Prof. Dr. Viatcheslav Mukhanov Winter term 2019/2020

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

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

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

$$\hat{a}\,|\,n\rangle = \sqrt{n}\,|\,n-1\rangle \quad \text{and} \quad \hat{a}^\dagger\,|\,n\rangle = \sqrt{n+1}\,|\,n+1\rangle\,, \tag{2}$$

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, $\left\langle 0 \,\middle|\, \hat{N} \,\middle|\, 0\right\rangle$, 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.

Solution

(i) Using the definition of conjugate momentum we find

$$p = \frac{\mathrm{d}\,L}{\mathrm{d}\dot{q}} = m\dot{q}.$$

And the Hamiltonian is

$$\begin{aligned} H(q,p,J(t)) &= \left[\dot{q}p - L(q,\dot{q},J(t))\right]_{\dot{q}=p} \\ &= \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2 - J(t)q. \end{aligned}$$

(ii) Defining creation and annihilation operators as,

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} - \frac{i}{m\omega}\hat{p}\right) \qquad \hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{i}{m\omega}\hat{p}\right),$$

we know from Question 22 that we can write the free Hamiltonian as

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2 = \frac{\hbar\omega}{2}\left(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\right) = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}\right).$$

Using the fact that $\hat{q} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right)$, we find

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}\right) - \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right)J(t). \tag{3}$$

(iii) Using the Heisenberg equation of motion

$$\begin{aligned}\frac{\mathrm{d}\,\hat{a}}{\mathrm{d}t} &= \frac{i}{\hbar}\left[\hat{H}, \hat{a}\right] \\ &= i\omega\left[\hat{a}^\dagger, \hat{a}\right]\hat{a} - \frac{i}{\sqrt{2\hbar m\omega}}\left[\hat{a}^\dagger, \hat{a}\right]J(t) \\ &= -i\omega\hat{a} + \frac{i}{\sqrt{2\hbar m\omega}}J(t),\end{aligned}$$

where we used that $\left[\hat{a}, \hat{a}^\dagger\right] = 1$. Therefore

$$\frac{\mathrm{d}\,\hat{a}}{\mathrm{d}t} = -i\omega\hat{a} + \frac{i}{\sqrt{2\hbar m\omega}}J(t), \qquad \frac{\mathrm{d}\,\hat{a}^\dagger}{\mathrm{d}t} = i\omega\hat{a}^\dagger - \frac{i}{\sqrt{2\hbar m\omega}}J(t) \tag{4}$$

where we found the equation of motion for $\hat{a}^\dagger$ by complex conjugation.

(iv) Using the hint that the solution of Eq. 4 for $\hat{a}$ has the form

$$\hat{a}(t) = (\hat{C}_0 + \hat{C}(t))\exp(-i\omega t).$$

where $A(t) = i\omega$, we can substitute into Eq. 4 to find,

$$\begin{aligned}-i\omega\hat{a} + \frac{i}{\sqrt{2\hbar m\omega}}J(t) &= -i\omega(\hat{C}_0 + \hat{C}(t))\exp(-i\omega t) + \frac{\mathrm{d}\,\hat{C}(t)}{\mathrm{d}t}\exp(-i\omega t) \\ &= -i\omega\hat{a} + \frac{\mathrm{d}\,\hat{C}(t)}{\mathrm{d}t}\exp(-i\omega t).\end{aligned}$$

Therefore,

$$\frac{\mathrm{d}\,\hat{C}(t)}{\mathrm{d}t} = \frac{i}{\sqrt{2\hbar m\omega}}J(t)\exp(i\omega t) \quad \Longrightarrow \quad \hat{C}(t) = \frac{i}{\sqrt{2\hbar m\omega}}\int_0^t dt'\; J(t')\exp(i\omega t'),$$

where we used that $J(t<0) = 0$. Hence we have

$$\hat{a}(t) = \left(\hat{C}_0 + \frac{i}{\sqrt{2\hbar m\omega}}\int_0^t dt'\; J(t')e^{i\omega t'}\right)e^{-i\omega t}. \tag{5}$$

