### 1.4. Evaluation of the path integral for harmonic oscillator

As a "crosscheck", we would now like to evaluate the path integral in Eq. (1.41) for the case of a harmonic oscillator, and check that we get the correct result in Eq. (1.17). To make the exercise more interesting, we carry out the evaluation in Fourier space (with respect to the time coordinate $\tau$) rather than in configuration space. Moreover, we would like to see if we can deduce the information contained in the divergent constant $C$ without making use of its actual value in Eq. (1.40).

Let us start by representing an arbitrary function $x(\tau)$, $0 < \tau < \beta\hbar$, with the property $x(\beta\hbar) = x(0)$, as a Fourier sum:

$$x(\tau) \equiv T \sum_{n=-\infty}^{\infty} x_n e^{i\omega_n \tau} \,, \tag{1.45}$$

where the factor $T$ is a convention. Periodicity requires

$$e^{i\omega_n \beta\hbar} = 1 \,, \quad \text{i.e.} \quad \omega_n \beta\hbar = 2\pi n \,, \quad n \in \mathbb{Z} \,. \tag{1.46}$$

The values $\omega_n = 2\pi T n/\hbar$ are called *Matsubara frequencies.*

Apart from periodicity, we also impose reality on $x(\tau)$:

$$x(\tau) \in \mathbb{R} \Rightarrow x^*(\tau) = x(\tau) \Rightarrow x_n^* = x_{-n} \,. \tag{1.47}$$

If we write $x_n = a_n + ib_n$, it follows that

$$x_n^* = a_n - ib_n = x_{-n} = a_{-n} + ib_{-n} \Rightarrow \left\{ \begin{array}{r} a_{-n} = a_n \\ b_{-n} = -b_n \end{array} \right. \tag{1.48}$$

In particular, $b_0 = 0$, and $x_{-n}x_n = a_n^2 + b_n^2$. Thereby, we now have the representation

$$x(\tau) = T\left\{ a_0 + \sum_{n=1}^{\infty} \Big[ (a_n + ib_n)e^{i\omega_n \tau} + (a_n - ib_n)e^{-i\omega_n \tau} \Big] \right\} . \tag{1.49}$$

Here, $a_0$ is called (the amplitude of) the Matsubara *zero-mode.*

With the representation of Eq. (1.49), general quadratic structures in configuration space can be written as

$$\begin{aligned} \frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau\, x(\tau)y(\tau) &= T^2 \sum_{m,n} x_n y_m \frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau\, e^{i(\omega_n + \omega_m)\tau} \\ &= T^2 \sum_{m,n} x_n y_m \, \frac{1}{T}\delta_{n,-m} = T\sum_n x_n y_{-n} \,. \end{aligned} \tag{1.50}$$

In particular, the argument of the exponential in Eq. (1.41) becomes

$$\begin{aligned} & -\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau\, \frac{m}{2}\left[ \frac{\mathrm{d}x(\tau)}{\mathrm{d}\tau}\frac{\mathrm{d}x(\tau)}{\mathrm{d}\tau} + \omega^2 x(\tau)x(\tau) \right] \\ \overset{\text{Eq. (1.50)}}{=} & \quad -\frac{mT}{2}\sum_{n=-\infty}^{\infty} x_n \Big[ i\omega_n\, i\omega_{-n} + \omega^2 \Big] x_{-n} \\ \overset{\omega_{-n} = -\omega_n}{=} & \quad -\frac{mT}{2}\sum_{n=-\infty}^{\infty} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2) \\ = & \quad -\frac{mT}{2}\omega^2 a_0^2 - mT\sum_{n=1}^{\infty} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2) \,. \end{aligned} \tag{1.51}$$

Next, we need to consider the *integration measure*. Let us make a change of variables from $x(\tau)$, $\tau \in (0, \beta\hbar)$, to the Fourier components $a_n, b_n$. As we have seen, the independent variables are then $a_0$ and $\{a_n, b_n\}$, $n \geq 1$.

