Imaginary Time Free Propagator for the Quantum Oscillator

Solution Problem 25.6

Pedro Dardengo Mesquita
Universidade Federal de Viçosa
June 16, 2020

There are two ways of solving this problem: using canonical quantization (less complicated) or using path integrals (more complicated).

Canonical Quantization Method

This method requires the realization that we may substitute (remember interaction picture for the harmonic oscillator):

$$\hat{x}(t) = \sqrt{\frac{1}{2m\omega}}\left(\hat{a}^\dagger(t) + \hat{a}(t)\right) = \sqrt{\frac{1}{2m\omega}}\left(\hat{a}^\dagger(0)e^{i\omega t} + \hat{a}(0)e^{-i\omega t}\right) \tag{1}$$

we need to make the substitution $t = -i\tau$ that leads to:

$$\hat{x}(\tau) = \sqrt{\frac{1}{2m\omega}}\left(\hat{a}^\dagger(\tau) + \hat{a}(\tau)\right) = \sqrt{\frac{1}{2m\omega}}\left(\hat{a}^\dagger(0)e^{\omega\tau} + \hat{a}(0)e^{-\omega\tau}\right) \tag{2}$$

naturally:

$$\hat{x}(0) = \sqrt{\frac{1}{2m\omega}}\left(\hat{a}^\dagger(0) + \hat{a}(0)\right) \tag{3}$$

Since we need to calculate $G_{\text{book}}(\tau) = -\langle \hat{T}\hat{x}(\tau)\hat{x}(0)\rangle$ (I'm using G_{book} cause the definition from the book has a minus sign, what I'll call G here is equal $-G_{\text{book}}$) we may start calculating the application of the time ordering operator:

$$G_{\text{book}}(\tau) = -\langle \hat{T}\hat{x}(\tau)\hat{x}(0)\rangle = -\left[\langle \hat{x}(\tau)\hat{x}(0)\rangle\theta(\tau) + \langle \hat{x}(0)\hat{x}(\tau)\rangle\theta(-\tau)\right] \tag{4}$$

Now we just substitute the terms stated before and use the commutation relation $[\hat{a}(t), \hat{a}^\dagger(t)] = 1$ to grind down the terms:

$$\langle \hat{x}(\tau)\hat{x}(0)\rangle = \frac{1}{2m\omega}\left(\hat{a}^\dagger(0)e^{\omega\tau} + \hat{a}(0)e^{-\omega\tau}\right)\left(\hat{a}^\dagger(0) + \hat{a}(0)\right) \tag{5}$$

$$= \frac{1}{2m\omega}\langle \hat{a}^\dagger(0)\hat{a}^\dagger(0)e^{\omega\tau} + \hat{a}^\dagger(0)\hat{a}(0)e^{\omega\tau} + (1 + \hat{a}^\dagger(0)\hat{a}(0))e^{-\omega\tau} + \hat{a}(0)\hat{a}(0)e^{-\omega\tau}\rangle \tag{6}$$

Notice that the thermal averages of the following operators $\langle \hat{a}^\dagger(0)\hat{a}^\dagger(0)\rangle = \langle \hat{a}(0)\hat{a}(0)\rangle = 0$ and $\langle \hat{a}^\dagger(0)\hat{a}(0)\rangle = \langle n\rangle$ where $\langle n\rangle$ is the Bose-Einstein distribution.

Then we can conclude:

$$\langle\hat{x}(\tau)\hat{x}(0)\rangle = \frac{1}{2m\omega}\left[\langle n\rangle e^{-\omega\tau} + (1+\langle n\rangle)e^{\omega\tau}\right] \tag{7}$$

and similarly:

$$\langle\hat{x}(0)\hat{x}(\tau)\rangle = \frac{1}{2m\omega}\left[\langle n\rangle e^{\omega\tau} + (1+\langle n\rangle)e^{-\omega\tau}\right] \tag{8}$$

Then we arrive at the solution:

$$G_{\text{book}}(\tau) = -\frac{1}{2m\omega}\left[\left[\langle n\rangle e^{-\omega\tau} + (1+\langle n\rangle)e^{\omega\tau}\right]\theta(\tau) + \left[\langle n\rangle e^{\omega\tau} + (1+\langle n\rangle)e^{-\omega\tau}\right]\theta(-\tau)\right] \tag{9}$$

The second item in the problem is just a matter of integration, so I'll skip this solution since it will appear naturally in the next method.