We can fix the constant $\hat{C}_0$ by matching solution, Eq. 5, to the one of a free harmonic oscillator at $t = 0$ with $\hat{a}_0$ and $\hat{a}_0^\dagger$. Also, by conjugation we can find the solution for $\hat{a}^\dagger(t)$. Finally, we arrive at

$$\begin{aligned}\hat{a}(t) &= \left(\hat{a}_0 + \frac{i}{\sqrt{2\hbar m\omega}}\int_0^t dt'\; J(t')e^{i\omega t'}\right)e^{-i\omega t} \\ \hat{a}^\dagger(t) &= \left(\hat{a}_0^\dagger - \frac{i}{\sqrt{2\hbar m\omega}}\int_0^t dt'\; J(t')e^{-i\omega t'}\right)e^{i\omega t}\end{aligned} \tag{6}$$

(v) Using that $\hat{a}_0 \,|\, 0\rangle = 0$ and $\langle 0 \,|\, \hat{a}_0^\dagger = 0$, we immediately have

$$\left\langle 0 \,\middle|\, \hat{N}(t) \,\middle|\, 0 \right\rangle = \left\langle 0 \,\middle|\, \frac{1}{2\hbar m\omega} \left| \int_0^t dt' \; J(t') e^{i\omega t'} \right|^2 \,\middle|\, 0 \right\rangle = \frac{1}{2\hbar m\omega} \left| \int_0^t dt' \; J(t') e^{i\omega t'} \right|^2 \geq 0.$$

We can interpret this result as excitation of the harmonic oscillator by the energy supplied from the driving force.
If we interpret the state $|\, n\rangle$ as a "n-particle"-state, the driving force would supply energy to create particles.

Exercise 44

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

$$I = \int_{\mathbb{R}^n} \exp\left[-\frac{1}{2}x^T A x + b^T x + c\right] d^n x = \sqrt{\frac{(2\pi)^n}{\det A}} \exp\left[\frac{1}{2} b^T A^{-1} b + c\right]. \tag{7}$$

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.

Solution

(i) First of all, since A is positive definite, it is invertible so we may change the integration variable to $y = x - A^{-1}b$. The Jacobian of this transformation is 1 so the integral becomes

$$I = \int_{\mathbb{R}^n} \exp\left[-\frac{1}{2}y^T A y + \frac{1}{2} b^T A^{-1} b + c\right] d^n y = \exp\left[\frac{1}{2} b^T A^{-1} b + c\right] \times \int_{\mathbb{R}^n} \exp\left[-\frac{1}{2} y^T A y\right] d^n y. \tag{8}$$

The remaining integral can be reduced to one-dimensional case by an orthogonal transformation: any symmetric positive-definite matrix A can be diagonalized by an orthogonal transformation O (with determinant 1) such that $A = O^T D O$ where D is a diagonal matrix with positive diagonal elements. Using this and changing the integration variable from y to $z = Oy$ (the determinant of this transformation is $+1$) we see that

$$\begin{aligned} I &= \exp\left[\frac{1}{2} b^T A^{-1} b + c\right] \times \int_{\mathbb{R}^n} \exp\left[-\frac{1}{2} z^T D z\right] d^n z & (9)\\ &= \exp\left[\frac{1}{2} b^T A^{-1} b + c\right] \times \prod_{j=1}^n \int_{\mathbb{R}} \exp\left[-\frac{1}{2} d_j z_j^2\right] dz_j & (10)\\ &= \exp\left[\frac{1}{2} b^T A^{-1} b + c\right] \times \prod_{j=1}^n \sqrt{\frac{2\pi}{d_j}} & (11)\\ &= \sqrt{\frac{(2\pi)^n}{\det A}} \exp\left[\frac{1}{2} b^T A^{-1} b + c\right]. & (12) \end{aligned}$$

(ii) We find the extremal value of the exponent in the integrand by first finding the extremum,

$$0 = \nabla_x \left[-\frac{1}{2} x^T A x + b^T x + c\right] = -Ax + b \tag{13}$$

so the extremal point is at $x_0 = A^{-1}b$. Plugging this back into the exponent (action), we find

$$-\frac{1}{2} x_0^T A x_0 + b^T x_0 + c = \frac{1}{2} b^T A^{-1} b + c \tag{14}$$

which is exactly the exponent of the result.

