Chapter 1
Quantum Mechanics

Abstract After recalling some basic concepts of statistical physics and quantum mechanics, the partition function of a harmonic oscillator is defined and evaluated in the standard canonical formalism. An imaginary-time path integral representation is subsequently developed for the partition function, the path integral is evaluated in momentum space, and the earlier result is reproduced upon a careful treatment of the zero-mode contribution. Finally, the concept of 2-point functions (propagators) is introduced, and some of their key properties are derived in imaginary time.

Keywords Partition function • Euclidean path integral • Imaginary-time formalism • Matsubara modes • 2-point function

1.1 Path Integral Representation of the Partition Function

Basic Structure

The properties of a quantum-mechanical system are defined by its *Hamiltonian*, which for non-relativistic spin-0 particles in one dimension takes the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \; , \tag{1.1}$$

where m is the particle mass. The dynamics of the states $|\psi\rangle$ is governed by the *Schrödinger equation*,

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle \; , \tag{1.2}$$

which can formally be solved in terms of a *time-evolution operator* $\hat{U}(t;t_0)$. This operator satisfies the relation

$$|\psi(t)\rangle = \hat{U}(t;t_0)|\psi(t_0)\rangle \; , \tag{1.3}$$

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and for a time-independent Hamiltonian takes the explicit form

$$\hat{U}(t;t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} \, . \tag{1.4}$$

It is useful to note that in the *classical limit*, the system of Eq. (1.1) can be described by the *Lagrangian*

$$\mathcal{L} = \mathcal{L}_M = \frac{1}{2}m\dot{x}^2 - V(x) \, , \tag{1.5}$$

which is related to the classical version of the Hamiltonian via a simple Legendre transform:

$$p \equiv \frac{\partial \mathcal{L}_M}{\partial \dot{x}} \, , \quad H = \dot{x}p - \mathcal{L}_M = \frac{p^2}{2m} + V(x) \, . \tag{1.6}$$

Returning to the quantum-mechanical setting, various *bases* can be chosen for the state vectors. The so-called $|x\rangle$-basis satisfies the relations

$$\langle x|\hat{x}|x'\rangle = x\langle x|x'\rangle = x\,\delta(x-x') \, , \quad \langle x|\hat{p}|x'\rangle = -i\hbar\,\partial_x\langle x|x'\rangle = -i\hbar\,\partial_x\,\delta(x-x') \, , \tag{1.7}$$

whereas in the energy basis we simply have

$$\hat{H}|n\rangle = E_n|n\rangle \, . \tag{1.8}$$

An important concrete realization of a quantum-mechanical system is provided by the *harmonic oscillator*, defined by the potential

$$V(\hat{x}) \equiv \frac{1}{2}m\omega^2\hat{x}^2 \, . \tag{1.9}$$

In this case the energy eigenstates $|n\rangle$ can be found explicitly, with the corresponding eigenvalues equalling

$$E_n = \hbar\omega\Big(n + \frac{1}{2}\Big) \, , \quad n = 0, 1, 2, \ldots \, . \tag{1.10}$$

All the states are non-degenerate.

It turns out to be useful to view (quantum) mechanics formally as *(1+0)-dimensional (quantum) field theory*: the operator $\hat{x}$ can be viewed as a field operator $\hat{\phi}$ at a certain point, implying the correspondence

$$\hat{x} \leftrightarrow \hat{\phi}(\mathbf{0}) \, . \tag{1.11}$$

In quantum field theory operators are usually represented in the Heisenberg picture; correspondingly, we then have

$$\hat{x}_H(t) \leftrightarrow \hat{\phi}_H(t, \mathbf{0}) \, . \tag{1.12}$$

In the following we adopt an implicit notation whereby showing the time coordinate t as an argument of a field automatically implies the use of the Heisenberg picture, and the corresponding subscript is left out.

Canonical Partition Function

Taking our quantum-mechanical system to a finite temperature T, the most fundamental quantity of interest is the partition function, $\mathcal{Z}$. We employ the canonical ensemble, whereby $\mathcal{Z}$ is a function of T; introducing units in which $k_\mathrm{B} = 1$ (i.e., $T_\text{here} \equiv k_\mathrm{B} T_\text{SI-units}$), the partition function is defined by

$$\mathcal{Z}(T) \;\equiv\; \mathrm{Tr}\,[e^{-\beta\hat{H}}] \, , \quad \beta \;\equiv\; \frac{1}{T} \, , \tag{1.13}$$

where the trace is taken over the full Hilbert space. From this quantity, other observables, such as the free energy F, entropy S, and average energy E can be obtained via standard relations:

$$F = -T \ln \mathcal{Z} \, , \tag{1.14}$$

$$S = -\frac{\partial F}{\partial T} = \ln \mathcal{Z} + \frac{1}{T\mathcal{Z}} \mathrm{Tr}\,[\hat{H} e^{-\beta\hat{H}}] = -\frac{F}{T} + \frac{E}{T} \, , \tag{1.15}$$

$$E = \frac{1}{\mathcal{Z}} \mathrm{Tr}\,[\hat{H} e^{-\beta\hat{H}}] \, . \tag{1.16}$$

