1. Quantum Mechanics

1.1. Basic structure

The properties of the system can be described by a *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 is governed by the *Schrödinger equation*,

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

Formally, the time evolution can be solved in terms of the *time-evolution operator*:

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

where, for a time-independent Hamiltonian,

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

For the state vectors $|\psi\rangle$, various *bases* can be chosen. In the $|x\rangle$-basis,

$$\langle x|\hat{x}|x'\rangle = x\langle x|x'\rangle = x\,\delta(x-x') \; , \quad \langle x|\hat{p}|x'\rangle = -i\hbar\partial_x\langle x|x'\rangle = -i\hbar\partial_x\,\delta(x-x') \; . \tag{1.5}$$

In the energy basis,

$$\hat{H}|n\rangle = E_n|n\rangle \; . \tag{1.6}$$

In the *classical limit*, the system of Eq. (1.1) can be described by the *Lagrangian*

$$\mathcal{L}_M = \frac{1}{2}m\dot{x}^2 - V(x) \; . \tag{1.7}$$

A Legendre transform leads to the classical Hamiltonian:

$$p = \frac{\partial \mathcal{L}_M}{\partial \dot{x}} \; , \quad H = \dot{x}p - \mathcal{L}_M = \frac{p^2}{2m} + V(x) \; . \tag{1.8}$$

A most important example of a quantum mechanical system is provided by a *harmonic oscillator*:

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

In this case the energy eigenstates can be found explicitly:

$$E_n = \hbar\omega\Big(n + \frac{1}{2}\Big) \; , \quad n = 1, 2, 3, \ldots \; . \tag{1.10}$$

All states are non-degenerate.

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

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

In quantum field theory operators are usually represented in the Heisenberg picture rather than in the Schrödinger picture; then

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

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

1.2. Canonical partition function

Taking now our quantum mechanical system to a finite temperature T, the basic quantity to compute is the partition function $\mathcal{Z}$. We employ the canonical ensemble, whereby $\mathcal{Z}$ is a function of T. Introducing units where $k_B = 1$ (i.e., $T_{\text{here}} \equiv k_B T_{\text{SI-units}}$), the partition function is defined by

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

From the partition function, other observables are obtained, for instance the free energy F, the entropy S, and the average energy E:

$$\begin{aligned} F &= -T\ln\mathcal{Z}\;, & (1.14)\\ S &= -\frac{\partial F}{\partial T} = \ln\mathcal{Z} + \frac{1}{T\mathcal{Z}}\mathrm{Tr}\,[\hat{H}e^{-\beta\hat{H}}] = -\frac{F}{T} + \frac{E}{T}\;, & (1.15)\\ E &= \frac{1}{\mathcal{Z}}\mathrm{Tr}\,[\hat{H}e^{-\beta\hat{H}}]\;. & (1.16) \end{aligned}$$

Let us now compute these quantities for the harmonic oscillator. This can be trivially done in the energy basis:

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

Consequently,

$$\begin{aligned} F &= T\ln\left(e^{\frac{\hbar\omega}{2T}} - e^{-\frac{\hbar\omega}{2T}}\right) = \frac{\hbar\omega}{2} + T\ln\left(1-e^{-\beta\hbar\omega}\right) & (1.18)\\ &\overset{T\ll\hbar\omega}{\approx} \frac{\hbar\omega}{2} & (1.19)\\ &\overset{T\gg\hbar\omega}{\approx} -T\ln\left(\frac{T}{\hbar\omega}\right)\;, & (1.20)\\ S &= -\ln\left(1-e^{-\beta\hbar\omega}\right) + \frac{\hbar\omega}{T}\frac{1}{e^{\beta\hbar\omega}-1} & (1.21)\\ &\overset{T\ll\hbar\omega}{\approx} \frac{\hbar\omega}{T}e^{-\frac{\hbar\omega}{T}} & (1.22)\\ &\overset{T\gg\hbar\omega}{\approx} 1 + \ln\frac{T}{\hbar\omega}\;, & (1.23)\\ E &= F + TS = \hbar\omega\left[\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\right] & (1.24)\\ &\overset{T\ll\hbar\omega}{\approx} \frac{\hbar\omega}{2} & (1.25)\\ &\overset{T\gg\hbar\omega}{\approx} T\;. & (1.26) \end{aligned}$$

Here we have also shown the behaviours of the various functions at low temperatures $T \ll \hbar\omega$ and at high temperatures $T \gg \hbar\omega$. Note how in most cases one can identify the contribution of the ground state, and of the thermal states, with their Bose-Einstein distribution function.