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

$$\mathcal{K}(q_F, T; q_I, 0) = \int_{\substack{q(0)=q_I \\ q(T)=q_F}} \mathcal{D}q(t) \exp\left[\frac{i}{\hbar}\int_0^T dt \left(\frac{1}{2} m\dot{q}(t)^2 - \frac{1}{2} m\omega^2 q(t)^2\right)\right]. \tag{15}$$

The final answer that we should find is

$$\mathcal{K}(q_F, T; q_I, 0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega T}} \exp\left[\frac{im\omega}{2\hbar\sin\omega T}\left((q_I^2 + q_F^2)\cos\omega T - 2q_I q_F\right)\right]. \tag{16}$$

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 (15) 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 (16).

(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

$$A_\omega = -\partial_t^2 - \omega^2 \tag{17}$$

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

(iv) Find the eigenfunctions and eigenvalues of (17). 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 the 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 (15) up to an ω-independent prefactor. Fix this prefactor by comparing the $\omega \to 0$ limit of the result to the 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 (16).

Solution

(i) First of all we need to find the saddle points - the classical extrema of the action. The Euler-Lagrange equations tell us that we must find the solutions of ordinary differential equation

$$\ddot{q}(t) + \omega^2 q(t) = 0$$

with boundary conditions $q(0) = q_I$ and $q(T) = q_F$. The general solution satisfying these boundary conditions is

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

[If we wrote the solution as a combination $q_0(t) = a\sin(\omega t) + b\cos(\omega t)$ the boundary condition determine $b = q_I$ and $a = \frac{q_F - q_I \cos(\omega T)}{\sin \omega T}$]. There can be a problem with this solution whenever $\omega T = \pi n$, $n \in \mathbb{N}$. There is a physical reason for this singularity: we are not solving an initial value problem with prescibed position and velocity at the initial time, but instead a boundary problem fixing the position of the particle at initial and final time. In this case the exisitence of solutions is not guaranteed. Indeed, because of the periodicity of classical solutions of the equations of motion, we know that after the period $2\pi/\omega$ the position of particle is always same as the initial position, no matter what initial velocity we choose, and after half-integer multiple of the period the particle is at the opposite position. This is the physical origin of the poles in the solution.

(ii) Now we evaluate the classical action at the solution that we found. The classical Lagrangian is

$$\begin{aligned}
\mathcal{L}(q_0(t), \dot{q}_0(t)) &= \frac{m}{2}\dot{q}_0^2(t) - \frac{m\omega^2}{2} q_0^2(t) \\
&= \frac{m\omega^2}{2\sin^2(\omega T)} \Big[q_I^2 \cos^2(\omega(T - t)) + q_F^2 \cos^2(\omega t) - 2q_I q_F \cos(\omega t)\cos(\omega(T - t)) \\
&- q_I^2 \sin^2(\omega(T - t)) - q_F^2 \sin^2(\omega t) - 2q_I q_F \sin(\omega t)\sin(\omega(T - t))\Big] \\
&= \frac{m\omega^2}{2\sin^2 \omega T} \left(q_F^2 \cos(2\omega t) + q_I^2 \cos 2\omega(T - t) - 2q_I q_F \cos(\omega(T - 2t))\right)
\end{aligned}$$

To go to the second line we used

$$\dot{q}_0(t) = \frac{\omega}{\sin(\omega T)} \left[-q_I \cos(\omega(T - t)) + q_F \cos(\omega t)\right]. \tag{18}$$

