



# Introduction to Feynman path integrals

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### Introduction to Feynman path integrals

### Motivation

Propagator

Derivation of path integral

Particle on a ring

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oscillator

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### Classical mechanics: Hamilton vs. Lagrange



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### Hamilton formalism

Hamiltonian H(q, p)

Poisson bracket  $\{q, p\} = 1$ equations of motion  $\dot{q} = \{q, H\}, \dot{p} = \{p, H\}$ 

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

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

### Lagrange formalism

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

action 
$$S = \int dt L(q, \dot{q})$$
  
equation of motion from  
Hamilton's principle  $\delta S = 0$ 

$$\downarrow$$

Dirac (1933), Feynman (1948)

Path integral formulation of quantum mechanics



# Why base quantum mechanics on Lagrange formalism?



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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
- lacksquare ...is very well suited to consider the semiclassical limit  $\mathcal{S}\gg\hbar$





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# Propagator



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

time evolution of a state

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

in position representation

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

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

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



# Propagator of a free particle



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

propagator of the free particle

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



# Digression: Fresnel integral



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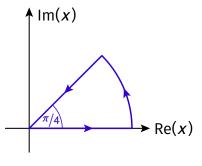
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$$\int_0^\infty dx e^{i\alpha x^2} = e^{i\pi/4} \int_0^\infty du e^{-\alpha u^2}$$
$$= \frac{1}{2} \sqrt{\frac{i\pi}{\alpha}}$$

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





# Propagator of a free particle and relation to classical properties



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

classical motion from position  $q_i$  to  $q_f$  in time t:

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

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

propagator of free particle in terms of classical properties

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



# Combining two propagators



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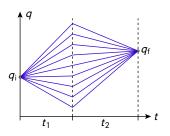
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### semigroup property

$$\begin{split} K(q_{\mathrm{f}},q_{\mathrm{i}},t_{2}+t_{1}) &= \langle q_{\mathrm{f}}|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht_{2}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht_{1}}|q_{\mathrm{i}}\rangle \\ &= \int_{-\infty}^{+\infty}\mathrm{d}q'\langle q_{\mathrm{f}}|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht_{2}}|q'\rangle\langle q'|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht_{1}}|q_{\mathrm{i}}\rangle \\ &= \int_{-\infty}^{+\infty}\mathrm{d}q'K(q_{\mathrm{f}},q',t_{2})K(q',q_{\mathrm{i}},t_{1}) \end{split}$$



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





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# Strategy for the derivation of the Feynman path integral



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### 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



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

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

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

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

⇒ 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



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

$$\Delta t = \frac{t}{N} \quad q_0 = q_i \quad q_N = q_f$$

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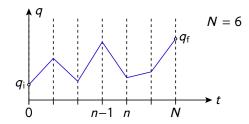
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$$\int_{-\infty}^{+\infty} \left( \prod_{n=1}^{N-1} dq_n \right) \langle q_f | \cdots | q_n \rangle \underbrace{\langle q_n | e^{-\frac{i}{\hbar}V\Delta t} e^{-\frac{i}{\hbar}T\Delta t} | q_{n-1} \rangle} \langle q_{n-1} | \cdots | q_i \rangle$$

$$\sqrt{rac{m}{2\pi \mathrm{i}\hbar\Delta t}}\exp\left[rac{\mathrm{i}}{\hbar}\left(rac{m(q_n-q_{n-1})^2}{2\Delta t}-V(q_n)\Delta t
ight)
ight]$$





# Splitting the propagator II



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

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

Ν

n-1





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

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

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

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

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



# Feynman path integral



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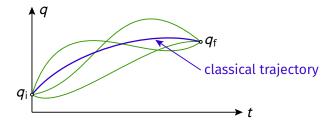
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propagator as functional integral (Feynman path integral)

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

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





# Evaluation of a Feynman path integral



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

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

- expansion in a complete set of functions
  - → see our later discussion of the harmonic oscillator

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



# **Physical interpretation**



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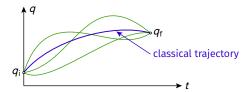
Motivation

# Derivation of path integral

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- 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.