Let us now explicitly compute these quantities for the harmonic oscillator. This becomes a trivial exercise in the energy basis, given that we can immediately write

$$\mathcal{Z} = \sum_{n=0}^{\infty} \langle n | e^{-\beta\hat{H}} | n \rangle = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(\frac{1}{2}+n)} = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} = \frac{1}{2\sinh\left(\frac{\hbar\omega}{2T}\right)} \, . \tag{1.17}$$

Consequently,

$$F = T \ln\left(e^{\frac{\hbar\omega}{2T}} - e^{-\frac{\hbar\omega}{2T}}\right) = \frac{\hbar\omega}{2} + T \ln\left(1 - e^{-\beta\hbar\omega}\right) \tag{1.18}$$

$$\approx \begin{cases} \dfrac{\hbar\omega}{2} \, , & T \ll \hbar\omega \\ -T \ln\left(\dfrac{T}{\hbar\omega}\right) \, , & T \gg \hbar\omega \end{cases} \, , \tag{1.19}$$

$$S = -\ln\left(1 - e^{-\beta\hbar\omega}\right) + \frac{\hbar\omega}{T}\frac{1}{e^{\beta\hbar\omega} - 1} \tag{1.20}$$

$$\approx \begin{cases} \dfrac{\hbar\omega}{T} e^{-\frac{\hbar\omega}{T}} \,, & T \ll \hbar\omega \\ 1 + \ln\dfrac{T}{\hbar\omega} \,, & T \gg \hbar\omega \end{cases} \,, \tag{1.21}$$

$$E = F + TS = \hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1}\right) \tag{1.22}$$

$$\approx \begin{cases} \dfrac{\hbar\omega}{2} \,, & T \ll \hbar\omega \\ T \,, & T \gg \hbar\omega \end{cases} \,. \tag{1.23}$$

Note how in most cases one can separate the contribution of the ground state, dominating at low temperatures $T \ll \hbar\omega$, from that of the thermally excited states, characterized by the appearance of the Bose distribution $n_{\rm B}(\hbar\omega) \equiv 1/[\exp(\beta\hbar\omega) - 1]$. Note also that E rises linearly with T at high temperatures; the coefficient is said to count the number of degrees of freedom of the system.

Path Integral for the Partition Function

In the case of the harmonic oscillator, the energy eigenvalues are known in an analytic form, and $\mathcal{Z}$ could be easily evaluated. In many other cases the E_n are, however, difficult to compute. A more useful representation of $\mathcal{Z}$ is obtained by writing it as a *path integral*.

In order to get started, let us recall some basic relations. First of all, it follows from the form of the momentum operator in the $|x\rangle$-basis that

$$\langle x|\hat{p}|p\rangle = p\langle x|p\rangle = -i\hbar\,\partial_x\langle x|p\rangle \Rightarrow \langle x|p\rangle = A\,e^{\frac{ipx}{\hbar}} \,, \tag{1.24}$$

where A is some constant. Second, we need completeness relations in both $|x\rangle$ and $|p\rangle$-bases, which take the respective forms

$$\int \mathrm{d}x\,|x\rangle\langle x| = \hat{\mathbb{1}} \,, \qquad \int \frac{\mathrm{d}p}{B}\,|p\rangle\langle p| = \hat{\mathbb{1}} \,, \tag{1.25}$$

where B is another constant. The choices of A and B are not independent; indeed,

$$\begin{aligned}\hat{\mathbb{1}} &= \int \mathrm{d}x \int \frac{\mathrm{d}p}{B} \int \frac{\mathrm{d}p'}{B} |p\rangle\langle p|x\rangle\langle x|p'\rangle\langle p'| = \int \mathrm{d}x \int \frac{\mathrm{d}p}{B} \int \frac{\mathrm{d}p'}{B} |p\rangle |A|^2 e^{\frac{i(p'-p)x}{\hbar}} \langle p'| \\ &= \int \frac{\mathrm{d}p}{B} \int \frac{\mathrm{d}p'}{B} |p\rangle |A|^2 2\pi\hbar\,\delta(p'-p)\langle p'| = \frac{2\pi\hbar|A|^2}{B} \int \frac{\mathrm{d}p}{B}\,|p\rangle\langle p| = \frac{2\pi\hbar|A|^2}{B}\,\hat{\mathbb{1}} \,, \end{aligned} \tag{1.26}$$

implying that $B = 2\pi\hbar|A|^2$. We choose $A \equiv 1$ in the following, so that $B = 2\pi\hbar$.

