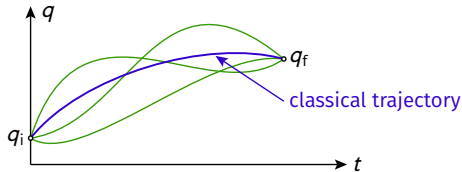
- All trajectories connecting initial to final point in the given time contribute to the propagator.

- 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.
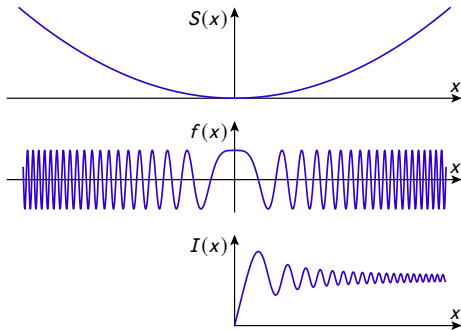
Conventional integral as an analogy:

$S(x) = x^2$

$x = 0$ corresponds to classical trajectory

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

$I(x) = \int_{-x}^{x} du \, \cos(S(u))$

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

particle of mass m on a ring of radius R

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

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

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

two ways to reach ϕ_f:
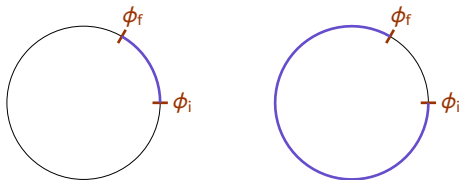
■ the two paths cannot be deformed into each other
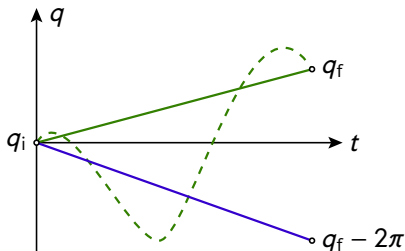
two ways to reach ϕ_f:
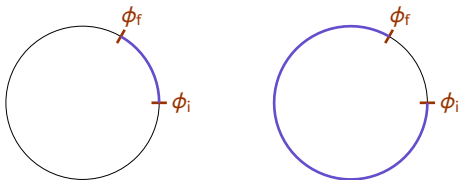
- the two paths cannot be deformed into each other
- two contributions:

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

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

but there is more …

ϕ_f ϕ_i $n = 1$

ϕ_f ϕ_i $n = -2$

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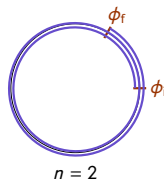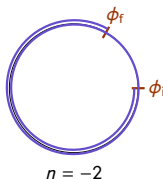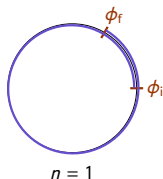
- the angles ϕ_f and $\phi_f + 2\pi n$ have to be identfied
- the propagator is a sum over all topologically distinct contributions

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

two different expressions for the propagator

winding number

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

angular momentum

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

compare with propagator of free particle

$$K(q_f, q_i, t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{dp}{\hbar} \exp\left(i\frac{p}{\hbar}(q_f - q_i) - i\frac{p^2}{2\hbar m}t\right)$$

Fourier representation of a periodic δ-comb

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

Exercise 3: Verify this relation.

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

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

$$= \frac{R}{2\pi} \sqrt{\frac{m}{2\pi i \hbar t}} \sum_{\ell=-\infty}^{+\infty} \exp^{-i\ell(\phi_f - \phi_i)} \int_{-\infty}^{+\infty} d\phi \exp\left(\frac{i}{\hbar} \frac{mR^2}{2t} \phi^2 + i\ell\phi\right)$$
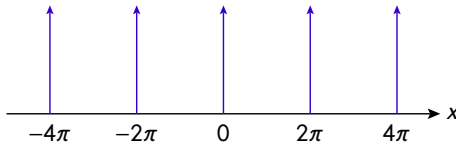
$$= \frac{1}{2\pi} \sum_{\ell=-\infty}^{+\infty} \exp\left(i\ell(\phi_f - \phi_i) - i\frac{\hbar \ell^2}{2mR^2} t\right) \quad \checkmark$$

Exercise 4: Fill in the missing details.

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

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

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

$$K(q_{\mathrm{f}}, q_{\mathrm{i}}, t) = \frac{2}{L} \sum_{j=1}^{\infty} \exp\left(-\mathrm{i}\frac{\hbar\pi^2 j^2}{2mL^2}t\right) \sin\left(\frac{\pi j}{L}q_{\mathrm{f}}\right) \sin\left(\frac{\pi j}{L}q_{\mathrm{i}}\right)$$
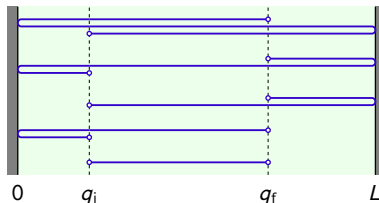
unfolding of the trajectories
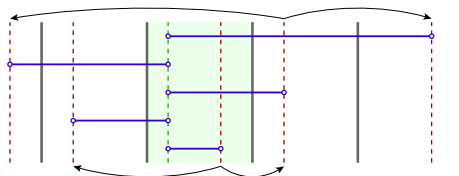
- sum over propagators of a free particle
- relative phase between the various contributions?
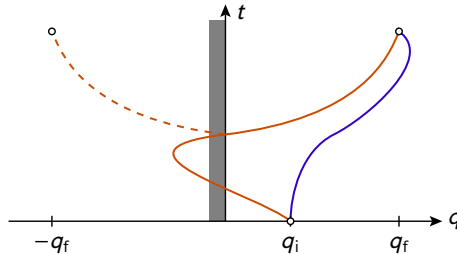
subtract the contribution of paths crossing the wall:

