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Quantum Many-Body Systems

5. Exercise Sheet

16 Path integral of the harmonic oscillator in an external force field

In this exercise, we consider a problem of an harmonic oscillator in an external force-field that is space-independent but depends in an arbitrary manner on time. The Hamiltonian describing such a system is given, in the Schrödinger representation, by

$$\hat{H}(t) = \hat{H} - f(t)\hat{x}, \tag{16.1}$$

where $\hat{H}_0$ is given, as before, by

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 = \hbar\omega_0\big(\hat{a}^\dagger\hat{a} + \frac{1}{2}\big). \tag{16.2}$$

We have here redefined $\hat{H}_0$ to include the zero-point energy contribution, so that we do not have to carry it explicitly in the definition of the propagators. Since the total Hamiltonian is time-dependent, the time-evolution operator, which satisfies the Schrödinger equation (??), has to be written as a time-ordered exponential, see equation (). For a perturbative expansion, the time-evolution operator in the interaction representation $\hat{S}(T,0)$ is important, which is given in this case by (we assume that the motion takes place in the interval $t\varepsilon[0,T]$)

$$\hat{S}(T,0) = \mathcal{T}\exp\big[\frac{i}{\hbar}\int_0^T dt\, f(t)\hat{x}(t)\big], \tag{16.3}$$

where $\hat{x}(t) = e^{i\hat{H}_0 t/\hbar}\hat{x}e^{-i\hat{H}_0 t/\hbar}$ is the position operator in the interaction representation (which coincides with the Heisenberg representation of the harmonic oscillator in the absence of an external field). We have that $\hat{U}(T,0) = e^{-i\hat{H}_0 t/\hbar}\hat{S}(T,0)$, see problem sheet 2.

It was shown in the lecture that the Green function of the quantum harmonic oscillator in the presence of an homogeneous time-dependent force $G_f^R(x,T;x_0,0) = -\frac{i}{\hbar}\langle x|\hat{U}(T,0)|x_0\rangle$ can be expressed as the following path-integral

$$G_f^R(x,T;x_0,0) = -\frac{i}{\hbar}\int \mathcal{D}[x(t)]\, e^{iS_f[x(t)]/\hbar}, \tag{16.4}$$

where the path integral is a sum over all piece-wise continuous trajectories that start at $t=0$ in point x_0 and end at $t=T$ in point x (*i.e.* $x(0)=x_0$ and $x(T)=X$). The action $S_f[x(t)] = \frac{1}{2}m\int_0^T dt\,[\dot{x}(t) - \omega_0^2 x^2(t)] + \int_0^T dt\, f(t)x(t)$ is computed over each of such trajectories (the action is said to be a *functional* of the trajectory) and each trajectory contributes with a different phase to the overall *sum over histories*. The objective of this exercise is to explicitly compute the propagator (16.4).

(a) Writing $x(t) = x_c(t) + \delta x(t)$, where $x_c(t)$ is a solution of the classical equation of motion $\ddot{x}_c(t) = -\omega_0^2 x_c(t) + \frac{f(t)}{m}$, with $x_c(0) = x_0$ and $x_c(T) = x$, and $\delta x(t)$ is the quantum fluctuation around such a solution, with $\delta x(0) = \delta x(T) = 0$, show that one can write $S[x(t)] = S_f[x_c(t)] + S_0[\delta x(t)]$, where $S_0[\delta x(t)]$ is the action of the quantum harmonic oscillator in the absence of an external force, see problem 15.
(**3 points**)
Hint: Use $x(t) = x_c(t)+\delta x(t)$ in $S_f[x(t)] = \frac{1}{2}m\int_0^T dt\,[\dot{x}(t) - \omega_0^2 x^2(t)] + \int_0^T dt\, f(t)x(t)$, integrate one of the terms by parts and use the classical equation of motion for $x_c(t)$ and the boundary conditions for $\delta x(t)$ at $t=0$ and $t=T$.