Note also that the average energy rises linearly with T at high temperatures, with a coefficient counting the number of degrees of freedom (i.e. the "degeneracy").

1.3. Path integral for the partition function

In the case of the harmonic oscillator, energy eigenvalues are known, and $\mathcal{Z}$ can easily be evaluated. In many other cases, however, E_n are 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,

$$\langle x|\hat{p}|p\rangle = p\langle x|p\rangle = -i\hbar\partial_x\langle x|p\rangle \Rightarrow \langle x|p\rangle = Ae^{\frac{ipx}{\hbar}} \ , \tag{1.27}$$

where A is some constant. Second, we will need completeness relations, which we write as

$$\int \mathrm{d}x \, |x\rangle\langle x| = \mathbb{1} \ , \quad \int \frac{\mathrm{d}p}{B} \, |p\rangle\langle p| = \mathbb{1} \ , \tag{1.28}$$

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

$$\begin{aligned} \mathbb{1} &= \int \mathrm{d}x \int \frac{\mathrm{d}p}{B} \int \frac{\mathrm{d}p'}{B} |p\rangle\langle p|x\rangle\langle x|p'\rangle\langle p'| = \int \mathrm{d}x \int \frac{\mathrm{d}p}{B} \int \frac{\mathrm{d}p'}{B} |p\rangle|A|^2 e^{\frac{i(p'-p)x}{\hbar}} \langle p'| & (1.29) \\ &= \int \frac{\mathrm{d}p}{B} \int \frac{\mathrm{d}p'}{B} |p\rangle|A|^2 2\pi\hbar\delta(p'-p)\langle p'| = \frac{2\pi\hbar|A|^2}{B} \int \frac{\mathrm{d}p}{B} |p\rangle\langle p| = \frac{2\pi\hbar|A|^2}{B} \mathbb{1} \ . & (1.30) \end{aligned}$$

Thereby $B = 2\pi\hbar|A|^2$; we choose $A \equiv 1$, so that $B = 2\pi\hbar$.

We then move to the evaluation of the partition function. We do this in the x-basis, whereby

$$\mathcal{Z} = \mathrm{Tr}\,[e^{-\beta\hat{H}}] = \int \mathrm{d}x \, \langle x|e^{-\beta\hat{H}}|x\rangle = \int \mathrm{d}x \, \langle x|e^{-\frac{\epsilon\hat{H}}{\hbar}} \cdots e^{-\frac{\epsilon\hat{H}}{\hbar}} |x\rangle \ . \tag{1.31}$$

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

The trick now is to insert

$$\mathbb{1} = \int \frac{\mathrm{d}p_i}{2\pi\hbar} |p_i\rangle\langle p_i| \ , \quad i = 1, \ldots, N \tag{1.32}$$

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

$$\mathbb{1} = \int \mathrm{d}x_i \, |x_i\rangle\langle x_i| \ , \quad i = 1, \ldots, N \tag{1.33}$$

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

$$\begin{aligned} \langle x_{i+1}|p_i\rangle\langle p_i|e^{-\frac{\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})}|x_i\rangle &= e^{\frac{ip_i x_{i+1}}{\hbar}} \langle p_i|e^{-\frac{\epsilon}{\hbar}H(p_i,x_i)+\mathcal{O}(\epsilon^2)}|x_i\rangle \\ &= \exp\left\{-\frac{\epsilon}{\hbar}\left[\frac{p_i^2}{2m} - ip_i\frac{x_{i+1}-x_i}{\epsilon} + V(x_i) + \mathcal{O}(\epsilon)\right]\right\} \ . \end{aligned} \tag{1.34}$$

Moreover we need to note that on the very right, we have

$$\langle x_1|x\rangle = \delta(x_1 - x) \ , \tag{1.35}$$

which allows to carry out the integral over x; and that on 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. (1.34) can be eliminated by sending $N \to \infty$.