Next, we move on to evaluate the partition function, which we do in the x-basis, so that our starting point becomes

$$\mathcal{Z} = \mathrm{Tr}\,[e^{-\beta\hat{H}}] = \int \mathrm{d}x\, \langle x|e^{-\beta\hat{H}}|x\rangle = \int \mathrm{d}x\, \langle x|e^{-\frac{\epsilon\hat{H}}{\hbar}} \cdots e^{-\frac{\epsilon\hat{H}}{\hbar}}|x\rangle\ . \tag{1.27}$$

Here we have split $e^{-\beta\hat{H}}$ into a product of $N \gg 1$ different pieces, defining $\epsilon \equiv \beta\hbar/N$.

A crucial trick at this point is to insert

$$\hat{\mathbb{1}} = \int \frac{\mathrm{d}p_i}{2\pi\hbar}\, |p_i\rangle\langle p_i|\ , \quad i = 1, \ldots, N\ , \tag{1.28}$$

on the *left side* of each exponential, with i increasing from right to left; and

$$\hat{\mathbb{1}} = \int \mathrm{d}x_i\, |x_i\rangle\langle x_i|\ , \quad i = 1, \ldots, N\ , \tag{1.29}$$

on the *right side* of each exponential, with again i increasing from right to left. Thereby we are left to consider matrix elements of the type

$$\begin{aligned}\langle x_{i+1}|p_i\rangle\langle p_i|e^{-\frac{\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})}|x_i\rangle &= e^{\frac{ip_ix_{i+1}}{\hbar}}\langle p_i|e^{-\frac{\epsilon}{\hbar}H(p_i,x_i)+\mathcal{O}(\epsilon^2)}|x_i\rangle \\ &= \exp\left\{-\frac{\epsilon}{\hbar}\left[\frac{p_i^2}{2m} - ip_i\frac{x_{i+1}-x_i}{\epsilon} + V(x_i) + \mathcal{O}(\epsilon)\right]\right\}\ . \end{aligned}\tag{1.30}$$

Moreover, we note that at the very right, we have

$$\langle x_1|x\rangle = \delta(x_1 - x)\ , \tag{1.31}$$

which allows us to carry out the integral over x. Similarly, at the very left, the role of $\langle x_{i+1}|$ is played by the state $\langle x| = \langle x_1|$. Finally, we remark that the $\mathcal{O}(\epsilon)$ correction in Eq. (1.30) can be eliminated by sending $N \to \infty$.

In total, we can thus write the partition function in the form

$$\mathcal{Z} = \lim_{N\to\infty}\int\left[\prod_{i=1}^{N}\frac{\mathrm{d}x_i\mathrm{d}p_i}{2\pi\hbar}\right]\exp\left\{-\frac{1}{\hbar}\sum_{j=1}^{N}\epsilon\left[\frac{p_j^2}{2m} - ip_j\frac{x_{j+1}-x_j}{\epsilon} + V(x_j)\right]\right\}\Bigg|_{x_{N+1}\equiv x_1,\,\epsilon\equiv\beta\hbar/N}\ , \tag{1.32}$$

which is often symbolically expressed as a "continuum" path integral

$$\mathcal{Z} = \int_{x(\beta\hbar)=x(0)}\frac{\mathcal{D}x\mathcal{D}p}{2\pi\hbar}\exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar}\mathrm{d}\tau\left[\frac{[p(\tau)]^2}{2m} - ip(\tau)\dot{x}(\tau) + V(x(\tau))\right]\right\}\ . \tag{1.33}$$

The integration measure here is understood as the limit indicated in Eq. (1.32); the discrete x_i's have been collected into a function $x(\tau)$; and the maximal value of the τ-coordinate has been obtained from $\epsilon N = \beta\hbar$.

Returning to the discrete form of the path integral, we note that the integral over the momenta p_i is Gaussian, and can thereby be carried out explicitly:

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}p_i}{2\pi\hbar} \exp\left\{-\frac{\epsilon}{\hbar}\left[\frac{p_i^2}{2m} - ip_i\frac{x_{i+1}-x_i}{\epsilon}\right]\right\} = \sqrt{\frac{m}{2\pi\hbar\epsilon}} \exp\left[-\frac{m(x_{i+1}-x_i)^2}{2\hbar\epsilon}\right]. \tag{1.34}$$

Using this, Eq. (1.32) becomes

$$\mathcal{Z} = \lim_{N\to\infty} \int \left[\prod_{i=1}^{N} \frac{\mathrm{d}x_i}{\sqrt{2\pi\hbar\epsilon/m}}\right] \exp\left\{-\frac{1}{\hbar}\sum_{j=1}^{N} \epsilon\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2 + V(x_j)\right]\right\}\Bigg|_{x_{N+1}\equiv x_1,\,\epsilon\equiv\beta\hbar/N}, \tag{1.35}$$

which may also be written in a continuum form. Of course the measure then contains a factor which appears quite divergent at large N,

$$C \equiv \left(\frac{m}{2\pi\hbar\epsilon}\right)^{N/2} = \exp\left[\frac{N}{2}\ln\left(\frac{mN}{2\pi\hbar^2\beta}\right)\right]. \tag{1.36}$$