Path Integral Method

The book mentions that we may use the generating functional to find thermal averages using:

$$\langle x(\tau_2)x(\tau_1)\rangle = \frac{1}{Z[0]}\frac{\delta^2 Z[J]}{\delta J(\tau_2)\delta J(\tau_1)}_{J=0} \tag{10}$$

using this result along with equation (4) will allow us to find the answer. This means we need to make the following steps in order to solve the proble this way:

1. Write the action for the harmonic oscilator and put it into the quadratic form:

$$S[x(t)] = \frac{m}{2}\int dt[\dot{x}^2(t) + \omega^2 x^2(t)] = \frac{m}{2}\int x(t)[-\partial_t^2 + \omega^2]x(t)dt \tag{11}$$

(see equation 23.36 in the book).

2. Add a source term to the action (the generating functional).

$$S[x(t),J(t)] = \frac{m}{2}\int x(t)[-\partial_t^2 + \omega^2]x(t)dt + \int J(t)x(t)dt \tag{12}$$

3. Write the path integral for the exponential of the action, which leads us to the real time propagator.

$$G = \int D[x(t)]\exp\{iS[x(t),J(t)]\} \tag{13}$$

4. Wick rotate the last path integral and then it becomes the partition function of the system. To do this we need to make the substitution $t = -i\tau$. This turns the action into:

$$S[x(\tau),J(\tau)] = \frac{m}{2}\int_0^\beta x(\tau)[-\partial_{-i\tau}^2 + \omega^2]x(\tau)(-i)d\tau + \int_0^\beta J(\tau)x(\tau)(-i)d\tau \tag{14}$$

$$= -i\left(\frac{m}{2}\int_0^\beta x(\tau)[-\partial_\tau^2 + \omega^2]x(\tau)d\tau + \int_0^\beta J(\tau)x(\tau)d\tau\right) \tag{15}$$

this imply that:

$$Z[J(\tau)] = \int D[x(\tau)]\exp\{S[x(\tau),J(\tau)]\} \tag{16}$$

5. Calculate the partition function using the functional integration methods.

To solve path integral (16) we can use the formula 23.30 in the book, but in order to do that we need to diagonalize the operator $A = [-\partial_\tau^2 + \omega^2]$ in order to easily find its inverse A^-1. Before telling the reader how to do it I want to say a word on how this situation is the continuous analogy of the discrete situation. Looking at equation (15) we may think that $x(\tau)$ is the continuous analogy of the component of a vector like x_i but since in our continuous analogy we need an infinite dimensional vector we also need a continuous index τ. The operator $A = [-\partial_\tau^2 + \omega^2]$ is the continuous analogy of a non diagonal matrix, in order to turn it diagonal we need to do a change of basis, this will change our continuous vectors and matrix, once we put it into diagonal form finding it‘s inverse A^{-1} is an easy task since the inverse of a diagonal matrix A is just a matrix composed of the inverse of its diagonal elements, just check $AA^{-1} = 1$.