This change of variables introduces a determinant,

$$\mathcal{D}x(\tau) = \left|\det\left[\frac{\delta x(\tau)}{\delta x_n}\right]\right| \, \mathrm{d}a_0 \Big[\prod_{n\geq 1} \mathrm{d}a_n \, \mathrm{d}b_n\Big] \; . \tag{1.52}$$

The change of bases is purely kinematical, however, and independent of the potential $V(x)$. Thus we can define

$$C' \equiv C \left|\det\left[\frac{\delta x(\tau)}{\delta x_n}\right]\right| \; , \tag{1.53}$$

and consider now $C'$ as an unknown coefficient.

Making use of the gaussian integral $\int_{-\infty}^{\infty} \mathrm{d}x \exp(-cx^2) = \sqrt{\pi/c}$, the expression in Eq. (1.41) now becomes

$$\begin{aligned} \mathcal{Z} &= C' \int_{-\infty}^{\infty} \mathrm{d}a_0 \int_{-\infty}^{\infty} \Big[\prod_{n\geq 1} \mathrm{d}a_n \, \mathrm{d}b_n\Big] \exp\Big[-\frac{1}{2} mT\omega^2 a_0^2 - mT \sum_{n\geq 1} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2)\Big] \\ &= C' \sqrt{\frac{2\pi}{mT\omega^2}} \prod_{n=1}^{\infty} \frac{\pi}{mT(\omega_n^2 + \omega^2)} \; , \quad \omega_n = \frac{2\pi T n}{\hbar} \; . \end{aligned} \tag{1.54}$$

It remains to determine $C'$. How to do this?

- Since $C'$ is independent of $\omega$, we can determine it in the limit $\omega = 0$, whereby the system simplifies.
- The integral over the zero-mode $a_0$ in Eq. (1.54) is, however, divergent for $\omega \to 0$. We call such a divergence an *infrared divergence*: the zero-mode is the *lowest-energy* mode.
- But we can still take $\omega \to 0$ if we momentarily *regulate* the integration over the zero-mode in some other way. We note from Eq. (1.49) that

  $$\frac{1}{\beta\hbar} \int_0^{\beta\hbar} \mathrm{d}\tau \, x(\tau) = T a_0 \; , \tag{1.55}$$

  so that $Ta_0$ represents the average value of $x(\tau)$. In terms of Eq. (1.31), we can identify the average value with the "boundary condition" $x$, over which we integrate.

  Let us then simply regulate the system by "putting it in a box", i.e. by restricting the values of $x$ to some (asymptotially wide by finite) interval $\Delta x$, and those of $a_0$ to the interval $\Delta x/T$.

With this setup, we can proceed to *match* for $C'$.

**Side A: "effective theory computation".** In the presence of the regulator, Eq. (1.54) becomes

$$\begin{aligned} \lim_{\omega\to 0} \mathcal{Z}_{\text{regulated}} &= C' \int_{\Delta x/T} \mathrm{d}a_0 \int_{-\infty}^{\infty} \Big[\prod_{n\geq 1} \mathrm{d}a_n \, \mathrm{d}b_n\Big] \exp\Big[-mT \sum_{n\geq 1} \omega_n^2 (a_n^2 + b_n^2)\Big] \\ &= C' \frac{\Delta x}{T} \prod_{n=1}^{\infty} \frac{\pi}{mT\omega_n^2} \; , \quad \omega_n = \frac{2\pi T n}{\hbar} \; . \end{aligned} \tag{1.56}$$

**Side B: "full theory computation".** In the presence of the regulator, and in the absence of $V(x)$, Eq. (1.31) can be computed in a very simple way:

$$\begin{aligned}
\lim_{\omega\to 0} \mathcal{Z}_{\text{regulated}} &= \int_{\Delta x} \mathrm{d}x\, \langle x| e^{-\frac{\hat p^2}{2mT}} |x\rangle \\
&= \int_{\Delta x} \mathrm{d}x \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar} \langle x| e^{-\frac{\hat p^2}{2mT}} |p\rangle \langle p|x\rangle \\
&= \int_{\Delta x} \mathrm{d}x \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar} e^{-\frac{p^2}{2mT}} \langle x|p\rangle \langle p|x\rangle \\
&= \Delta x \frac{1}{2\pi\hbar} \sqrt{2\pi m T}\,. \qquad (1.57)
\end{aligned}$$