This factor is, however, *independent of the properties of the potential* $V(x_j)$ and thereby contains *no dynamical information*, so that we do not need to worry too much about the apparent divergence. For the moment, then, we can simply write down a continuum "functional integral",

$$\mathcal{Z} = C \int_{x(\beta\hbar)=x(0)} \mathcal{D}x \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau \left[\frac{m}{2}\left(\frac{\mathrm{d}x(\tau)}{\mathrm{d}\tau}\right)^2 + V(x(\tau))\right]\right\}. \tag{1.37}$$

Let us end by giving an "interpretation" to the result in Eq. (1.37). We recall that the usual quantum-mechanical path integral at zero temperature contains the exponential

$$\exp\left(\frac{i}{\hbar}\int \mathrm{d}t\,\mathcal{L}_M\right), \quad \mathcal{L}_M = \frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x). \tag{1.38}$$

We note that Eq. (1.37) can be obtained from its zero-temperature counterpart with the following recipe [1]:

(i) Carry out a Wick rotation, denoting $\tau \equiv it$.
(ii) Introduce

$$L_E \equiv -\mathcal{L}_M(\tau = it) = \frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + V(x). \tag{1.39}$$

(iii) Restrict τ to the interval $(0, \beta\hbar)$.
(iv) Require periodicity of $x(\tau)$, i.e. $x(\beta\hbar) = x(0)$.

With these steps (and noting that $i\mathrm{d}t = \mathrm{d}\tau$), the exponential becomes

$$\exp\left(\frac{i}{\hbar}\int \mathrm{d}t\,\mathcal{L}_M\right) \overset{\text{(i)}-\text{(iv)}}{\longrightarrow} \exp\left(-\frac{1}{\hbar}S_E\right) \equiv \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar}\mathrm{d}\tau\,L_E\right), \tag{1.40}$$

where the subscript E stands for "Euclidean". Because of step (i), the path integral in Eq. (1.40) is also known as the *imaginary-time formalism*. It turns out that this recipe works, with few modifications, also in quantum field theory, and even for spin-1/2 and spin-1 particles, although the derivation of the path integral itself looks quite different in those cases. We return to these issues in later chapters of the book.

1.2 Evaluation of the Path Integral for the Harmonic Oscillator

As an independent crosscheck of the results of Sect. 1.1, we now explicitly evaluate the path integral of Eq. (1.37) in the case of a harmonic oscillator, and compare the result with Eq. (1.17). To make the exercise more interesting, we carry out the evaluation in Fourier space with respect to the time coordinate τ. Moreover we would like to deduce the information contained in the divergent constant C without making use of its actual value, given in Eq. (1.36).

Let us start by representing an arbitrary function $x(\tau)$, $0 < \tau < \beta\hbar$, with the property $x((\beta\hbar)^-) = x(0^+)$ (referred to as "periodicity") as a Fourier sum

$$x(\tau) \equiv T\sum_{n=-\infty}^{\infty} x_n\, e^{i\omega_n\tau}\,, \tag{1.41}$$

where the factor T is a convention. Imposing periodicity requires that

$$e^{i\omega_n\beta\hbar} = 1\,, \quad \text{i.e.} \quad \omega_n\beta\hbar = 2\pi n\,, \quad n \in \mathbb{Z}\,, \tag{1.42}$$

where the values $\omega_n = 2\pi T n/\hbar$ are called *Matsubara frequencies*. The corresponding amplitudes x_n are called *Matsubara modes*.

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

$$x(\tau) \in \mathbb{R} \;\Rightarrow\; x^*(\tau) = x(\tau) \;\Rightarrow\; x_n^* = x_{-n}\,. \tag{1.43}$$

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

$$x_n^* = a_n - ib_n = x_{-n} = a_{-n} + ib_{-n} \Rightarrow \begin{cases} a_n = a_{-n} \\ b_n = -b_{-n} \end{cases} , \tag{1.44}$$

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

$$x(\tau) = T\left\{ a_0 + \sum_{n=1}^{\infty} \left[(a_n + ib_n)e^{i\omega_n\tau} + (a_n - ib_n)e^{-i\omega_n\tau} \right] \right\} , \tag{1.45}$$

where a_0 is called (the amplitude of) the Matsubara *zero mode*.

With the representation of Eq. (1.41), general quadratic structures can be expressed as

$$\begin{aligned} \frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau\, x(\tau)y(\tau) &= T^2 \sum_{m,n} x_n y_m \frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau\, e^{i(\omega_n+\omega_m)\tau} \\ &= T^2 \sum_{m,n} x_n y_m \frac{1}{T}\, \delta_{n,-m} = T \sum_n x_n y_{-n} \, . \end{aligned} \tag{1.46}$$

