Introduction to Feynman path integrals

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github.com/gertingold/feynman-intro

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Hamilton formalism

Hamiltonian $H(q,p)$

Poisson bracket $\{q,p\}=1$

equations of motion

$\dot{q}=\{q,H\}, \dot{p}=\{p,H\}$

$\Vert$

canonical quantization

$[\hat{q},\hat{p}]=\mathrm{i}\hbar$

$\Downarrow$

Heisenberg, Schrödinger, …(1925)

Schrödinger equation

$\hat{H}|\Psi\rangle=\mathrm{i}\hbar\frac{\partial}{\partial t}|\Psi\rangle$

Lagrange formalism

Lagrangian $L(q,\dot{q})$

action $S=\int \mathrm{d}t\, L(q,\dot{q})$

equation of motion from

Hamilton's principle $\delta S=0$

$\Vert$

?

$\Downarrow$

Dirac (1933), Feynman (1948)

Path integral formulation of quantum mechanics

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 $S \gg \hbar$

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

time evolution of a state

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

in position representation

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

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

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

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

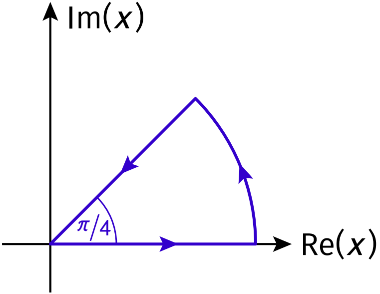
propagator of the free particle

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

Digression: Fresnel integral

$$\int_0^\infty \mathrm{d}x\, e^{\mathrm{i}\alpha x^2} = e^{\mathrm{i}\pi/4} \int_0^\infty \mathrm{d}u\, e^{-\alpha u^2}$$
$$= \frac{1}{2}\sqrt{\frac{\mathrm{i}\pi}{\alpha}}$$

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



Propagator of a free particle and relation to classical properties

propagator

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

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

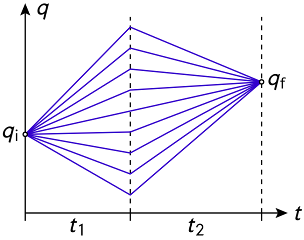
propagator of free particle in terms of classical properties

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

Combining two propagators

semigroup property

$$
\begin{aligned}
K(q_\mathrm{f}, q_\mathrm{i}, t_2 + t_1) &= \langle q_\mathrm{f}| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht_2} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht_1} |q_\mathrm{i}\rangle \\
&= \int_{-\infty}^{+\infty} \mathrm{d}q' \langle q_\mathrm{f}| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht_2} |q'\rangle\langle q'| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht_1} |q_\mathrm{i}\rangle \\
&= \int_{-\infty}^{+\infty} \mathrm{d}q' K(q_\mathrm{f}, q', t_2) K(q', q_\mathrm{i}, t_1)
\end{aligned}
$$



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

Strategy for the derivation of the Feynman path integral

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

Baker-Campbell-Hausdorff formula and Lie-Trotter formula

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

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

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

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

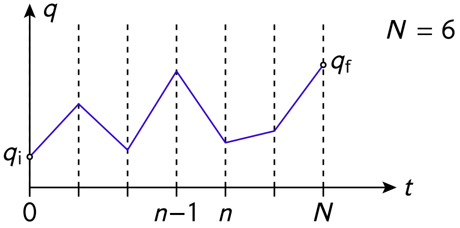
$$\exp\left(-\frac{\mathrm{i}}{\hbar}(T+V)t\right) = \lim_{N\to\infty}\left[\exp\left(-\frac{\mathrm{i}}{\hbar}V\frac{t}{N}\right)\exp\left(-\frac{\mathrm{i}}{\hbar}T\frac{t}{N}\right)\right]^N$$

Splitting the propagator I

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

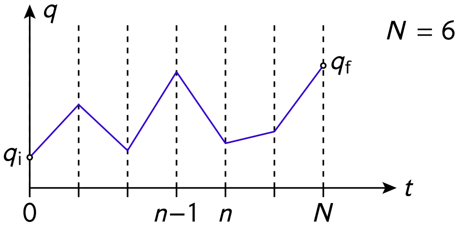
$$\langle q_\mathrm{f}|U(t)|q_\mathrm{i}\rangle =$$