**Matching the two sides.** Equating Eqs. (1.56) and (1.57), the regulator $\Delta x$ drops out, and we find

$$C' = \frac{T}{2\pi\hbar}\sqrt{2\pi m T}\prod_{n=1}^{\infty}\frac{mT\omega_n^2}{\pi}\,. \qquad (1.58)$$

Since the infrared regulator has dropped out, we may called $C'$ an "ultraviolet" coefficient.

Now we can continue with the full Eq. (1.54). Inserting $C'$ from Eq. (1.58), we get

$$\begin{aligned}
\mathcal{Z} &= \frac{T}{\hbar\omega}\prod_{n=1}^{\infty}\frac{1}{1+\frac{\omega^2}{\omega_n^2}} \qquad (1.59)\\
&= \frac{T}{\hbar\omega}\frac{1}{\prod_{n=1}^{\infty}\Big[1+\frac{(\hbar\omega/2\pi T)^2}{n^2}\Big]}\,. \qquad (1.60)
\end{aligned}$$

Making use of

$$\frac{\sinh \pi x}{\pi x} = \prod_{n=1}^{\infty}\left(1+\frac{x^2}{n^2}\right)\,, \qquad (1.61)$$

then yields directly Eq. (1.17): the result is correct!

Thus, we have indeed managed to reproduce the correct result from the path integral, without ever making recourse to Eq. (1.40) or, for that matter, to the discretization that was present in Eqs. (1.36), (1.39).

Let us end with a couple of final remarks. First of all, in Quantum Mechanics, the partition function $\mathcal{Z}$, and all other observables, are certainly finite and well-defined functions of the parameters $T, m$, and $\omega$, if computed properly. We saw that with path integrals this is not always obvious at every intermediate step, but at the end does work out. In Quantum Field Theory, on the contrary, divergences may remain, even if we compute everything correctly. These are then taken care of by renormalization. It is important to realise, however, that the "ambiguity" of the functional integration measure (through $C'$) is not in itself the source of these divergences, as our quantum mechanical example has demonstrated!

As the second remark, it is appropriate to stress that in many physically relevant observables, the coefficient $C'$ drops out completely, and the procedure is thereby simpler. An example of such a quantity is discussed in Exercise 1.

As a final remark, it should be noted that many of the concepts and techniques that were introduced with this simple example — zero-modes, infrared divergences, their regulation, matching computations, etc — will also play a role in much less trivial quantum field theoretic examples later on, so it is important to master them as early as possible.

### 1.5. Exercise 1

Defining

$$\hat{x}(\tau) \equiv e^{\frac{\hat{H}\tau}{\hbar}} \hat{x} e^{-\frac{\hat{H}\tau}{\hbar}} \;, \quad 0 < \tau < \beta\hbar \;, \tag{1.62}$$

we define a "2-point Green's function" as

$$G(\tau) \equiv \frac{1}{\mathcal{Z}} \mathrm{Tr} \left[ e^{-\beta\hat{H}} \hat{x}(\tau)\hat{x}(0) \right] \;. \tag{1.63}$$

The corresponding path integral reads

$$G(\tau) = \frac{\int_{x(\beta\hbar)=x(0)} \mathcal{D}x \, x(\tau)x(0) \exp[-S_E/\hbar]}{\int_{x(\beta\hbar)=x(0)} \mathcal{D}x \, \exp[-S_E/\hbar]} \;, \tag{1.64}$$

whereby the coefficient $C'$ has dropped out. The task is to compute explicitly $G(\tau)$ for the harmonic oscillator, by making use of

(a) the canonical formalism [expressing $\hat{H}$, $\hat{x}$ in terms of $\hat{a}$, $\hat{a}^\dagger$].

(b) the path integral formalism, in Fourier space.