In particular, the argument of the exponential in Eq. (1.37) becomes

$$\begin{aligned} & -\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau\, \frac{m}{2}\left[\frac{\mathrm{d}x(\tau)}{\mathrm{d}\tau}\frac{\mathrm{d}x(\tau)}{\mathrm{d}\tau} + \omega^2\, x(\tau)x(\tau) \right] \\ & \overset{(1.46)}{=} \quad -\frac{mT}{2} \sum_{n=-\infty}^{\infty} x_n \left[i\omega_n\, i\omega_{-n} + \omega^2 \right] x_{-n} \\ & \overset{\omega_{-n}=-\omega_n}{=} \quad -\frac{mT}{2} \sum_{n=-\infty}^{\infty} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2) \\ & \overset{(1.45)}{=} \quad -\frac{mT}{2}\, \omega^2 a_0^2 - mT \sum_{n=1}^{\infty} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2) \, . \end{aligned} \tag{1.47}$$

Next, we need to consider the *integration measure*. To this end, 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 a_0 and $\{a_n, b_n\}$, $n \geq 1$, whereby the measure becomes

$$\mathcal{D}x(\tau) = \left| \det\left[\frac{\delta x(\tau)}{\delta x_n} \right] \right| \, \mathrm{d}a_0 \left[\prod_{n\geq 1} \mathrm{d}a_n\, \mathrm{d}b_n \right] . \tag{1.48}$$

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

$$C' \equiv C \left| \det\left[\frac{\delta x(\tau)}{\delta x_n}\right] \right| , \tag{1.49}$$

and regard now C' as an unknown coefficient.

Making use of the Gaussian integral $\int_{-\infty}^{\infty} \mathrm{d}x \exp(-cx^2) = \sqrt{\pi/c}$, $c > 0$, as well as the above integration measure, the expression in Eq. (1.37) becomes

$$\mathcal{Z} = C' \int_{-\infty}^{\infty} \mathrm{d}a_0 \int_{-\infty}^{\infty} \Big[\prod_{n\geq 1} \mathrm{d}a_n\, \mathrm{d}b_n\Big] \exp\Big[-\frac{1}{2} mT\omega^2 a_0^2 - mT \sum_{n\geq 1} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2)\Big] \tag{1.50}$$

$$= C' \sqrt{\frac{2\pi}{mT\omega^2}} \prod_{n=1}^{\infty} \frac{\pi}{mT(\omega_n^2 + \omega^2)} , \quad \omega_n = \frac{2\pi T n}{\hbar} . \tag{1.51}$$

The remaining task is to determine C'. This can be achieved via the following observations:

- Since C' is independent of ω [which only appears in $V(x)$], we can determine it in the limit $\omega = 0$, whereby the system simplifies.
- The integral over the zero mode a_0 in Eq. (1.50) is, however, divergent for $\omega \to 0$. We may call such a divergence an *infrared divergence*: the zero mode is the *lowest-energy* mode.
- We can still take the $\omega \to 0$ limit, if we momentarily *regulate* the integration over the zero mode in some way. Noting from Eq. (1.45) that

$$\frac{1}{\beta\hbar} \int_0^{\beta\hbar} \mathrm{d}\tau\, x(\tau) = T a_0 , \tag{1.52}$$

  we see that Ta_0 represents the average value of $x(\tau)$ over the τ-interval. We may thus regulate the system by "putting it in a periodic box", i.e. by restricting the (average) value of $x(\tau)$ to some (large but finite) interval Δx.

With this setup, we can now proceed to find C' via *matching*.

"Effective theory computation": In the $\omega \to 0$ limit but in the presence of the regulator, Eq. (1.50) becomes

$$\lim_{\omega\to 0} \mathcal{Z}_{\text{regulated}} = C' \int_{\Delta x/T} \mathrm{d}a_0 \int_{-\infty}^{\infty} \Big[\prod_{n\geq 1} \mathrm{d}a_n\, \mathrm{d}b_n\Big] \exp\Big[-mT \sum_{n\geq 1} \omega_n^2 (a_n^2 + b_n^2)\Big]$$

$$= C' \frac{\Delta x}{T} \prod_{n=1}^{\infty} \frac{\pi}{mT\omega_n^2} , \quad \omega_n = \frac{2\pi T n}{\hbar} . \tag{1.53}$$

"Full theory computation": In the presence of the regulator, and in the absence of $V(x)$ (implied by the $\omega \to 0$ limit), Eq. (1.27) can be computed in a very simple way:

$$\begin{aligned}
\lim_{\omega\to 0} \mathcal{Z}_{\text{regulated}} &= \int_{\Delta x} \mathrm{d}x \, \langle x| e^{-\frac{\hat{p}^2}{2mT}} |x\rangle \\
&= \int_{\Delta x} \mathrm{d}x \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar} \langle x| e^{-\frac{\hat{p}^2}{2mT}} |p\rangle \langle p|x\rangle \\
&= \int_{\Delta x} \mathrm{d}x \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar} e^{-\frac{p^2}{2mT}} \underbrace{\langle x|p\rangle \langle p|x\rangle}_{1} \\
&= \frac{\Delta x}{2\pi\hbar} \sqrt{2\pi m T} \, . \qquad (1.54)
\end{aligned}$$

Matching the two sides: Equating Eqs. (1.53) and (1.54), we find the formal expression

$$C' = \frac{T}{2\pi\hbar} \sqrt{2\pi m T} \prod_{n=1}^{\infty} \frac{mT\omega_n^2}{\pi} \, . \qquad (1.55)$$

Since the regulator Δx has dropped out, we may call C' an "ultraviolet" matching coefficient.