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



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 $N \to \infty$

Action

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

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

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

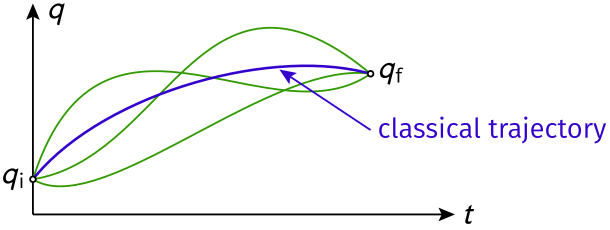
which takes a function $q(s)$ and returns a number S

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

propagator as functional integral (Feynman path integral)

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

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



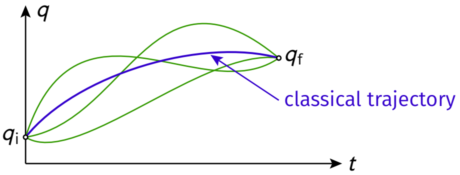
- evaluate discretized version as an N-dimensional integral
  for linear systems, the following relation is useful:

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

- 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?

Physical interpretation

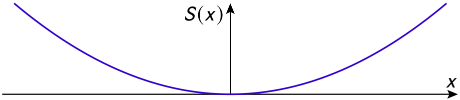


- All trajectories connecting initial to final point in the given time contribute to the propagator.
- Almost all of these trajectories are not solutions of the corresponding classical equation of motion.
- Each trajectory contributes with a phase factor depending on the action associated with the trajectory,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

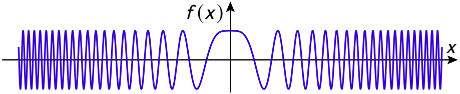
Conventional integral as an analogy:

$S(x) = x^2$

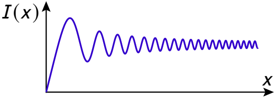
$x = 0$ corresponds to classical trajectory



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



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



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

Standard approach

particle of mass m on a ring of radius R

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

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

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

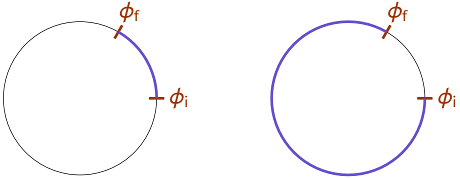
eigenenergies

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

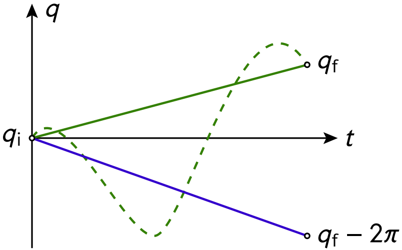
propagator

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

two ways to reach ϕ_f:

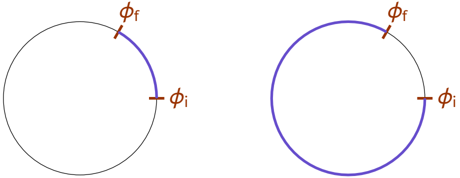


- the two paths cannot be deformed into each other



More than one way

two ways to reach ϕ_f:



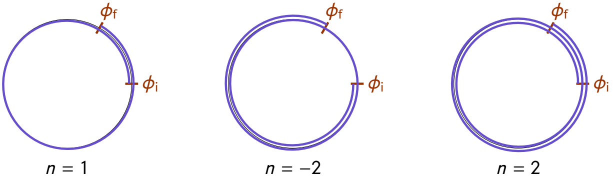
- the two paths cannot be deformed into each other
- two contributions:

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

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

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

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

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

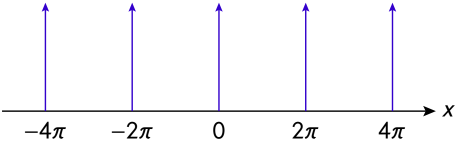
$$K(\phi_\mathrm{f}, \phi_\mathrm{i}, t) = \frac{1}{2\pi} \sum_{\ell=-\infty}^{+\infty} \exp\left(\mathrm{i}\ell(\phi_\mathrm{f}-\phi_\mathrm{i}) - \mathrm{i}\frac{\hbar\ell^2}{2mR^2}t\right)$$