Integrating this over time, we find for the classical action

$$S[q_0(t)] = \frac{m\omega}{2\sin \omega T} \left((q_I^2 + q_F^2)\cos \omega T - 2q_I q_F\right).$$

We used the integrals

$$\int_0^T \cos(2\omega t)dt = \int_0^T \cos(2\omega(T - t))dt = \frac{\sin(2\omega T)}{2\omega}$$

and

$$\int_0^T \cos(\omega(T - 2t))dt = \frac{\sin(\omega T)}{\omega}.$$

(iii) It remains to compute the determinant prefactor (the one-loop determinant). In order to do this, we need to integrate over the quadratic fluctuations around the classical trajectory. Expanding the action to the quadratic order around $q(t)$

$$S[q_0(t) + \delta q(t)] = S[q_0(t)] + \frac{1}{2}\int dt \int dt' \frac{\delta^2 S[q(t)]}{\delta q(t)\delta q(t')}\Big|_{q\to q_0} \delta q(t)\delta q(t') + \dots$$

Note that the first term vanishes because $q_0(t)$ extremizes the action. In our case the action is quadratic so the three dots are actually zero.

More explicitly, plugging in $q(t) = q_0(t) + \delta q(t)$ we find

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

So we need to compute the determinant of operator

$$-\partial_t^2 - \omega^2 \tag{19}$$

in the space of functions $\delta q(t)$ satisfying the boundary conditions $\delta q(0) = 0 = \delta q(T)$ (this comes from the fact that from the beginning we were evaluating the Feynman path integral over trajectories with fixed end points).

(iv) The eigenfunctions of the operator (19) are easily found to be

$$f_k(t) = \sin\frac{\pi k t}{T}$$

where $k = 1, 2, \dots$ with corresponding eigenvalues

$$\lambda_k = \frac{\pi^2 k^2}{T^2} - \omega^2$$

This means that the determinant we are after is

$$\det(A_\omega) \sim \prod_{k=1}^{\infty}\left(\omega^2 - \frac{\pi^2 k^2}{T^2}\right) \tag{20}$$

This product diverges for large values of k. It makes sense, however, to compare the ratio of these determinants for different values of ω,

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

In this way, we can understand the ω-dependence of the determinant, although we cannot fix the overall prefactor. Using now the product formula for the sine function

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

we find

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

(v) Combining the result of the classical action and of the determinant, we find that

$$\mathcal{K}(q_F, T; q_I, 0) \sim \sqrt{\frac{\omega}{\sin \omega T}}\exp\left[\frac{im\omega}{2\hbar \sin \omega T}\left((q_I^2 + q_F^2)\cos \omega T - 2 q_I q_F\right)\right]. \tag{21}$$

To fix the normalization constant, we compare this and the result for the free particle propagator,

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

which is the $\omega \to 0$ limit of the harmonic oscillator. Comapring this with (21) we find the final answer

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

Exercise 46

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

$$\mathcal{K}(q_F, T_1 + T_2, q_I, 0) = \int_{-\infty}^{+\infty} \mathcal{K}(q_F, T_1 + T_2, q, T_1)\mathcal{K}(q, T_1, q_I, 0)dq. \tag{22}$$

Parametrize the propagator of the harmonic oscillator as

$$\mathcal{K}(q_f, T, q_I, 0) = A(T) \exp\left[\frac{im\omega}{2\hbar \sin(\omega T)} \left((q_I^2 + q_F^2)\cos(\omega T) - 2q_I q_F\right)\right] \tag{23}$$

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

$$A(T_1 + T_2) = A(T_1)A(T_2)\sqrt{\frac{2\pi i\hbar \sin(\omega T_1)\sin(\omega T_2)}{m\omega \sin(\omega(T_1 + T_2))}} \tag{24}$$

which determines the prefactor to be

$$A(T) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}}. \tag{25}$$

Solution We need to evaluate the one-dimensional integral

$$\int_{-\infty}^{+\infty} dq A(T_1)A(T_2) \exp\left[\frac{im\omega}{2\hbar \sin(\omega T_1)} \left((q_I^2 + q^2)\cos(\omega T_1) - 2q_I q\right)\right] \times$$
$$\times \exp\left[\frac{im\omega}{2\hbar \sin(\omega T_2)} \left((q_F^2 + q^2)\cos(\omega T_2) - 2q_F q\right)\right]. \tag{26}$$