# Classical trajectory and quantum fluctuations



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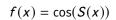
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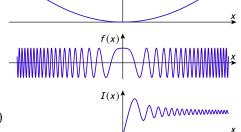
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Conventional integral as an analogy:

$$S(x) = x^2$$
  
 $x = 0$  corresponds to classical trajectory



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



S(x)'

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





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# Standard approach



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Harmonio oscillator particle of mass m on a ring of radius R

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

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

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

eigenenergies

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

propagator

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



## More than one way



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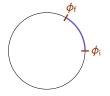
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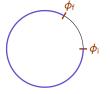
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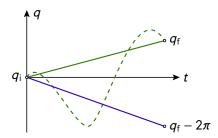
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two ways to reach  $\phi_{\rm f}$ :





the two paths cannot be deformed into each other





# More than one way



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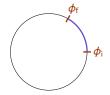
Derivation of path integral

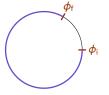
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two ways to reach  $\phi_{\rm f}$ :





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

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



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# $\phi_{\rm f}$

n = 1





- the angles  $\phi_{\rm f}$  and  $\phi_{\rm f} + 2\pi n$  have to be identified
- the propagator is a sum over all topologically distinct contributions

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



# **Dual representations**



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two different expressions for the propagator

### winding number

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

### angular momentum

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

compare with propagator of free particle

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



## A useful relation



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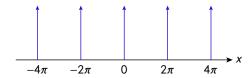
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### Fourier representation of a periodic $\delta$ -comb



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

Exercise: Verify this relation.



# Relating the two representations



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$$\begin{split} K(\phi_{\rm f},\phi_{\rm i},t) &= R \sqrt{\frac{m}{2\pi {\rm i}\hbar t}} \sum_{n=-\infty}^{+\infty} \exp\biggl(\frac{{\rm i}}{\hbar} \frac{mR^2}{2} \frac{(\phi_{\rm f}-\phi_{\rm i}-2\pi n)^2}{t}\biggr) \\ &= R \sqrt{\frac{m}{2\pi {\rm i}\hbar t}} \int_{-\infty}^{+\infty} {\rm d}\phi \exp\biggl(\frac{{\rm i}}{\hbar} \frac{mR^2}{2t} \phi^2\biggr) \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \delta \bigl(\phi - (\phi_{\rm f}-\phi_{\rm i}-2\pi n)\bigr) \\ &= \frac{R}{2\pi} \sqrt{\frac{m}{2\pi {\rm i}\hbar t}} \sum_{\ell=-\infty}^{+\infty} \exp \biggl({\rm i}\ell(\phi_{\rm f}-\phi_{\rm i}) \int_{-\infty}^{+\infty} {\rm d}\phi \exp\biggl(\frac{{\rm i}}{\hbar} \frac{mR^2}{2t} \phi^2 + {\rm i}\ell\phi\biggr) \\ &= \frac{1}{2\pi} \sum_{\ell=-\infty}^{+\infty} \exp\biggl({\rm i}\ell(\phi_{\rm f}-\phi_{\rm i}) - {\rm i}\frac{\hbar\ell^2}{2mR^2} t\biggr) \qquad \checkmark \end{split}$$

Exercise: Fill in the missing details.





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# Standard approach



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

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

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

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

eigenenergies

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

propagator

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



# Possible trajectories



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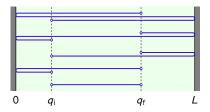
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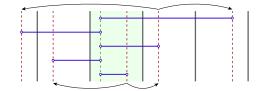
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### unfolding of the trajectories



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

### Influence of a wall



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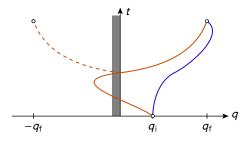
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subtract the contribution of paths crossing the wall:

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

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



# Propagator for particle in a box



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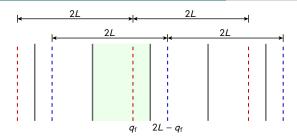
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even number of reflections at  $q = q_f + 2nL$ odd number of reflections at  $q = 2nL - q_f$ 

propagator

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



# Two versions of the propagator



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

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

and

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

*Exercise*: 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.





### Introduction to Feynman path integrals

Motivation

Propagator

Derivation of path integral

Particle on a ring

Particle in a box

Harmonic oscillator

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- 5 Particle in a box
- 6 Harmonic oscillator



# Path integral for the harmonic oscillator



Introduction to Feynman path integrals

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Harmonic oscillator path integral representation of the propagator of the harmonic oscillator

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

How do we integrate over all functions satisfying the boundary conditions  $q(0) = q_i$  and  $q(t) = q_f$ ?