The question remains, what change of basis we need to do? The answer is to Fourier transform equation (15):

$$x(\tau) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} e^{-i\omega_n \tau} \tilde{x}(\omega_n) \qquad J(\tau) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} e^{-i\omega_n \tau} \tilde{J}(\omega_n) \tag{17}$$

where, $\omega_n = \dfrac{2\pi n}{\beta}$ this leads us to:

$$S[\tilde{x}(\omega_n), \tilde{J}(\omega_n)] = -i\frac{1}{\beta} \sum_{\omega_n, \omega_m} \left(\frac{m}{2} \int_0^\beta \tilde{x}(\omega_n) e^{-i\omega_n \tau} [-\partial_\tau^2 + \omega^2] \tilde{x}(\omega_m) e^{-i\omega_m \tau} d\tau + \int_0^\beta \tilde{J}(\omega_n) e^{-i\omega_n \tau} \tilde{x}(\omega_m) e^{-i\omega_m \tau} d\tau \right) \tag{18}$$

$$= -i\frac{1}{\beta} \sum_{\omega_n, \omega_m} \left(\frac{m}{2} \tilde{x}(\omega_n) [(\omega_m)^2 + \omega^2] \tilde{x}(\omega_m) + \tilde{J}(\omega_n) \tilde{x}(\omega_m) \right) \int_0^\beta e^{-i\omega_n \tau} e^{-i\omega_m \tau} d\tau \tag{19}$$

since:

$$\int_0^\beta e^{-i\omega_n \tau} e^{-i\omega_m \tau} d\tau = \beta \delta_{m,-n} \tag{20}$$

we get:

$$S[\tilde{x}(\omega_n), \tilde{J}(\omega_n)] = -i \sum_{\omega_n} \left(\frac{m}{2} \tilde{x}(\omega_n) [\omega_n^2 + \omega^2] \tilde{x}(\omega_{-n}) + \tilde{J}(\omega_n) \tilde{x}(\omega_{-n}) \right) \tag{21}$$

The term $D[x(\tau)]$ will also be transform, but this will lead only to terms that will be normalized in equation (10). The last equation allows us to use equation 23.30 to solve the path integral (16):

$$Z[J(\omega_n)] = N \exp\left\{ \frac{1}{2} \sum_{\omega_n} \frac{\tilde{J}(\omega_n) \tilde{J}(-\omega_n)}{m[\omega_n^2 + \omega^2]} \right\} \tag{22}$$

where N are all the terms that will be normalized in equation (10). This result already allows us to obtain the result of the second item of the problem:

$$G(i\omega_n) = \frac{1}{m} \frac{1}{(i\omega_n)^2 - \omega^2} \tag{23}$$

the minus sign appers because of how the propagator is defined in equation 25.46. The reason our answer is hidden here has to do with Wick’s Theorem, but this will be made clear at the last step of this solution.

Since the functional derivatives are derivatives in the complex time we need to put the partition function in the complex time space. To do this we notice that:

$$\tilde{J}(\omega_n) = \frac{1}{\sqrt{\beta}} \int_0^\beta J(\tau) e^{i\omega_n \tau} d\tau \tag{24}$$

then the partition function becomes:

$$Z[J(\tau)] = N \exp\left\{ \frac{1}{2} \int_0^\beta J(\tau_2) \sum_{\omega_n} \frac{e^{-i\omega_n(\tau_2 - \tau_1)}}{\beta m[\omega_n^2 + \omega^2]} J(\tau_1) d\tau_1 d\tau_2 \right\} \tag{25}$$

to completely eliminate the dependence in the Matsubara frequencies we need to calculate the frequency sum in the last equation. But before we do that I want to stress the fact that we could have obtained the same result in equation (25) by directly using the nondiagonal matrix and this relation $A(\tau_2 - \tau_1) A^{-1}(\tau_2 - \tau_1) = \delta(\tau_2 - \tau_1)$:

$$A(\tau_2 - \tau_1) A^{-1}(\tau_2 - \tau_1) = [-\partial_\tau^2 + \omega^2] A^{-1}(\tau_2 - \tau_1) = \delta(\tau_2 - \tau_1) \tag{26}$$

since:

$$\delta(\tau_2-\tau_1)=\frac{1}{\beta}\sum_{\omega_n}e^{i\omega_n(\tau_2-\tau_1)} \quad ; \quad A^{-1}(\tau_2-\tau_1)=\sum_{\omega_n}\tilde{A}^{-1}(\omega_n)e^{-i\omega_n(\tau_2-\tau_1)} \tag{27}$$

we can use this relations in equation (26) and get:

$$A^{-1}(\tau_2-\tau_1)=\frac{1}{\beta m}\sum_{\omega_n}\frac{e^{-i\omega_n(\tau_2-\tau_1)}}{\omega_n^2+\omega^2} \tag{28}$$

and then we could use this to solve equation 23.30 and we would be back to equation (25).