This is a Gaussian integral with

$$a = \frac{-im\omega}{\hbar}\left(\frac{\cos(\omega T_1)}{\sin(\omega T_1)} + \frac{\cos(\omega T_2)}{\sin(\omega T_2)}\right) = \frac{-im\omega}{\hbar}\frac{\sin(\omega(T_1 + T_2))}{\sin(\omega T_1)\sin(\omega T_2)} \tag{27}$$

$$b = -\frac{iq_I m\omega}{\hbar \sin(\omega T_1)} - \frac{iq_F m\omega}{\hbar \sin(\omega T_2)} \tag{28}$$

$$c = \frac{im\omega}{2\hbar}\left(\frac{q_I^2 \cos(\omega T_1)}{\sin(\omega T_1)} + \frac{q_F^2 \cos(\omega T_2)}{\sin(\omega T_2)}\right). \tag{29}$$

We can concentrate on the prefactor (the classical action in the exponent will give us the correct expression that we already know). From the Gaussian integration formula the prefactor of the result depends only on a and is equal to

$$A(T_1)A(T_2)\sqrt{\frac{2\pi}{a}} = A(T_1)A(T_2)\sqrt{\frac{2\pi i\hbar \sin(\omega T_1)\sin(\omega T_2)}{m\omega \sin(\omega(T_1 + T_2))}}. \tag{30}$$

which should be equal to $A(T_1 + T_2)$ and this is the relation we wanted.

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 $T \to -i\hbar\beta$ 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

$$\mathcal{K}(q_F, -i\hbar\beta, q_I, 0) = \alpha^{\frac{1}{2}}\sqrt{\frac{m\omega}{\hbar\pi(1-\alpha^2)}} \exp\left[-\frac{m\omega}{\hbar(1-\alpha^2)}\left((q_I^2 + q_F^2)\frac{1+\alpha^2}{2} - 2q_I q_F \alpha\right)\right]. \tag{31}$$

(iii) Read off the spectrum of the Hamiltonian from the expression for the propagator you just found. The (unnormalized) density matrix should have an expansion of the form

$$\mathcal{K}(q_F, -i\hbar\beta, q_I, 0) = \sum_{n=0}^{\infty} \alpha^{\frac{1}{2}+n} f_n(q_F, q_I). \tag{32}$$

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

$$\varphi_n(q_F)\varphi_n^*(q_I) = \lim_{\beta\to\infty} \frac{1}{n!}\left(-\frac{1}{\hbar\omega} e^{\hbar\omega\beta} \frac{d}{d\beta}\right)^n \left[e^{\frac{1}{2}\hbar\omega\beta}\mathcal{K}(q_F, -i\hbar\beta, q_I, 0)\right]. \tag{33}$$

Solution

(i) We start with the propagator $\mathcal{K}(q_F, T, q_I, 0)$ evaluated above and replace $T \to -i\hbar\beta$. The result is

$$\mathcal{K}(q_F, -i\hbar\beta, q_I, 0) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\hbar\omega\beta)}} \exp\left[-\frac{m\omega}{2\hbar\sinh(\hbar\beta\omega)}\left((q_I^2+q_F^2)\cosh(\hbar\beta\omega) - 2q_Iq_F\right)\right]. \tag{34}$$

where we used the formula $\sin(ix) = i\sinh(x)$.