With C' determined, we can now continue with Eq. (1.51), obtaining the finite expression

$$\begin{aligned}
\mathcal{Z} &= \frac{T}{\hbar\omega} \prod_{n=1}^{\infty} \frac{\omega_n^2}{\omega_n^2 + \omega^2} \qquad (1.56) \\
&= \frac{T}{\hbar\omega} \frac{1}{\prod_{n=1}^{\infty} \left[1 + \frac{(\hbar\omega/2\pi T)^2}{n^2}\right]} \, . \qquad (1.57)
\end{aligned}$$

Making use of the identity

$$\frac{\sinh \pi x}{\pi x} = \prod_{n=1}^{\infty} \left(1 + \frac{x^2}{n^2}\right) \qquad (1.58)$$

we directly reproduce our earlier result for the partition function, Eq. (1.17). Thus, we have managed to correctly evaluate the path integral without ever making recourse to Eq. (1.36) or, for that matter, to the discretization that was present in Eqs. (1.32) and (1.35).

Let us end with a few remarks:

- In quantum mechanics, the partition function $\mathcal{Z}$ as well as all other observables are finite functions of the parameters T, m, and ω, if computed properly. We saw that with path integrals this is not obvious at every intermediate step, but at the end it did work out. In quantum field theory, on the contrary, "ultraviolet" (UV) divergences may remain in the results even if we compute everything correctly. These are then taken care of by renormalization. However, as our quantum-mechanical example demonstrated, the "ambiguity" of the functional integration measure (through C') is not in itself a source of UV divergences.
- It is appropriate to stress that in many physically relevant observables, the coefficient C' drops out completely, and the above procedure is thereby even simpler. An example of such a quantity is given in Eq. (1.60) below.
- Finally, some of the concepts and techniques that were introduced with this simple example—zero modes, infrared divergences, their regularization, matching computations, etc.—also play a role in non-trivial quantum field theoretic examples that we encounter later on.

Appendix: 2-Point Function

Defining a Heisenberg-like operator (with $it \to \tau$)

$$\hat{x}(\tau) \;\equiv\; e^{\frac{\hat{H}\tau}{\hbar}}\,\hat{x}\,e^{-\frac{\hat{H}\tau}{\hbar}}\;, \quad 0 < \tau < \beta\hbar\;, \tag{1.59}$$

we define a "2-point Green's function" or a "propagator" through

$$G(\tau) \;\equiv\; \frac{1}{\mathcal{Z}}\,\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{x}(\tau)\hat{x}(0)\right]. \tag{1.60}$$

The corresponding path integral can be shown to read

$$G(\tau) = \frac{\int_{x(\beta\hbar)=x(0)}\mathcal{D}x\, x(\tau)x(0)\exp[-S_E/\hbar]}{\int_{x(\beta\hbar)=x(0)}\mathcal{D}x\,\exp[-S_E/\hbar]}\;, \tag{1.61}$$

whereby the normalization of $\mathcal{D}x$ plays no role. In the following, we compute $G(\tau)$ explicitly for the harmonic oscillator, by making use of

(a) the canonical formalism, i.e. expressing $\hat{H}$ and $\hat{x}$ in terms of the annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$,
(b) the path integral formalism, working in Fourier space.

Starting with the canonical formalism, we write all quantities in terms of $\hat{a}$ and $\hat{a}^\dagger$:

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \quad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger), \quad [\hat{a}, \hat{a}^\dagger] = 1 . \tag{1.62}$$

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

$$e^{\hat{A}}\hat{B}\,e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \frac{1}{3!}[\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + \dots . \tag{1.63}$$

Noting that

$$\begin{aligned}
[\hat{H}, \hat{a}] &= \hbar\omega[\hat{a}^\dagger\hat{a}, \hat{a}] = -\hbar\omega\hat{a} , \\
[\hat{H}, [\hat{H}, \hat{a}]] &= (-\hbar\omega)^2\hat{a} , \\
[\hat{H}, \hat{a}^\dagger] &= \hbar\omega[\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger , \\
[\hat{H}, [\hat{H}, \hat{a}^\dagger]] &= (\hbar\omega)^2\hat{a}^\dagger ,
\end{aligned} \tag{1.64}$$

and so forth, we can write

$$\begin{aligned}
e^{\frac{\hat{H}\tau}{\hbar}}\hat{x}\,e^{-\frac{\hat{H}\tau}{\hbar}} &= \sqrt{\frac{\hbar}{2m\omega}}\left\{\hat{a}\left[1 - \omega\tau + \frac{1}{2!}(-\omega\tau)^2 + \dots\right]\right. \\
&\quad \left. + \hat{a}^\dagger\left[1 + \omega\tau + \frac{1}{2!}(\omega\tau)^2 + \dots\right]\right\} \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}\,e^{-\omega\tau} + \hat{a}^\dagger e^{\omega\tau}\right) .
\end{aligned} \tag{1.65}$$

