Prof. Dr. Viatcheslav Mukhanov

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Exercises on Quantum Mechanics II (TM1/TV)Problem set 7, discussed December 2 - December 6, 2019

Exercise 43

Consider the Lagrangian for a driven harmonic oscillator in one dimension

$$L(q, \dot{q}, J(t)) = \frac{\dot{m}q^2}{2} - \frac{m\omega^2}{2}q^2 + J(t)q,$$
(1)

with ω being a constant and J(t) being a time dependent driving force.

(i) Derive expressions for the conjugate momentum p and the Hamiltonian H of the system.

We now quantize the system by promoting q and p to operators \hat{q} and \hat{p} , respectively. These operators satisfy the usual commutation relation.

- (ii) Write the Hamiltonian in terms of creation and annihilation operators \hat{a} and \hat{a}^{\dagger} . Hint: Recall your results from Question 22.
- (iii) Find the equations of motion for the the operators \hat{a} and \hat{a}^{\dagger} , respectively. They should have the form

$$\frac{\mathrm{d}\,\hat{y}(t)}{\mathrm{d}t} + A(t)\hat{y}(t) = B(t),$$

where y(t) represents $\hat{a}(t)$ or $\hat{a}^{\dagger}(t)$.

(iv) Assuming the driving force satisfies J(t < 0) = 0, solve the equations of motion. You may assume that the solution has the form

$$y(t) = (C_0 + C(t)) \exp\left(-\int A(t)dt\right).$$

find C(t) and then fix C_0 with the boundary condition at t = 0 arising from J(t < 0) = 0. Remark: The general form of the solution can be derived using the method of variation of constants.

Given that the operators \hat{a} and \hat{a}^{\dagger} act on the "*n*-particle" state $|n\rangle$ as

$$\hat{a} | n \rangle = \sqrt{n} | n - 1 \rangle$$
 and $\hat{a}^{\dagger} | n \rangle = \sqrt{n+1} | n+1 \rangle$, (2)

we can define a number operator $\hat{N} = \hat{a}^{\dagger}\hat{a}$ such that $\hat{N} | n \rangle = n | n \rangle$.

(v) Find the vacuum expectation value of the number operator, $\langle 0 | \hat{N} | 0 \rangle$, where the vacuum is defined by $\hat{a}_0 | 0 \rangle = 0$ and \hat{a}_0 is the annihilation operator of the free harmonic oscillator. Comment on your result.

Exercise 44

(i) Prove the following *n*-dimensional Gaussian integration formula:

$$I = \int_{\mathbb{R}^n} \exp\left[-\frac{1}{2}x^T A x + b^T x + c\right] d^n x = \sqrt{\frac{(2\pi)^n}{\det A}} \exp\left[\frac{1}{2}b^T A^{-1}b + c\right].$$
(3)

Here A is a symmetric positive definite $n \times n$ matrix.

(ii) Show that the argument of the exponential in the result is the extremal value of the exponent in the integrand.

Exercise 45 (central tutorial)

In this problem we will evaluate the propagator of the harmonic oscillator using the path integral. The Lagrangian is

$$\mathcal{L} = \frac{1}{2}m\dot{q}(t)^2 - \frac{1}{2}m\omega^2 q(t)^2$$

and the path integral that we are going to compute is

$$\mathcal{K}(q_F, T; q_I, 0) = \int_{\substack{q(0)=q_I\\q(T)=q_F}} \mathcal{D}q(t) \exp\left[\frac{i}{\hbar} \int_0^T dt \left(\frac{1}{2}m\dot{q}(t)^2 - \frac{1}{2}m\omega^2 q(t)^2\right)\right].$$
(4)

The final answer that we should find is

$$\mathcal{K}(q_F, T; q_I, 0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} \exp\left[\frac{im\omega}{2\hbar \sin \omega T} \left((q_I^2 + q_F^2) \cos \omega T - 2q_I q_F\right)\right].$$
(5)

We will work directly in the continuum limit, integrating over all paths. The main fact that we are going to use is that for harmonic oscillator the integral (4) is Gaussian (exponential of a quadratic function of integration variables), so that we will be able to use the continuous generalization of the Gaussian integration formula (see Exercise 44)

$$\int_{\mathbb{R}^n} d^n x \exp\left[-\frac{1}{2}x^T A x + b^T x + c\right] = \sqrt{\frac{(2\pi)^n}{\det A}} \exp\left[\frac{1}{2}b^T A^{-1}b + c\right]$$

valid for A a positive definite symmetric matrix A and b an arbitrary real vector. In our continuum computation we will have to determine the analogue of the exponential factor on the right hand side and of the determinant det A.

(i) To determine the stationary point, find the stationary path $q_0(t)$ of the action (there will be only one), i.e. solve the classical Euler-Lagrange equations with boundary conditions $q(0) = q_I$ and $q(T) = q_F$. You should get

$$q_0(t) = \frac{1}{\sin \omega T} \left(q_F \sin \omega t + q_I \sin \omega (T - t) \right)$$

The result is singular for $\omega T = \pi n$, $n \in \mathbb{N}$ - explain the origin of these singularities.