(b) Show that $S_f[x(t)] = \frac{1}{2}m\int_0^T dt\,[\dot{x}_c(t) - \omega_0^2 x_c^2(t)] + \int_0^T dt\, f(t)x_c(t)$ can be written as $S_f[x(t)] = \frac{1}{2}m[x_c(T)\dot{x}_c(T) - x_c(0)\dot{x}_c(0)] + \frac{1}{2}\int_0^T dt\, f(t)x_c(t)$.
(**2 points**)
Hint: Integrate one of the terms in $S[x_c(t)]$ by parts and use the classical equation of motion.

(c) Show that the solution of the classical equation of motion in the presence of an external force can be written as $x_c(t) = x_c^h(t) + x_c^p(t)$, where $x_c^h(t)$ is a solution of the equation of motion in the absence of an external force, with the boundary conditions $x_c^h(0) = x_0$, $x_c^h(T) = x$ and $x_c^p(t)$ is a solution of the equation of motion in the presence of an external force $\ddot{x}_c^p(t) = -\omega_0^2 x_c^p(t) + \frac{f(t)}{m}$, but with the particular boundary conditions $x_c^p(0) = x_c^p(T) = 0$. Furthermore, show that $x_c^h(t)$ can be written as

$$x_c^h(t) = \frac{1}{\sin(\omega_0 T)}\big[x_0 \sin(\omega_0(T-t)) + x\sin(\omega_0 t)\big]. \tag{16.5}$$

Deduce that

$$\dot{x}_c^h(t) = \frac{\omega_0}{\sin(\omega_0 T)}\big[x_0 \cos(\omega_0 t) + x\cos(\omega_0(T-t))\big], \tag{16.6}$$

with

$$\begin{aligned}\dot{x}_c^h(0) &= \frac{\omega_0[x - x_0\cos(\omega_0 T)]}{\sin(\omega_0 T)}\\ \dot{x}_c^h(T) &= \frac{\omega_0[x\cos(\omega_0 T) - x_0]}{\sin(\omega_0 T)}.\end{aligned} \tag{16.7}$$

(**5 points**)
Hint: The first part of the exercise is a particular case of a general result that applies for linear differential equations, while the second part is a mere repetition of exercise 15(d).

(d) Argue that the solution $x_c^p(t)$ can be written within the interval $t\varepsilon[0,T]$ in terms of the Fourier series

$$x_c^p(t) = \sum_{n=1}^{\infty} x_n^p \sin\Big(\frac{n\pi t}{T}\Big). \tag{16.8}$$

(**2 points**)
Hint: Any function within the interval $t\varepsilon[0,2T]$ (which includes the interval [0,T]), can be written as a Fourier series which involves a sum over both sines and cosines, since the Fourier basis is complete. What is the form of this series if we wish to enforce the boundary conditions $x_c^p(0) = x_c^p(T) = 0$?

(e) By substituting (16.8) in the equation $\ddot{x}_c(t) = -\omega_0^2 x_c^p(t) + \dfrac{f(t)}{m}$, show that the coefficients x_n^p are given by

$$x_n^p = \frac{2T}{m[(\omega_0 T)^2 - (n\pi)^2]}\int_0^T du\, f(u)\sin\Big(\frac{n\pi u}{T}\Big). \tag{16.9}$$

We explicitly assume that $\omega_0 T \neq n\pi$, for $n\varepsilon\mathbb{Z}$.
(**2 points**)
Hint: $\dfrac{2}{T}\int_0^T du\, \sin\big(\dfrac{n\pi u}{T}\big)\sin\big(\dfrac{l\pi u}{T}\big) = \delta_{n,l}$, where l is, like n, a positive integer.