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

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

$\boxed{\textit{Exercise 4:}\ \text{Fill in the missing details.}}$

Standard approach

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

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

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

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

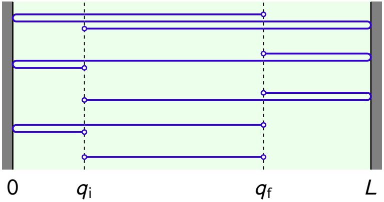
eigenenergies

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

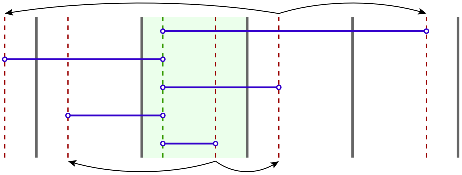
propagator

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

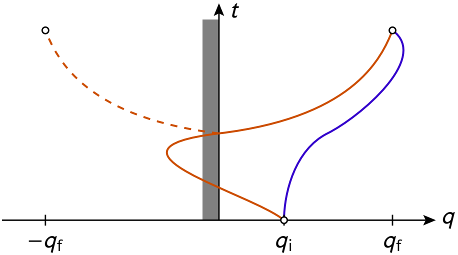
Possible trajectories



unfolding of the trajectories



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

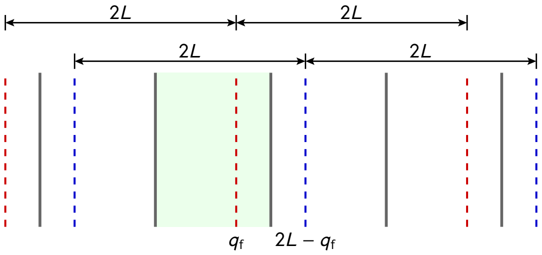


subtract the contribution of paths crossing the wall:

$$K_{\mathrm{wall}}(q_\mathrm{f}, q_\mathrm{i}, t) = K_{\mathrm{free}}(q_\mathrm{f}, q_\mathrm{i}, t) - K_{\mathrm{free}}(-q_\mathrm{f}, q_\mathrm{i}, t)$$

- 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)



even number of reflections at $q = q_\mathrm{f} + 2nL$

odd number of reflections at $q = 2nL - q_\mathrm{f}$

propagator

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

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.

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

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

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

action

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

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

Universität Augsburg University

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

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

Classical solution

general solution of the equation of motion of the harmonic oscillator

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

boundary conditions

$$\begin{aligned} q_{\text{cl}}(0) &= q_{\text{i}} = A \\ q_{\text{cl}}(t) &= q_{\text{f}} = A\cos(\omega t) + B\sin(\omega t) \end{aligned}$$

classical solution satisfying the boundary conditions

$$\begin{aligned} q_{\text{cl}}(s) &= q_{\text{i}}\cos(\omega s) + \frac{q_{\text{f}} - q_{\text{i}}\cos(\omega t)}{\sin(\omega t)}\sin(\omega s) \\ &= q_{\text{i}}\frac{\sin\big(\omega(t-s)\big)}{\sin(\omega t)} + q_{\text{f}}\frac{\sin(\omega s)}{\sin(\omega t)} \end{aligned}$$

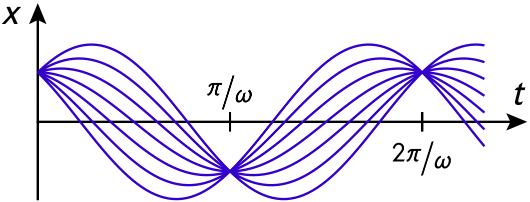
Existence of classical solution

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

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

boundary value problems …

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



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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

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

fluctuation part of the action

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

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

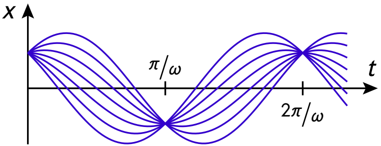
expand the fluctuations in the complete set of eigenfunctions of $\frac{\mathrm{d}^2}{\mathrm{d}s^2} + \omega^2$ vanishing at the boundaries:

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

Eigenfunctions and -values

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

- $0 \leq \omega t < \pi$: $\quad \lambda_n > 0$ 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



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

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

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

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

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

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

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.

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

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

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

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

Literature

- G.-L. Ingold
  Path Integrals and Their Application to Dissipative Quantum Systems
  Lect. Notes Phys. **611**, 1 (2002) [`arXiv:quant-ph/0208026`]
- H. Kleinert
  Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets
  (World Scientific, 2009)