**Solution to Exercise 1**

(a) In terms of $\hat{a}, \hat{a}^\dagger$, we can write

$$\hat{H} = \hbar\omega\Big(\hat{a}^\dagger\hat{a} + \frac{1}{2}\Big) , \quad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) , \quad [\hat{a}, \hat{a}^\dagger] = 1 . \tag{1.65}$$

In order to construct $\hat{x}(\tau)$, we make use of the expansion

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \frac{1}{3!}[\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + ... . \tag{1.66}$$

In particular,

$$\begin{aligned} [\hat{H}, \hat{a}] &= \hbar\omega[\hat{a}^\dagger\hat{a}, \hat{a}] = -\hbar\omega\hat{a} , \\ [\hat{H}, [\hat{H}, \hat{a}]] &= (-\hbar\omega)^2\hat{a} , \\ [\hat{H}, \hat{a}^\dagger] &= \hbar\omega[\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger , \\ [\hat{H}, [\hat{H}, \hat{a}^\dagger]] &= (\hbar\omega)^2\hat{a}^\dagger , \end{aligned} \tag{1.67}$$

and so forth, so that we can write

$$\begin{aligned} e^{\frac{\hat{H}\tau}{\hbar}}\hat{x}e^{-\frac{\hat{H}\tau}{\hbar}} &= \sqrt{\frac{\hbar}{2m\omega}}\bigg\{\hat{a}\Big[1 - \omega\tau + \frac{1}{2!}(\omega\tau)^2 + ...\Big] + \hat{a}^\dagger\Big[1 + \omega\tau + \frac{1}{2!}(\omega\tau)^2 + ...\Big]\bigg\} \\ &= \sqrt{\frac{\hbar}{2m\omega}}\Big(\hat{a}e^{-\omega\tau} + \hat{a}^\dagger e^{\omega\tau}\Big) . \end{aligned} \tag{1.68}$$

Inserting $\mathcal{Z}$ from Eq. (1.17), we then get

$$G(\tau) = 2\sinh\Big(\frac{\beta\hbar\omega}{2}\Big)\sum_{n=0}^{\infty}\langle n|e^{-\beta\hbar\omega(n+\frac{1}{2})}\frac{\hbar}{2m\omega}\Big(\hat{a}e^{-\omega\tau} + \hat{a}^\dagger e^{\omega\tau}\Big)\big(\hat{a} + \hat{a}^\dagger\big)|n\rangle . \tag{1.69}$$

We now use $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ to identify the non-zero matrix elements,

$$\langle n|\hat{a}\hat{a}^\dagger|n\rangle = n + 1 , \quad \langle n|\hat{a}^\dagger\hat{a}|n\rangle = n . \tag{1.70}$$

Thereby

$$G(\tau) = \frac{\hbar}{m\omega}\sinh\Big(\frac{\beta\hbar\omega}{2}\Big)\exp\Big(-\frac{\beta\hbar\omega}{2}\Big)\sum_{n=0}^{\infty}e^{-\beta\hbar\omega n}\Big[e^{-\omega\tau} + n\Big(e^{-\omega\tau} + e^{\omega\tau}\Big)\Big] . \tag{1.71}$$

The sums are simple,

$$\begin{aligned} \sum_{n=0}^{\infty}e^{-\beta\hbar\omega n} &= \frac{1}{1 - e^{-\beta\hbar\omega}} , \\ \sum_{n=0}^{\infty}ne^{-\beta\hbar\omega n} &= -\frac{1}{\beta\hbar}\frac{\mathrm{d}}{\mathrm{d}\omega}\frac{1}{1 - e^{-\beta\hbar\omega}} = \frac{e^{-\beta\hbar\omega}}{(1 - e^{-\beta\hbar\omega})^2} . \end{aligned} \tag{1.72}$$