- (ii) Evaluate the classical action at the stationary point. The result should reproduce the exponential factor of the final result (5).
- (iii) It remains to evaluate the prefactor, in particular we should understand a continuous generalization of the determinant $\det A$. This determinant comes from integrating over the quadratic fluctuations around the stationary path. We make a shift of the integration variable

$$q(t) = q_0(t) + \delta q(t).$$

where $q_0(t)$ is the stationary point found previously and δq now satisfies the boundary conditions $\delta q(0) = 0 = \delta q(T)$. Why? What is the Jacobian of this change of integration variable? Show that the action is now

$$S[q(t)] = S[q_0(t)] - \frac{m}{2} \int_0^T \delta q(t) \left[\partial_t^2 + \omega^2\right] \delta q(t)$$

(why there is no term linear in δq ?) so that we need to find the determinant of the operator

$$A_{\omega} = -\partial_t^2 - \omega^2 \tag{6}$$

acting in the space of functions which satisfy $\delta q(0) = 0 = \delta q(T)$.

(iv) Find the eigenfunctions and eigenvalues of (6). The determinant should be their product. Show that this is formally

$$\det A_{\omega} = \prod_{k=1}^{\infty} \left(\frac{\pi^2 k^2}{T^2} - \omega^2 \right)$$

which is divergent as $k \to \infty$. But the ratio of these two formal expressions at different values of ω is convergent. Using the product formula for sine function

$$\frac{\sin \pi z}{\pi z} = \prod_{n>0} \left(1 - \frac{z^2}{n^2} \right)$$

show that

$$\det(A_{\omega}) = \frac{\Omega \det(A_{\Omega})}{\sin \Omega T} \frac{\sin \omega T}{\omega}$$

(v) In this way, we evaluated the functional integral (4) up to an ω -independent prefactor. Fix this prefactor by comparing the $\omega \to 0$ limit of the result to free particle propagator

$$\mathcal{K}_{free}(q_F, T; q_I, 0) = \sqrt{\frac{m}{2\pi i \hbar T}} \exp\left[-\frac{m(q_F - q_I)^2}{2i\hbar T}\right]$$

The result you should find is (5).

Exercise 46

There is another way to determine the prefactor of the harmonic oscillator propagator using the property of composition of two propagators

$$\mathcal{K}(q_F, T_1 + T_2, q_I, 0) = \int_{-\infty}^{+\infty} \mathcal{K}(q_F, T_1 + T_2, q, T_1) \mathcal{K}(q, T_1, q_I, 0) dq.$$
(7)

Parametrize the propagator of the harmonic oscillator as

$$\mathcal{K}(q_f, T, q_I, 0) = A(T) \exp\left[\frac{im\omega}{2\hbar\sin(\omega T)} \left((q_I^2 + q_F^2)\cos(\omega T) - 2q_I q_F\right)\right]$$
(8)

and show that the composition property implies an equation for the prefactor

$$A(T_1 + T_2) = A(T_1)A(T_2)\sqrt{\frac{2\pi i\hbar\sin(\omega T_1)\sin(\omega T_2)}{m\omega\sin(\omega(T_1 + T_2))}}$$
(9)

which determines the prefactor to be

$$A(T) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega T)}}.$$
(10)

Exercise 47 (central tutorial)

In this problem we want to extract wave functions and energies of the harmonic oscillator from the propagator that we calculated using the path integral.

- (i) Find the Euclidean propagator (unnormalized density matrix) of the harmonic oscillator by analytic continuation $T \rightarrow -i\hbar\beta$ where β is the inverse temperature.
- (ii) What is the leading order low temperature behavior as $\beta \to \infty$? It is convenient to introduce a variable $\alpha = e^{-\hbar\beta\omega}$ such that $\alpha \to 0$ as $\beta \to \infty$.

At this point, the Euclidean propagator expressed in terms of α should look like

$$\mathcal{K}(q_F, -i\hbar\beta, q_I, 0) = \alpha^{\frac{1}{2}} \sqrt{\frac{m\omega}{\hbar\pi(1-\alpha^2)}} \exp\left[-\frac{m\omega}{\hbar(1-\alpha^2)} \left((q_I^2 + q_F^2)\frac{1+\alpha^2}{2} - 2q_I q_F \alpha\right)\right].$$
 (11)

(iii) Read off the spectrum of the Hamiltonian from the previous expression. The (unnormalized) density matrix should have an expansion of the form

$$\mathcal{K}(q_F, -i\hbar\beta, q_I, 0) = \sum_{n=0}^{\infty} \alpha^{\frac{1}{2}+n} f_n(q_F, q_I).$$
(12)

Interpret the quantities $f_n(q_F, q_I)$ in terms of eigenfunctions of the Hamiltonian.

- (iv) For one-dimensional quantum mechanical problems with discrete spectrum the wave functions can be chosen to be real. Detemine the ground state wave function from the leading order coefficient of \mathcal{K} as $\beta \to \infty$.
- (v) Determine the wave function of the first excited state.
- (vi) Show that for the harmonic oscillator we have in general

$$\varphi_n(q_F)\varphi_n^*(q_I) = \lim_{\beta \to \infty} \frac{1}{n!} \left(-\frac{1}{\hbar\omega} e^{\hbar\omega\beta} \frac{d}{d\beta} \right)^n \left[e^{\frac{1}{2}\hbar\omega\beta} \mathcal{K}(q_F, -i\hbar\beta, q_I, 0) \right].$$
(13)