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

- compare with method of images in electrostatics
- each reflection yields a factor -1
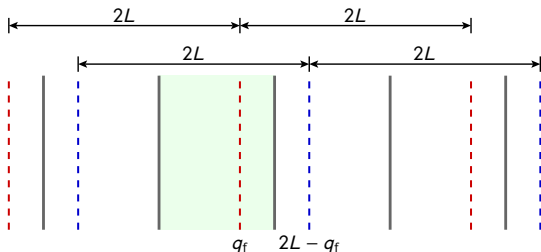
even number of reflections at $q = q_f + 2nL$
odd number of reflections at $q = 2nL - q_f$

propagator

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

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

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

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.

path integral representation of the propagator of the
harmonic oscillator

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

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

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

with $\quad q(0) = q_i, q(t) = q_f \quad$ and $\quad \xi(0) = \xi(t) = 0$

action

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

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

integration by parts

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

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

Expansion around classical solution

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Harmonic oscillator

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

action

$$S[q] = \int_0^t ds \frac{m}{2} \left[\left(\frac{dq_{cl}}{ds} \right)^2 - \omega^2 q_{cl}^2 + \left(\frac{d\xi}{ds} \right)^2 - \omega^2 \xi^2 \right]$$

$$= S_{cl} + \int_0^t ds \frac{m}{2} \left[\left(\frac{d\xi}{ds} \right)^2 - \omega^2 \xi^2 \right]$$

- 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

general solution of the equation of motion of the harmonic oscillator

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

boundary conditions

$$q_{cl}(0) = q_i = A$$
$$q_{cl}(t) = q_f = A \cos(\omega t) + B \sin(\omega t)$$

classical solution satisfying the boundary conditions

$$q_{cl}(s) = q_i \cos(\omega s) + \frac{q_f - q_i \cos(\omega t)}{\sin(\omega t)} \sin(\omega s)$$
$$= q_i \frac{\sin\left(\omega(t-s)\right)}{\sin(\omega t)} + q_f \frac{\sin(\omega s)}{\sin(\omega t)}$$

$$q_{cl}(s) = q_i \frac{\sin\big(\omega(t-s)\big)}{\sin(\omega t)} + q_f \frac{\sin(\omega s)}{\sin(\omega t)}$$

What happens for $t = \dfrac{2\pi n}{\omega}$?

boundary value problems ...

- ... do not necessarily have a solution
- ... may have more than one solution
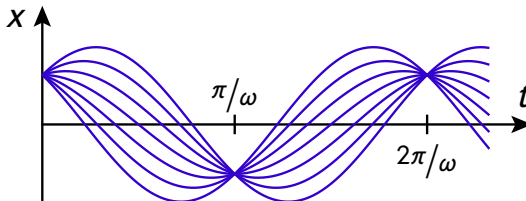
$$S_{\mathrm{cl}} = \int_0^t \mathrm{d}s \frac{m}{2} \left(\dot{q}_{\mathrm{cl}}^2(s) - \omega^2 q_{\mathrm{cl}}^2(s) \right)$$

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

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

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:

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

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

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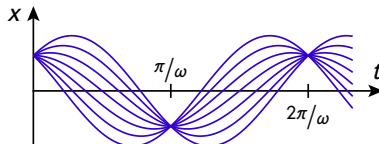
- $\pi < \omega t < 2\pi$: $\lambda_1 < 0$, $\lambda_n > 0$ for $n = 2, 3, \ldots$
  classical action is a saddle point

- …

action

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

propagator

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

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

fluctuation determinant

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

the prefactor unknown so far does not depend on ω
$\rightarrow$ 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

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

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

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

propagator of the harmonic oscillator

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

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

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.

$$K(q_f, q', \tfrac{3\pi}{2\omega}) = \int_{-\infty}^{+\infty} dq' K(q_f, q', \tfrac{3\pi}{4\omega}) K(q', q_i, \tfrac{3\pi}{4\omega})$$

Exercises for the harmonic oscillator

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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.

action

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

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

$$S = \int_0^t ds \left(\frac{m}{2}(\dot{q}_{cl}^2 + 2\dot{q}_{cl}\dot{\xi} + \dot{\xi}^2) - V(q_{cl}) - V'(q_{cl})\xi - \frac{1}{2}V''(q_{cl})\xi^2 + \ldots \right)$$

$$= S_{cl} - \int_0^t ds \underbrace{\left(m\ddot{q}_{cl} + V'(q_{cl}) \right)}_{=0} \xi - \frac{1}{2} \int_0^t ds\, \xi \left(m\frac{d^2}{ds^2} + V''(q_{cl}) \right) \xi + \ldots$$

- 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

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

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

- 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