We need now to solve the frequency sum:

$$S=-\frac{1}{\beta}\sum_{\omega_n}\frac{e^{-i\omega_n(\tau_2-\tau_1)}}{[(i\omega_n)^2-\omega^2]}=-\frac{1}{\beta}\sum_{\omega_n}f(i\omega_n) \tag{29}$$

The trick of the Matsubara sum is realize this sum can be done using a contour integration in the complex plane:

$$I=-\frac{1}{2\pi i\beta}\oint_C f(z)h(z)dz \tag{30}$$

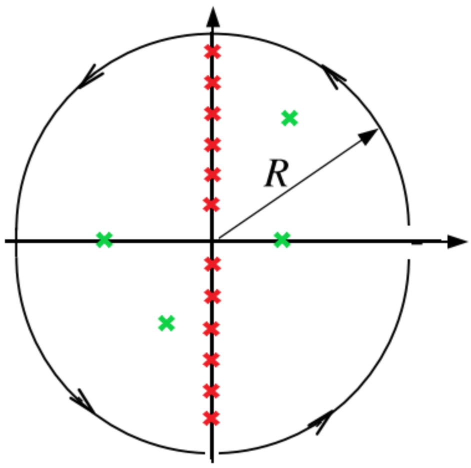

Figure 1: The contour of integration where $R\to\infty$ and the green poles are the poles of the function $f(z)$ the red poles are the poles from the function $h(z)$.

where $h(z)$ will be a function specially built to find the value of the sum. The function $h(z)$ must have some properties:

- Have poles in the Matsubara frequencies ω_n.
- f(z)h(z) must be vanish at infinity.
- Be such that $\mathrm{Res}\{f(z)h(z)\}=f(z)$ at the Matsubara frequency poles.

Since the countour is a circle of infinite radius the Integral must vanish:

$$I=-\frac{1}{\beta}\left(\sum_{\text{poles of } f(z)}\mathrm{Res}\{f(z)h(z)\}+\sum_{\text{poles of } h(z)}\mathrm{Res}\{f(z)h(z)\}\right) \tag{31}$$

$$=-\frac{1}{\beta}\left(\sum_{\text{poles of } f(z)}\mathrm{Res}\{f(z)h(z)\}+\sum_{i\omega_n}f(i\omega_n)\right)=0 \tag{32}$$

recognizing our sum in the last equation we arrive at:

$$S=\frac{1}{\beta}\sum_{\text{poles of } f(z)}\mathrm{Res}\{f(z)h(z)\} \tag{33}$$

This is exactly what we seek, since calculating the sum of the residues over the finite number of poles of $f(z)$ (generaly they are very few, like in our case they are only two) is much easier than doing our original sum that is an infinite sum. The only thing left now is to determine $h(z)$, we need to be careful since the exponential in our sum may lead to divergences at infinity depending if the term $\tau_2-\tau_1$ is negative or positive. The function that accomplishes the job is:

$$h(z)=\beta n_B(z)\theta(\tau_2-\tau_1)+\beta[1+n_B(z)]\theta(\tau_1-\tau_2),\ \text{where } n_B(z)=\frac{1}{e^{\beta z}-1} \tag{34}$$

This may seem completely out of the blue at first, but remember a general rule: $h(z)=\beta n_B(z)$ always when $f(z)$ is divergent in the right side and that $h(z)=\beta(1+n_B(z))$ always when $f(z)$ is divergent in the left side.