Inserting now $\mathcal{Z}$ from Eq. (1.17), Eq. (1.60) becomes

$$G(\tau) = 2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\sum_{n=0}^{\infty}\langle n|e^{-\beta\hbar\omega(n+\frac{1}{2})}\frac{\hbar}{2m\omega}\left(\hat{a}\,e^{-\omega\tau} + \hat{a}^\dagger e^{\omega\tau}\right)\left(\hat{a} + \hat{a}^\dagger\right)|n\rangle . \tag{1.66}$$

With the relations $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ we can identify the non-zero matrix elements,

$$\langle n|\hat{a}\hat{a}^\dagger|n\rangle = n + 1 , \quad \langle n|\hat{a}^\dagger\hat{a}|n\rangle = n . \tag{1.67}$$

Thereby we obtain

$$G(\tau) = \frac{\hbar}{m\omega}\sinh\left(\frac{\beta\hbar\omega}{2}\right)\exp\left(-\frac{\beta\hbar\omega}{2}\right)\sum_{n=0}^{\infty}e^{-\beta\hbar\omega n}\left[e^{-\omega\tau} + n\left(e^{-\omega\tau} + e^{\omega\tau}\right)\right] , \tag{1.68}$$

where the sums are quickly evaluated as geometric sums,

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n} = \frac{1}{1-e^{-\beta\hbar\omega}} \,,$$

$$\sum_{n=0}^{\infty} n e^{-\beta\hbar\omega n} = -\frac{1}{\beta\hbar}\frac{\mathrm{d}}{\mathrm{d}\omega}\frac{1}{1-e^{-\beta\hbar\omega}} = \frac{e^{-\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^2} \,. \tag{1.69}$$

In total, we then have

$$\begin{aligned} G(\tau) &= \frac{\hbar}{2m\omega}\Big(1-e^{-\beta\hbar\omega}\Big)\Bigg[\frac{e^{-\omega\tau}}{1-e^{-\beta\hbar\omega}} + \Big(e^{-\omega\tau}+e^{\omega\tau}\Big)\frac{e^{-\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^2}\Bigg] \\ &= \frac{\hbar}{2m\omega}\frac{1}{1-e^{-\beta\hbar\omega}}\Big[e^{-\omega\tau}+e^{\omega(\tau-\beta\hbar)}\Big] \\ &= \frac{\hbar}{2m\omega}\frac{\cosh\Big[\Big(\frac{\beta\hbar}{2}-\tau\Big)\,\omega\Big]}{\sinh\Big[\frac{\beta\hbar\omega}{2}\Big]} \,. \end{aligned} \tag{1.70}$$

As far as the path integral treatment goes, we employ the same representation as in Eq. (1.50), noting that C' drops out in the ratio of Eq. (1.61). Recalling the Fourier representation of Eq. (1.45),

$$x(\tau) = T\Bigg\{a_0 + \sum_{k=1}^{\infty}\Big[(a_k+ib_k)e^{i\omega_k\tau} + (a_k-ib_k)e^{-i\omega_k\tau}\Big]\Bigg\} \,, \tag{1.71}$$

$$x(0) = T\Bigg\{a_0 + \sum_{l=1}^{\infty} 2a_l\Bigg\} \,, \tag{1.72}$$

the observable of our interest becomes

$$G(\tau) \;=\; \big\langle x(\tau)x(0)\big\rangle \;\equiv\; \frac{\int \mathrm{d}a_0 \int \prod_{n\geq 1}\mathrm{d}a_n\,\mathrm{d}b_n\,x(\tau)\,x(0)\exp[-S_E/\hbar]}{\int \mathrm{d}a_0 \int \prod_{n\geq 1}\mathrm{d}a_n\,\mathrm{d}b_n\,\exp[-S_E/\hbar]} \,. \tag{1.73}$$

At this point, we employ the fact that the exponential is quadratic in $a_0, a_n, b_n \in \mathbb{R}$, which immediately implies

$$\langle a_0 a_k\rangle = \langle a_0 b_k\rangle = \langle a_k b_l\rangle = 0 \,, \quad \langle a_k a_l\rangle = \langle b_k b_l\rangle \propto \delta_{kl} \,, \tag{1.74}$$

with the expectation values defined in the sense of Eq. (1.73). Thereby we obtain

$$G(\tau) = T^2\Big\langle a_0^2 + \sum_{k=1}^{\infty} 2a_k^2\left(e^{i\omega_k\tau}+e^{-i\omega_k\tau}\right)\Big\rangle \,, \tag{1.75}$$