(f) By substituting (16.9) in (16.8), show that one can write $x_c^p(t)$ as

$$x_c^p(t) = \frac{T}{2m}\int_0^T du\, f(u)[H(t-u) - H(t+u)], \tag{16.10}$$

where $H(x) = \sum_{n=-\infty}^{\infty} \dfrac{1}{(\omega_0 T)^2 - (n\pi)^2} \cos\left(\dfrac{n\pi|x|}{T}\right)$.
(**3 points**)
Hint: Express the product of sines in terms of a difference of cosines and recall that the cosine is an even function.

(g) Show that $H(x) = \oint_{\mathcal{C}} \dfrac{dz}{2\pi i} \dfrac{1}{\sinh(z)} \dfrac{\cosh[z(1-|x|/T)]}{(\omega_0 T)^2 + z^2}$, where the contour is the union of the circles that surround each pole of $\dfrac{1}{\sinh(z)}$ (thus the poles of $\dfrac{1}{(\omega_0 T)^2 + z^2}$ at $z = \pm i\omega_0 T$ are excluded from such a contour).
(**2 points**)
Hint: $\cos(n\pi(1-y)) = (-1)^n \cos(n\pi y)$.

(h) Show that the integral over a circle with a very large radius R, $\oint_{\odot} \dfrac{dz}{2\pi i} \dfrac{1}{\sinh(z)} \dfrac{\cosh[z(1-|x|/T)]}{(\omega_0 T)^2 + z^2} = 0$, for R chosen appropriately. Hence, show that $H(x) = \dfrac{\cos[\omega_0(T-|x|))]}{\omega_0 T \sin(\omega_0 T)}$.
(**3 points**)
Hint: Have a look at the solution of exercise 12.

(i) Verify explicitly that the expression obtained for $x_c^p(t)$,

$$x_c^p(t) = \frac{1}{2m\omega_0 \sin(\omega_0 T)} \int_0^T du\, f(u) \{\cos[\omega_0(T-|t-u|)] - \cos[\omega_0(T-|t+u|)]\}, \tag{16.11}$$

fulfills the boundary conditions $x_c^p(0) = x_c^p(T) = 0$.
(**1 point**)

(j) Show that the derivative of $x_c^p(t)$ is given by

$$\dot{x}_c^p(t) = \frac{1}{2m \sin(\omega_0 T)} \int_0^T du\, f(u) \{\sin[\omega_0(T-|t-u|)]\mathrm{sgn}(t-u) - \sin[\omega_0(T-t-u)]\}, \tag{16.12}$$

where $\mathrm{sgn}(x) = 1$ if $x > 0$ and $\mathrm{sgn}(x) = -1$ if $x < 0$.
(**2 points**)
Hint: Note that $|t+u| = t+u$ if t and u are in $[0, T]$, $\dfrac{d|x|}{dx} = \mathrm{sgn}(x)$, and apply the chain rule of differentiation.

(k) Show in particular that

$$\begin{aligned} \dot{x}_c^p(0) &= -\frac{1}{m \sin(\omega_0 T)} \int_0^T du\, f(u) \sin[\omega_0(T-u)], \\ \dot{x}_c^p(T) &= \frac{1}{m \sin(\omega_0 T)} \int_0^T du\, f(u) \sin(\omega_0 u). \end{aligned} \tag{16.13}$$

(**2 points**)

(l) By differentiation (16.12), show that $x_c^p(t)$ satisfies the classical equation of motion in the presence of an external force. Thus, $x_c(t) = x_c^h(t) + x_c^p(t)$, with $x_c^h(t)$ as given by (16.5) and $x_c^p(t)$ as given by (16.11), is the full solution with the boundary conditions $x_c(0) = x_0$, $x_c(T) = x$.
(**2 points**)
Hint: $\mathrm{sgn}^2(x) = 1$ and $\dfrac{d\mathrm{sgn}(x)}{dx} = 2\delta(x)$.