Knowing this it is easy to see why the need of the step functions. Calculating (33):

$$\frac{S}{m} = G(\tau_2 - \tau_1) = \frac{1}{2m\omega}\left[e^{-\omega(\tau_2-\tau_1)}n_B(\omega) + e^{\omega(\tau_2-\tau_1)}(1+n_B(\omega))\right]\theta(\tau_2-\tau_1) + \frac{1}{2m\omega}\left[e^{\omega(\tau_2-\tau_1)}n_B(\omega) + e^{-\omega(\tau_2-\tau_1)}(1+n_B(\omega))\right]\theta(\tau_1-\tau_2)$$

this is already our answer (with the exception of the minus sign added in the definition of the book), we just need to set $\tau_2 = \tau$ and $\tau_1 = 0$, just like we did in equation (23). Just like it was said before, the reason for the answer already appearing here when we haven‘t even finished calculating (10) it‘s the version of Wick‘s Theorem for functional integration, proving this theorem here is beyond my scope but you can get a very good sense of what‘s happening in the exercise 23.2 of the book. I will continue from now on the sole purpose of proving that finishing the calculation will lead to the same result in this particular case, hopefully it will be useful to those who have any particular doubt on the steps that follow.

6. Using equation (4) with equation (10), do the functional derivatives an then find the propagator.

Plugging our results into equation (10) and since $Z(0) = N$ (from equation (25)) we find that:

$$\langle x(\tau)x(0)\rangle = \frac{1}{Z[0]}\frac{\delta^2 Z[J]}{\delta J(\tau)\delta J(0)}_{J=0} = \frac{\delta^2}{\delta J(\tau)\delta J(0)}_{J=0}\exp\left\{\frac{1}{2}\int_0^\beta J(\tau_2)G(\tau_2-\tau_1)J(\tau_1)d\tau_1 d\tau_2\right\} = \frac{\delta^2 F[J(\tau_2),J(\tau_1)]}{\delta J(\tau)\delta J(0)}_{J=0}$$

this is just a functional derivative that can be done using the techniques taught in chapter 1:

$$\frac{\delta}{\delta J(0)}F[J] = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(F[J(\tau_2)+\varepsilon\delta(\tau_2-0),J(\tau_1)+\varepsilon\delta(\tau_1-0)] - F[J(\tau_2),J(\tau_1)]\right) = F[J(\tau_2),J(\tau_1)]\frac{1}{2}\left(\int J(\tau')G(0-\tau')d\tau' + \int J(\tau')G(\tau'-0)d\tau'\right)$$

doing the next derivative in much the same we way:

$$\langle x(\tau)x(0)\rangle = \frac{\delta^2 F[J(\tau_2),J(\tau_1)]}{\delta J(\tau)\delta J(0)}_{J=0} = \frac{1}{2}(G(\tau)+G(-\tau)) = \frac{\delta^2 F[J(\tau_2),J(\tau_1)]}{\delta J(0)\delta J(\tau)}_{J=0} = \langle x(0)x(\tau)\rangle \tag{35}$$

using our result for $G(\tau)$ obtained previously allow us to notice that:

$$\frac{1}{2}(G(\tau)-G(-\tau)) = G(\tau) \tag{36}$$

from equation (4) now:

$$G_{\text{book}}(\tau) = -\left[\langle\hat{x}(\tau)\hat{x}(0)\rangle\theta(\tau) + \langle\hat{x}(0)\hat{x}(\tau)\rangle\theta(-\tau)\right] = -G(\tau)[\theta(\tau)+\theta(-\tau)] = -G(\tau) \tag{37}$$

finally obtaining the result from the book:

$$G_{\text{book}}(\tau) = -\frac{1}{2m\omega}\left[\left[n_B(\omega)e^{-\omega\tau} + (1+n_B(\omega))e^{\omega\tau}\right]\theta(\tau) + \left[n_B(\omega)e^{\omega\tau} + (1+n_B(\omega))e^{-\omega\tau}\right]\theta(-\tau)\right] \tag{38}$$