In total, then,

$$\begin{aligned} G(\tau) &= \frac{\hbar}{2m\omega}\Big(1 - e^{-\beta\hbar\omega}\Big)\bigg[e^{-\omega\tau}\frac{1}{1 - e^{-\beta\hbar\omega}} + \Big(e^{-\omega\tau} + e^{\omega\tau}\Big)\frac{e^{-\beta\hbar\omega}}{(1 - e^{-\beta\hbar\omega})^2}\bigg] \\ &= \frac{\hbar}{2m\omega}\frac{1}{1 - e^{-\beta\hbar\omega}}\Big[e^{-\omega\tau} + e^{\omega(\tau - \beta\hbar)}\Big] \\ &= \frac{\hbar}{2m\omega}\frac{\cosh\Big[\Big(\frac{\beta\hbar}{2} - \tau\Big)\omega\Big]}{\sinh\Big[\frac{\beta\hbar\omega}{2}\Big]} . \end{aligned} \tag{1.73}$$

(b) Integration measure:

$$C' \int_{-\infty}^{\infty} \mathrm{d}a_0 \int_{-\infty}^{\infty} \Big[\prod_{n\ge 1} \mathrm{d}a_n \, \mathrm{d}b_n\Big] \; . \tag{1.74}$$

Exponential:

$$\exp\biggl[-\frac{1}{2}\, mT\omega^2 a_0^2 - mT\sum_{n\ge1}(\omega_n^2+\omega^2)(a_n^2+b_n^2)\biggr] = \exp\biggl[-\frac{1}{2}\, T \sum_{n=-\infty}^{\infty} m(\omega_n^2+\omega^2)|x_n|^2\biggr] \; . \tag{1.75}$$

Fourier representation:

$$\begin{aligned} x(\tau) &= T\biggl\{a_0 + \sum_{k=1}^{\infty}\Bigl[(a_k+ib_k)e^{i\omega_k\tau} + (a_k - ib_k)e^{-i\omega_k\tau}\Bigr]\biggr\} \; , & (1.76)\\ x(0) &= T\biggl\{a_0 + \sum_{l=1}^{\infty} 2a_l\biggr\} \; . & (1.77)\end{aligned}$$

Observable:

$$G(\tau) = \langle x(\tau) x(0)\rangle \equiv \frac{\int \mathrm{d}a_0 \int \prod_{n\ge1} \mathrm{d}a_n \, \mathrm{d}b_n \, x(\tau)\, x(0) \exp[\cdots]}{\int \mathrm{d}a_0 \int \prod_{n\ge1} \mathrm{d}a_n \, \mathrm{d}b_n \; \exp[\cdots]} \; . \tag{1.78}$$

Since the exponential is quadratic in $a_0, a_n, b_n \in \mathbb{R}$, we have

$$\langle a_0 a_k\rangle = \langle a_0 b_k\rangle = \langle a_k b_l\rangle = 0 \; , \quad \langle a_k a_l \rangle = \langle b_k b_l\rangle \propto \delta_{kl} \; . \tag{1.79}$$

Thereby

$$G(\tau) = T^2 \left\langle a_0^2 + \sum_{k=1}^{\infty} 2a_k^2 \left(e^{i\omega_k\tau} + e^{-i\omega_k\tau}\right)\right\rangle \; . \tag{1.80}$$

Here

$$\begin{aligned} \langle a_0^2\rangle &= \frac{\int \mathrm{d}a_0 \, a_0^2 \, \exp\left(-\frac{1}{2}\, mT\omega^2 a_0^2\right)}{\int \mathrm{d}a_0 \, \exp\left(-\frac{1}{2}\, mT\omega^2 a_0^2\right)} \\ &= -\frac{2}{m\omega^2}\frac{\mathrm{d}}{\mathrm{d}T}\biggl[\ln \int \mathrm{d}a_0 \, \exp\biggl(-\frac{1}{2}\, mT\omega^2 a_0^2\biggr)\biggr] = -\frac{2}{m\omega^2}\frac{\mathrm{d}}{\mathrm{d}T}\biggl[\ln \sqrt{\frac{2\pi}{m\omega^2 T}}\biggr] \\ &= \frac{1}{m\omega^2 T} \; , & (1.81) \\ \langle a_k^2\rangle &= \frac{\int \mathrm{d}a_k \, a_k^2 \, \exp\left[-mT(\omega_k^2+\omega^2)a_k^2\right]}{\int \mathrm{d}a_k \, \exp\left[-mT(\omega_k^2+\omega^2)a_k^2\right]} \\ &= \frac{1}{2m(\omega_k^2+\omega^2)T} \; . & (1.82)\end{aligned}$$