- 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



Introduction to Feynman path integrals

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integral

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Particle in a box

Harmonic oscillator

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

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

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

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

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



## **Expansion around classical solution**



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

action

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

- $\blacksquare$  expansion around the classical path makes linear term in  $\xi$  disappear because  $\delta S = 0$  for classical paths
- for the harmonic oscillator:
  - lacksquare classical action  $\mathcal{S}_{ ext{cl}}$  contains the full dependence on  $q_{ ext{i}}$  and  $q_{ ext{f}}$
  - fluctuation part is independent of q<sub>i</sub> and q<sub>f</sub> and only contributes to the prefactor



## **Classical solution**



Introduction to Feynman path integrals

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......

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Harmonic oscillator general solution of the equation of motion of the harmonic oscillator

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

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

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



### Existence of classical solution



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Particle in a box

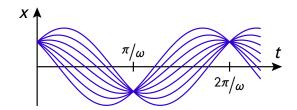
Harmonic oscillator

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

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

boundary value problems ...

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





# **Classical action**



#### Introduction to Feynman path integrals

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Harmonic oscillator

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

integration by parts

$$= \frac{m}{2} q_{cl}(s) \dot{q}_{cl}(s) \Big|_{0}^{t} - \int_{0}^{t} ds \frac{m}{2} q_{cl}(s) \left( \ddot{q}_{cl}(s) + \omega^{2} q_{cl}(s) \right)$$

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

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

classical action of the harmonic oscillator

$$\mathcal{S}_{\text{cl}} = \frac{m\omega}{2} \frac{\left(q_{\text{f}}^2 + q_{\text{i}}^2\right) \cos(\omega t) - 2q_{\text{f}}q_{\text{i}}}{\sin(\omega t)}$$



# **Expansion of the fluctuations**



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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  $\frac{d^2}{ds^2} + \omega^2$  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**



Introduction to Feynman path integrals

Motivation

. ropugua

Derivation of path integral

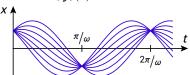
Particle on a ring

Particle in a box

Harmonic oscillator

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

- $0 \le \omega t < \pi$ :  $\lambda_n > 0$  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, ... classical action is a saddle point
- ...



# Total action and propagator



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Harmonic oscillator

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

propagator

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

fluctuation determinant

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



## **Prefactor**



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Harmonic oscillator the prefactor unknown so far does not depend on  $\omega$   $\rightarrow$  compare with propagator of the free particle

#### classical action

$$\lim_{\omega \to 0} \frac{m}{2} \underbrace{\frac{\omega}{\sin(\omega t)}}_{\to 1/t} \underbrace{\left( (q_f^2 + q_i^2) \cos(\omega t) - 2q_f q_i \right)}_{\to (q_f - q_i)^2} = \frac{m}{2} \frac{(q_f - q_i)^2}{t}$$

### prefactor

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

with

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



### 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

$$\begin{split} K(q_{\rm f},q_{\rm i},t) &= \sqrt{\frac{m\omega}{2\pi {\rm i}\hbar\sin(\omega t)}} \exp\left({\rm i}\frac{m\omega}{2\hbar}\frac{(q_{\rm f}^2+q_{\rm i}^2)\cos(\omega t)-2q_{\rm i}q_{\rm f}}{\sin(\omega t)}\right) \\ &= \sqrt{\frac{m\omega}{2\pi\hbar|\sin(\omega t)|}} \exp\left({\rm i}\frac{m\omega}{2\hbar}\frac{(q_{\rm f}^2+q_{\rm i}^2)\cos(\omega t)-2q_{\rm i}q_{\rm f}}{\sin(\omega t)} - {\rm i}\left(\frac{\pi}{4}+n\frac{\pi}{2}\right)\right) \end{split}$$

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.

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



# Nonlinear potentials



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

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

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

- the quadratic contribution in the fluctuations generally depends on  $q_f$  and  $q_i$
- it leads again to a determinant
- $\blacksquare$  the expansion of  $\xi$  does not necessarily need to be done in terms of eigenfunctions



# Fluctuation amplitude



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Harmonic oscillator 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