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Path integrals in quantum theory

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ABSTRACT: Notes.

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1 Path integrals in quantum mechanics

1.1 Introduction

In the 1940s, Feynman introduced a new formulation of Quantum Mechanics based on previous insights of Dirac. In Feynman's formulation, the basic quantity is the quantum-mechanical propagator (1.9). Feynman discovered that such an amplitude can be described by an integration over all possible "paths" interpolating between these two events in spacetime, with a weight $\exp(iS/\hbar)$, where S is the classical action of the path. In the classical limit in which the action is large as compared to Planck's constant, one recovers the principle of least action of classical mechanics.

It turns out that one can reformulate Quantum Mechanics by taking as the basic object the quantum propagator and Feynman's path integral formula for it. Starting from this postulate, one can reconstruct non-relativistic Quantum Mechanics, including the time-dependent

Schrödinger equation. This was shown in detail by Feynman in his 1965 book with Hibbs. Therefore, Feynman's approach provides a logically independent formulation of Quantum Mechanics. Certain aspects of Quantum Mechanics are more transparent in this formulation. For example, the fact that probability amplitudes of quadratic Lagrangians involve the classical action, as we showed in Examples 1.1 and 1.2, is an immediate consequence of the path integral formulation. Conversely, deriving the energy spectrum of even simple Hamiltonians turns out to be more difficult, since one has to calculate first the propagator, and then extract the energy eigenvalues from the spectral decomposition (1.13).

The path integral formulation has become of fundamental importance in modern theoretical physics, since it turns out to be much more convenient for the quantization of classical field theories. It is also extremely useful in condensed matter physics. In particular, it leads to a diagrammatic approach to perturbation theory (the famous Feynman diagrams) which has become the dominant language in many areas of physics. Perhaps the best introduction to the path integral formulation and to Feynman diagrams is to study them in the context of Quantum Mechanics, where all results derived in this way can be carefully tested and checked against traditional methods. This is our purpose in this Chapter.

1.2 The quantum-mechanical propagator

In quantum mechanics, time evolution between an initial time t_0 and a final time t_f is implemented by the unitary operator

$$\mathbf{U}(t_f, t_0), \quad (1.1)$$

which connects the quantum state of the system at time $t = t_0$ with the state at $t = t_f$:

$$\mathbf{U}(t_f, t_0)|\psi(t_0)\rangle = |\psi(t_f)\rangle. \quad (1.2)$$

It obviously satisfies the convolution law,

$$\mathbf{U}(t_f, t_0) = \mathbf{U}(t_f, t_1)\mathbf{U}(t_1, t_0). \quad (1.3)$$

Let \mathbf{H} be the Hamiltonian operator of the quantum system. By using Schrödinger's equation,

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \mathbf{H}|\psi(t)\rangle, \quad (1.4)$$

we deduce the evolution equation for the operator $\mathbf{U}(t, t_0)$:

$$i\hbar \frac{\partial \mathbf{U}(t, t_0)}{\partial t} = \mathbf{H}\mathbf{U}(t, t_0), \quad (1.5)$$

with initial condition

$$\mathbf{U}(t_0, t_0) = \mathbf{1}. \quad (1.6)$$

When the Hamiltonian \mathbf{H} is time-independent (as we will assume in this book), we can solve the evolution equation as

$$\mathbf{U}(t_f, t_0) = e^{-\frac{i}{\hbar}\mathbf{H}(t_f-t_0)}. \quad (1.7)$$

In this case, the evolution operator is invariant under time translation and only depends on the difference

$$T = t_f - t_0. \quad (1.8)$$

It is convenient to work in the position representation for the position operator. The corresponding eigenstates will be denoted by $|\mathbf{q}\rangle$, where $\mathbf{q} \in \mathbb{R}^d$. The integral kernel of the evolution operator in the position representation is called the *quantum-mechanical (QM) propagator*:

$$K(\mathbf{q}_f, \mathbf{q}_0; t_f, t_0) = \langle \mathbf{q}_f | U(t_f, t_0) | \mathbf{q}_0 \rangle. \quad (1.9)$$

The QM propagator can be regarded as a wavefunction at time $t = t_f$,

$$\psi(\mathbf{q}, t_f) = K(\mathbf{q}, \mathbf{q}_0; t_f, t_0), \quad (1.10)$$

which is obtained by evolving in time the state $|\mathbf{q}_0\rangle$ at $t = t_0$. This initial state is described by the wavefunction

$$\psi(\mathbf{q}, t_0) = \delta(\mathbf{q} - \mathbf{q}_0) \quad (1.11)$$

and it is an eigenfunction of the position operator with eigenvalue \mathbf{q}_0 . The QM propagator has a direct physical interpretation: it gives the probability amplitude that a particle is at the point \mathbf{q}_f at the time t_f , given that it has been at the point \mathbf{q}_0 at the time t_0 .