(ii) Introducing the variable α as suggested, the Euclidean propagator takes the form

$$\mathcal{K}(q_F, -i\hbar\beta, q_I, 0) = \alpha^{\frac{1}{2}}\sqrt{\frac{m\omega}{\hbar\pi(1-\alpha^2)}} \exp\left[-\frac{m\omega}{\hbar(1-\alpha^2)}\left((q_I^2+q_F^2)\frac{1+\alpha^2}{2} - 2q_Iq_F\alpha\right)\right]. \tag{35}$$

(iii) The prefactor $\alpha^{\frac{1}{2}}$ controls the leading order behavior at low temperatures (corresponding to the contribution of the ground state) while the rest can be Taylor expanded in positive powers of α. This means that the right-hand side has a Taylor expansion of the form

$$\sum_{n=0}^{\infty} f_n(q_F, q_I)\alpha^{\frac{1}{2}+n} = \sum_{n=0}^{\infty} f_n(q_F, q_I)e^{-\beta\hbar\omega(\frac{1}{2}+n)} = \sum_{n=0}^{\infty} f_n(q_F, q_I)e^{-\beta E_n} \tag{36}$$

which corresponds to the well-known energy spectrum $E_n = \hbar\omega\left(\frac{1}{2}+n\right)$. Inserting the complete set of states in the definition of the Euclidean propagator we find a general expression

$$\mathcal{K}(q_F, -i\hbar\beta, q_I, 0) = \sum_{n=0}^{\infty} \langle q_F \,|\, n\rangle\, e^{-\beta E_n}\, \langle n \,|\, q_I\rangle = \sum_{n=0}^{\infty} e^{-\beta E_n}\varphi_n(q_F)\varphi_n^*(q_I) \tag{37}$$

so the expressions $f_n(q_F, q_I)$ are just the matrix elements of projectors on eigenfunctions, i.e. $f_n(q_F, q_I) = \langle q_F \,|\, n\rangle \langle n \,|\, q_I\rangle$ which in terms of wave functions is just $\varphi_n(q_F)\varphi_n^*(q_I)$.

(iv) We can extract the leading order coefficient by putting $\alpha = 0$ everywhere except for the prefactor $\alpha^{\frac{1}{2}}$. We thus find

$$\varphi_0(q_F)\varphi_0^*(q_I) = \sqrt{\frac{m\omega}{\hbar\pi}} \exp\left[-\frac{m\omega}{2\hbar}(q_I^2+q_F^2)\right] \tag{38}$$

and from here we can read off the ground state wave function to be

$$\varphi_0(q) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \exp\left[-\frac{m\omega}{2\hbar}q^2\right] \tag{39}$$

which is indeed the well-known result.

(v) To find the information about the first excited state with energy $E_1 = \frac{3\hbar\omega}{2}$, we know from the previous questions that the wave function can be obtained by expanding the function in (35) to first order in α. Fortunately, for this calculation we can ignore all α^2 terms and we find simply

$$\varphi_1(q_F)\varphi_1^*(q_I) = \sqrt{\frac{m\omega}{\hbar\pi}} \exp\left[-\frac{m\omega}{\hbar}\left(\frac{q_I^2+q_F^2}{2}\right)\right]\frac{2m\omega q_Iq_F}{\hbar} = \varphi_0(q_F)\varphi_0^*(q_I)\frac{2m\omega q_Iq_F}{\hbar}. \tag{40}$$

(vi) From the expression for the density matrix (36) we see that the wave functions can be calculated as

$$\varphi_n(q_F)\varphi_n^*(q_I) = \frac{1}{n!}\frac{d^n}{d\alpha^n}\bigg|_{\alpha=0}\left[\alpha^{-\frac{1}{2}}\mathcal{K}(q_F, -i\hbar\beta, q_I, 0)\right] \tag{41}$$

Changing the variable from α to $\beta = -\frac{1}{\hbar\omega}\log\alpha$ we can write this as

$$\varphi_n(q_F)\varphi_n^*(q_I) = \lim_{\beta\to\infty}\frac{1}{n!}\left(-\frac{1}{\hbar\omega}e^{\hbar\omega\beta}\frac{d}{d\beta}\right)^n\left[e^{\frac{1}{2}\hbar\omega\beta}\mathcal{K}(q_F, -i\hbar\beta, q_I, 0)\right]. \tag{42}$$