where

$$\langle a_0^2 \rangle = \frac{\int \mathrm{d}a_0\, a_0^2 \, \exp\left(-\frac{1}{2}mT\omega^2 a_0^2\right)}{\int \mathrm{d}a_0 \, \exp\left(-\frac{1}{2}mT\omega^2 a_0^2\right)}$$
$$= -\frac{2}{m\omega^2}\frac{\mathrm{d}}{\mathrm{d}T}\left[\ln \int \mathrm{d}a_0 \, \exp\left(-\frac{1}{2}mT\omega^2 a_0^2\right)\right] = -\frac{2}{m\omega^2}\frac{\mathrm{d}}{\mathrm{d}T}\left[\ln\sqrt{\frac{2\pi}{m\omega^2 T}}\right]$$
$$= \frac{1}{m\omega^2 T} , \tag{1.76}$$

$$\langle a_k^2 \rangle = \frac{\int \mathrm{d}a_k\, a_k^2 \, \exp\left[-mT(\omega_k^2+\omega^2)a_k^2\right]}{\int \mathrm{d}a_k \, \exp\left[-mT(\omega_k^2+\omega^2)a_k^2\right]}$$
$$= \frac{1}{2m(\omega_k^2+\omega^2)T} . \tag{1.77}$$

Inserting these into Eq. (1.75) we get

$$G(\tau) = \frac{T}{m}\left(\frac{1}{\omega^2} + \sum_{k=1}^{\infty}\frac{e^{i\omega_k\tau}+e^{-i\omega_k\tau}}{\omega_k^2+\omega^2}\right) = \frac{T}{m}\sum_{k=-\infty}^{\infty}\frac{e^{i\omega_k\tau}}{\omega_k^2+\omega^2} , \tag{1.78}$$

where we recall that $\omega_k = 2\pi kT/\hbar$.

There are various ways to evaluate the sum in Eq. (1.78). We encounter a generic method in Sect. 2.2, so let us present a different approach here. We start by noting that

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+\omega^2\right)G(\tau) = \frac{T}{m}\sum_{k=-\infty}^{\infty} e^{i\omega_k\tau} = \frac{\hbar}{m}\,\delta(\tau \bmod \beta\hbar) , \tag{1.79}$$

where we made use of the standard summation formula $\sum_{k=-\infty}^{\infty} e^{i\omega_k\tau} = \beta\hbar\,\delta(\tau \bmod \beta\hbar)$.[1]

Next, we solve Eq. (1.79) for $0 < \tau < \beta\hbar$, obtaining

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+\omega^2\right)G(\tau) = 0 \quad \Rightarrow \quad G(\tau) = A\,e^{\omega\tau} + B\,e^{-\omega\tau} , \tag{1.80}$$

[1] "Proof": $\sum_{k=-\infty}^{\infty} e^{i\omega_k\tau} = 1 + \lim_{\epsilon\to 0}\sum_{k=1}^{\infty}[(e^{i\frac{2\pi\tau}{\beta\hbar}-\epsilon})^k + (e^{-i\frac{2\pi\tau}{\beta\hbar}-\epsilon})^k] = \lim_{\epsilon\to 0}\Big[\frac{1}{1-e^{i\frac{2\pi\tau}{\beta\hbar}-\epsilon}} - \frac{1}{1-e^{i\frac{2\pi\tau}{\beta\hbar}+\epsilon}}\Big]$. If $\tau \neq 0 \bmod \beta\hbar$, then the limit $\epsilon \to 0$ can be taken, and the two terms cancel against each other. But if $\frac{2\pi\tau}{\beta\hbar} \approx 0$, we can expand to leading order in a Taylor series, obtaining $\lim_{\epsilon\to 0}\Big[\frac{i}{\frac{2\pi\tau}{\beta\hbar}+i\epsilon} - \frac{i}{\frac{2\pi\tau}{\beta\hbar}-i\epsilon}\Big] = 2\pi\delta(\frac{2\pi\tau}{\beta\hbar}) = \beta\hbar\,\delta(\tau)$.

where A, B are unknown constants. The solution can be further restricted by noting that the definition of $G(\tau)$, Eq. (1.78), indicates that $G(\beta\hbar - \tau) = G(\tau)$. Using this condition to obtain B, we then get

$$G(\tau) = A\left[e^{\omega\tau} + e^{\omega(\beta\hbar-\tau)}\right] . \tag{1.81}$$

The remaining unknown A can be obtained by integrating Eq. (1.79) over the source at $\tau = 0$ and making use of the periodicity of $G(\tau)$, $G(\tau + \beta\hbar) = G(\tau)$. This finally produces

$$G'((\beta\hbar)^-) - G'(0^+) = \frac{\hbar}{m} \quad \Rightarrow \quad 2\omega A\left(e^{\omega\beta\hbar} - 1\right) = \frac{\hbar}{m} , \tag{1.82}$$

which together with Eq. (1.81) yields our earlier result, Eq. (1.70).

The agreement of the two different computations, Eqs. (1.60) and (1.61), once again demonstrates the equivalence of the canonical and path integral approaches to solving thermodynamic quantities in a quantum-mechanical setting.

Reference

1. R.P. Feynman, A.R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965)