Inserting into Eq. (1.80), we get

$$G(\tau) = \frac{T}{m}\biggl(\frac{1}{\omega^2} + \sum_{k=1}^{\infty}\frac{e^{i\omega_k\tau}+e^{-i\omega_k\tau}}{\omega_k^2+\omega^2}\biggr) = \frac{T}{m}\sum_{k=-\infty}^{\infty}\frac{e^{i\omega_k\tau}}{\omega_k^2+\omega^2} \; , \tag{1.83}$$

where $\omega_k = 2\pi k T/\hbar$.

There are various ways to evaluate the sum in Eq. (1.83). We will encounter one generic method in the later sections, so let us here present a different approach. We start by noting that

$$\biggl(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \omega^2\biggr) G(\tau) = \frac{T}{m}\sum_{k=-\infty}^{\infty} e^{i\omega_k\tau} = \frac{\hbar}{m}\delta(\tau \bmod \beta\hbar) \; , \tag{1.84}$$

where we made use of a standard summation formula.[1]

We now first solve Eq. (1.84) for $0 < \tau < \beta\hbar$:

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \omega^2\right) G(\tau) = 0 \quad \Rightarrow \quad G(\tau) = A e^{\omega\tau} + B e^{-\omega\tau} \,, \tag{1.85}$$

where $A, B$ are unknown constants. The definition, Eq. (1.83), indicates that $G(\beta\hbar - \tau) = G(\tau)$, which allows to related $A$ and $B$:

$$G(\tau) = A \left[ e^{\omega\tau} + e^{\omega(\beta\hbar - \tau)} \right] \,. \tag{1.86}$$

The remaining unknown $A$ can be obtained by approaching the limit $\tau \to 0^+$. Then, from (1.83),

$$\begin{aligned} G(0) &= A\left(1 + e^{\omega\beta\hbar}\right) \\ &= \frac{T}{m} \sum_{k=-\infty}^{\infty} \frac{1}{\omega_k^2 + \omega^2} = \frac{T}{m} \frac{\hbar^2}{(2\pi T)^2} \sum_{k=-\infty}^{\infty} \frac{1}{k^2 + \left(\frac{\hbar\omega}{2\pi T}\right)^2} \\ &= \frac{\hbar}{2m\omega} \frac{\cosh\left(\frac{\hbar\omega}{2T}\right)}{\sinh\left(\frac{\hbar\omega}{2T}\right)} \,, \end{aligned} \tag{1.87}$$

where we made use of $\sum_{k=-\infty}^{\infty} 1/(k^2 + x^2) = \pi/x \tanh(\pi x)$. Solving for $A$, and inserting into Eq. (1.86), yields the important final result:

$$G(\tau) = \frac{\hbar}{2m\omega} \frac{\cosh\left[\left(\frac{\beta\hbar}{2} - \tau\right)\omega\right]}{\sinh\left[\frac{\beta\hbar\omega}{2}\right]} \,. \tag{1.88}$$

[1] Proof: Clearly $\sum_{k=-\infty}^{\infty} e^{ikx} = C\delta(x \bmod 2\pi)$, where $C$ is some constant. In order to determine $C$, let us integrate both sides of this equation from $0^-$ to $2\pi + 0^-$. On the left-hand side we get $2\pi\delta_{k,0}$, on the right-hand side $C$. Thus, $C = 2\pi$. Replacing now $x$ by $2\pi T\tau/\hbar$, and using $\delta(ax) = \delta(x)/|a|$ on the right-hand side, yields $\sum_{k=-\infty}^{\infty} e^{i\omega_k\tau} = \beta\hbar\,\delta(\tau \bmod \beta\hbar)$.