(m) Substitute $x_c(t)$ in the expression for $S[x_c(t)]$ as given in **(b)**, to obtain the complete expression for the classical action of an oscillator in the presence of an external force, namely

$$\begin{aligned} S_f[x_c(t)] = &\frac{m\omega_0}{2\sin(\omega_0 T)}[x^2\cos(\omega_0 T) - 2xx_0 + x_0^2\cos(\omega_0 T)] + \Phi_0 \\ &+ \frac{1}{\sin(\omega_0 T)}\int_0^T dt\, f(t)\{x\sin(\omega_0 t) + x_0\sin[\omega_0(T-t)]\}, \end{aligned} \tag{16.14}$$

where Φ_0 is given by

$$\begin{aligned} \Phi_0 = &\frac{1}{4m\omega_0\sin(\omega_0 T)}\int_0^T dt\int_0^T du\, f(t)f(u)\{\cos[\omega_0(T-|t-u|)] \\ &- \cos[\omega_0(T-|t+u|)]\}. \end{aligned} \tag{16.15}$$

(**5 points**)
Hint: Use the expressions (16.7) and (16.13) to obtain $\dot{x}_c(0)$ and $\dot{x}_c(T)$.

(n) Show from the results obtained above that

$$G_f^R(x,T;x_0,0) = -\frac{i}{\hbar}A(T)e^{iS_f[x_c(t)]/\hbar}, \tag{16.16}$$

where $S_f[x_c(t)]$ is given by (16.14) and

$$A(T) = \int \mathcal{D}[\delta x(t)]e^{iS_f[\delta x(t)]/\hbar} = \sqrt{\frac{m\omega_0}{2\pi i\hbar\sin(\omega_0 T)}}. \tag{16.17}$$

(**2 points**)
Hint: The exercise is a mere repetition of 15(f).

17 Matrix elements of the time-evolution operator of the harmonic oscillator in a field in the interaction representation

The purpose of this exercise is two establish two identities that will be useful later on. Consider the matrix elements $S(x,T;x_0,0) = \langle x|\hat{S}(T,0)|x_0\rangle$, where $\hat{S}(T,0)$ is given by (16.3).

(a) Show that one can write $S(x, T; x_0, 0)$ as

$$S(x, T; x_0, 0) = \hbar^2 \int_{-\infty}^{\infty} dy\, \overline{G}_0^R(y, T; x, 0) G_f^R(y, T; x_0, 0), \tag{17.1}$$

where $\overline{G}_0^R(y, T; x, 0)$ is the complex conjugate of the propagator of the one-dimensional harmonic oscillator, given by expression (15.5) from the previous exercise sheet and $G_f^R(y, T; x_0, 0)$ is given by (16.16).
(**3 points**)
Hint: Use $\hat{S}(T, 0) = e^{i\hat{H}_0 T}\hat{U}(T, 0)$ is the matrix element $\langle x|\hat{S}(T, 0)|x_0\rangle$ and use the representation of the identity in terms of position eigenstates.

(b) Consider the generating functional for the correlation functions of the position operator

$$Z[f(t)] = \frac{1}{Z_\beta} \mathrm{Tr}\Big(e^{-\beta\hat{H}_0}\hat{S}(T, 0)\Big), \tag{17.2}$$

where $\hat{H}_0$ is given by (16.2). This quantity is a functional of the external field $f(t)$. By functionally differentiating it with respect to $f(t)$ at zero applied field, we can obtain all the causal Green functions involving the position operator in thermal equilibrium. Show that one can express $Z[f(t)]$ as

$$Z[f(t)] = \frac{i\hbar}{Z_\beta} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx_0 dx\, G_0^R(x_0, -i\hbar\beta; x, 0) S(x, T; x_0, 0). \tag{17.3}$$

(**3 points**)
Hint: Use the representation of the trace in terms of position eigenstates and use again the representation of the identity in terms of these eigenstates.

These results and those exercise 16 will be used in the next problem sheet to explicitly compute $Z[f(t)]$.