Problem 2.1: Path integral of the partition function

Learning objective

In the lecture you saw how the transition amplitude \( T(\mathbf{x}_i,t_i) \rightarrow (\mathbf{x}_f,t_f) \) can be expressed as a path integral. In this formulation, the action in the exponent appears with an extra factor of \( i \) which can lead to some problems with convergence. In this exercise you will derive the path integral formulation of the partition function for the single particle case.

Show that the partition function \( Z = \text{Tr} \left[ e^{-\beta \hat{H}} \right] \) can be expressed as

\[
Z \propto \int_{x(\beta)=x(0)} D\mathbf{x} e^{-\int_0^\beta d\tau \left( \frac{1}{2} m (\partial_\tau x)^2 + U(x) \right)}.
\]  

(1)

The Hamiltonian \( \hat{H} = \hat{T}(\mathbf{p}) + \hat{U}(\mathbf{x}) \) can be separated in a kinetic term \( \hat{T} \) and a potential term \( \hat{U} \).

Problem 2.2: Harmonic oscillator propagator with path integral

Learning objective

As a second example of applications with path integrals, we are going to obtain the propagator for the harmonic oscillator. Additionally, we shall see how the partition function \( Z \) can be naturally obtained within this formalism.

The propagator for a particle of mass \( m \) in a (one-dimensional) harmonic potential \( V(x) = \frac{1}{2} m \omega^2 x^2 \) is given by

\[
G(x',t';x,t) = \sqrt{\frac{m \omega}{2 \pi i \hbar \sin(\omega T)}} \times 
\exp \left\{ \frac{i m \omega}{2 \hbar \sin(\omega T)} \left[ (x^2 + x'^2) \cos(\omega T) - 2xx' \right] \right\},
\]  

(2)

where \( T = t' - t \).

a) In the path integral formulation, the propagator is calculated from the action \( S[x] \) as

\[
G(x',t';x,t) = \int_x^{x'} D\mathbf{x} \ e^{iS[x]/\hbar}
\]  

(3)
where \( x : [t, t'] \to \mathbb{R} \) denotes trajectories of the particle with \( x(t) = x \) and \( x(t') = x' \).

Express these trajectories \( x(t) = \pi(t) + y(t) \) as a sum of the classical path \( \pi(t) \) and fluctuations \( y(t) \). Write the action as the sum of the classical action and the contribution of the fluctuations.

What are the boundary conditions for the fluctuations?

Show that
\[
G (x', t'; x, t) = F(T) e^{iS[\pi]/\hbar},
\]
and demonstrate that \( F(T) \) is independent of the initial and final positions \( x \) and \( x' \).

b) Show that the classical solution of the harmonic oscillator takes the form
\[
\pi(t) = \frac{x' - x \cos(\omega t')}{\sin(\omega t')} \sin(\omega t) + x \cos(\omega t).
\]

Evaluate the classical action of this solution to obtain the factor \( e^{iS[\pi]/\hbar} \).

* c) Without loss of generality, consider \( T = t' \). Show that the prefactor is given by
\[
F(t') = \sqrt{\frac{m \omega}{2 \pi \hbar i}} \frac{1}{\sqrt{\sin(\omega t')}}
\]
using the expansion of the fluctuations
\[
y(t) = \sum_{n=1}^{\infty} a_n y_n(t),
\]
with
\[
y_n(t) = \sqrt{\frac{2}{t'}} \sin(n \pi t/t').
\]

Hint:
- Use the eigenvalue equation \((-\partial^2_t - \omega^2)y_n(t) = \lambda_n y_n(t)\) and the orthonormality of \( y_n \) to evaluate \( S[y] \).
- Use the parametrization \( D y = J \prod_{n=1}^{\infty} da_n \), where \( J \) is a (yet) undetermined normalization constant. Calculate \( F(t') \) as a function of \( J \) and \( \lambda_n \).
- To get rid of \( J \), study the limit \( \omega \to 0 \) of the propagator. In this limit, one must obtain the solution for a free particle and can derive \( F_0(t') = \lim_{\omega \to 0} F(t') \). Use this finding to obtain the result for arbitrary \( \omega \) as \( F(t') = \frac{F(t')}{F_0(t')} F_0(t') \). The fraction \( \frac{F(t')}{F_0(t')} \) can be simplified using the identity \( \sin(x) = x \prod_{k=1}^{\infty} \left( 1 - \frac{x^2}{k^2 \pi^2} \right) \).

Now that we have the propagator for the harmonic oscillator, we can take a look at how we can use this quantity to calculate the partition function from statistical mechanics.

d) As a first reminder, obtain the partition function for this system using
\[
Z = \text{tr} e^{-\beta \hat{H}}
\]
in the eigenbasis of \( \hat{H} \).
Problem 2.3: Gaussian integration with Grassmann variables

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**Learning objective**

On the previous sheet we derived the results of various Gaussian integrals over the real and complex numbers. Here, we will do the same for Grassmann variables.

Let us first recall the defining properties of Grassmann numbers,

\[ \psi_\alpha \psi_\beta = -\psi_\beta \psi_\alpha, \]  
\[ \int d\psi = 0, \]  
\[ \int d\psi \psi = 1. \]

Using these properties, show that

\[ \int \prod_{\alpha=1}^N d\psi_\alpha' d\psi_\alpha e^{-\psi_\alpha'' A_{\alpha\beta} \psi_\beta' + f_{\alpha}' \psi_\alpha + \psi_\alpha' f_{\alpha}} = \det(A) e^{f_{\alpha}' A^{-1}_{\alpha\beta} f_{\beta}}, \]  

where \( \psi_\alpha, \psi_\alpha' \in \mathcal{A} \) are Grassmann variables from the Grassmann algebra \( \mathcal{A} \), and \( A^T = A \).

**Hint:** Follow the same strategies in the previous list, i.e., solve the unshifted Gaussian integral to find that it is given by \( \det(A) \), and argue that shifting the integration variables as

\[ \psi_\alpha \rightarrow \psi_\alpha - A^{-1}_{\alpha\beta} f_{\beta} \]
\[ \psi_\alpha' \rightarrow \psi_\alpha' - f_{\beta}' A^{-1}_{\beta\alpha} \]

does not change the result, in order to get the additional term \( e^{f_{\alpha}' A^{-1}_{\alpha\beta} f_{\beta}} \).