In total, then, we can write the partition function as

$$\mathcal{Z} = \lim_{N\to\infty} \int \left[\prod_{i=1}^{N} \frac{\mathrm{d}x_i \mathrm{d}p_i}{2\pi\hbar}\right] \exp\left\{-\frac{1}{\hbar}\sum_{j=1}^{N} \epsilon \left[\frac{p_j^2}{2m} - ip_j\frac{x_{j+1}-x_j}{\epsilon} + V(x_j)\right]\right\}\Bigg|_{x_{N+1}\equiv x_1, \epsilon\equiv\beta\hbar/N} \ . \tag{1.36}$$

Oftentimes this is symbolically written as a "continuum" path integral, as

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

Note that in this form, the integration measure is well-defined (as a limit of that in Eq. (1.36)).

The integral over the momenta p_i is gaussian, and can be carried out explicitly:

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}p_i}{2\pi\hbar} \exp\left\{-\frac{\epsilon}{\hbar}\left[\frac{p_i^2}{2m} - ip_i\frac{x_{i+1}-x_i}{\epsilon}\right]\right\} = \sqrt{\frac{m}{2\pi\hbar\epsilon}} \exp\left[-\frac{m(x_{i+1}-x_i)^2}{2\hbar\epsilon}\right] . \tag{1.38}$$

Thereby Eq. (1.36) becomes

$$\mathcal{Z} = \lim_{N\to\infty} \int \left[\prod_{i=1}^{N} \frac{\mathrm{d}x_i}{\sqrt{2\pi\hbar\epsilon/m}}\right] \exp\left\{-\frac{1}{\hbar}\sum_{j=1}^{N} \epsilon \left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2 + V(x_j)\right]\right\}\Bigg|_{x_{N+1}\equiv x_1, \epsilon\equiv\beta\hbar/N} . \tag{1.39}$$

We may also try to write this in a continuum form, like in Eq. (1.37). Of course, the measure contains then a factor which appears quite divergent at large N,

$$C \equiv \left(\frac{m}{2\pi\hbar\epsilon}\right)^{N/2} = \exp\left[\frac{N}{2}\ln\left(\frac{mN}{2\pi\hbar^2\beta}\right)\right] . \tag{1.40}$$

This factor is, however, completely *independent of the properties of the potential* $V(x_j)$. Thereby it contains *no dynamical information*, and we actually do not need to worry too much about the apparent divergence — in any case, we will return to C from another angle in the next section. For the moment, then, we can again write a continuum form for the functional integral,

$$\mathcal{Z} = C \int_{x(\beta\hbar)=x(0)} \mathcal{D}x \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau \left[\frac{m}{2}\left(\frac{\mathrm{d}x(\tau)}{\mathrm{d}\tau}\right)^2 + V(x(\tau))\right]\right\} . \tag{1.41}$$

Let us end by giving an "interpretation" to the result in Eq. (1.41). We recall that the usual path integral at zero temperature has the exponential

$$\exp\left(\frac{i}{\hbar}\int \mathrm{d}t\,\mathcal{L}_M\right) , \quad \mathcal{L}_M = \frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x) . \tag{1.42}$$

We note that Eq. (1.41) could be obtained with the following recipe:

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

(ii) Introduce

$$\mathcal{L}_E \equiv -\mathcal{L}_M(\tau = it) = \frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + V(x) . \tag{1.43}$$

(iii) Restrict τ to the interval $0...\beta\hbar$.

(iv) Require periodicity over τ.

With these steps, the exponential becomes

$$\exp\left(-\frac{1}{\hbar}S_E\right) \equiv \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau\,\mathcal{L}_E\right) . \tag{1.44}$$

where the subscript E stands for "Euclidean", in contrast to "Minkowskian". It will turn out that this recipe works, almost without modifications, also in 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.