The evolution operator and the QM propagator contain detailed information about the spectrum and eigenfunctions of the Hamiltonian. Indeed, let us assume that H has a discrete and non-degenerate spectrum E_n , $n \geq 0$, with orthonormal eigenfunctions $|\phi_n\rangle$. Then, we have the spectral decompositions,

$$U(t_f, t_0) = \sum_{n \geq 0} |\phi_n\rangle e^{-iE_n(t_f - t_0)/\hbar} \langle \phi_n|, \quad (1.12)$$

or, equivalently,

$$K(\mathbf{q}_f, \mathbf{q}_0; t_f, t_0) = \sum_{n \geq 0} \phi_n(\mathbf{q}_f) e^{-iE_n(t_f - t_0)/\hbar} \phi_n^*(\mathbf{q}_0). \quad (1.13)$$

The evolution operator in QM is closely related to other useful quantities. The first one is the (unnormalized) density operator for the canonical ensemble. This is defined by

$$\rho(\beta) = e^{-\beta H}, \quad (1.14)$$

and we recall that $k_B\beta$ is the inverse temperature of the system. The density operator can be obtained from the evolution operator by the so-called *Euclidean continuation* or *Wick rotation*:

$$T = -iu, \quad u = \beta\hbar. \quad (1.15)$$

Therefore, if we know the evolution operator, we know the density operator, and if we know the QM propagator, we know the integral kernel of the density operator, sometimes called *density matrix*,

$$\langle \mathbf{q} | \rho(\beta) | \mathbf{q}' \rangle = \rho(\mathbf{q}, \mathbf{q}'; \beta). \quad (1.16)$$

More precisely, for a theory with a time-independent Hamiltonian, we have

$$\rho(\mathbf{q}, \mathbf{q}'; \beta) = K(\mathbf{q}, \mathbf{q}'; -i\hbar\beta, 0). \quad (1.17)$$

Note that the unnormalized density matrix satisfies the differential equation

$$-\frac{\partial \rho(\beta)}{\partial \beta} = H\rho, \quad (1.18)$$

which is sometimes called *Bloch equation*. The initial condition is

$$\rho(\beta = 0) = \mathbf{1}. \quad (1.19)$$

This is of course the analogue of (1.5). The canonical partition function is easily obtained from the unnormalized density operator,

$$Z(\beta) = \text{Tr } \rho(\beta) = \int_{\mathbb{R}^d} d\mathbf{q} \rho(\mathbf{q}, \mathbf{q}; \beta). \quad (1.20)$$

The density matrix is even more useful than the QM propagator to extract the spectral information, since it has the spectral decomposition

$$\rho(\mathbf{q}, \mathbf{q}'; \beta) = \sum_{n \geq 0} \phi_n(\mathbf{q}) e^{-\beta E_n} \phi_n^*(\mathbf{q}'). \quad (1.21)$$

This means that we can extract the energies and eigenfunctions by performing a low temperature expansion (i.e. by considering the limit $\beta \rightarrow \infty$). The leading term gives the energy and wavefunction of the ground state, the next-to-leading term contains information about the first excited state, and so on.

Let us now present three important examples where the quantum-mechanical propagator can be computed in closed form: the free particle, the harmonic oscillator, and a particle in a linear potential.

Example 1.1. *Propagator for the free particle.* The QM propagator can be easily computed for a free particle in one dimension. Indeed, we have

$$\begin{aligned} K(q_f, q_0; t_f, t_0) &= \langle q_f | \exp \left[-\frac{i(t_f - t_0) \mathbf{p}^2}{2m\hbar} \right] | q_0 \rangle = \int_{\mathbb{R}} \langle q_f | p \rangle \langle p | \exp \left[-\frac{i(t_f - t_0) \mathbf{p}^2}{2m\hbar} \right] | q_0 \rangle dp \\ &= \frac{1}{2\pi\hbar} \int_{\mathbb{R}} e^{ip(q_f - q_0)/\hbar} e^{-\frac{i(t_f - t_0)p^2}{2m\hbar}} dp \\ &= \left(\frac{m}{2\pi i \hbar (t_f - t_0)} \right)^{1/2} \exp \left[\frac{im}{2\hbar(t_f - t_0)} (q_f - q_0)^2 \right], \end{aligned} \quad (1.22)$$

where we have used the Gaussian integral formula (A.1) and the result for the plane waves

$$\langle q | p \rangle = \psi_p(q) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipq/\hbar}. \quad (1.23)$$

We can also deduce from (1.22) the canonical density matrix for a free particle,

$$\rho(q, q'; \beta) = \left(\frac{m}{2\pi\beta\hbar^2} \right)^{1/2} \exp \left[-\frac{m}{2\beta\hbar^2} (q - q')^2 \right], \quad (1.24)$$

and we recover in this way the thermal partition function for a free particle in D dimensions:

$$Z(\beta) = \left(\frac{m}{2\pi\beta\hbar^2} \right)^{D/2} V_D, \quad (1.25)$$

where V_D is the volume where the particle lives. □

Example 1.2. *Propagator for the harmonic oscillator.* Let us consider a quantum harmonic oscillator in one dimension, with Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + \frac{m\omega^2 \mathbf{q}^2}{2}. \quad (1.26)$$

Here, \mathbf{q} and \mathbf{p} are canonically conjugate Heisenberg operators, satisfying the commutation relation

$$[\mathbf{q}, \mathbf{p}] = i\hbar. \quad (1.27)$$

We will set $t_0 = 0$, which we can always do when H is time independent. Let us remind that the time-dependent Heisenberg operators associated to \mathbf{q} , \mathbf{p} are given by

$$\mathbf{q}_H(t) = e^{iHt/\hbar} \mathbf{q} e^{-iHt/\hbar}, \quad \mathbf{p}_H(t) = e^{iHt/\hbar} \mathbf{p} e^{-iHt/\hbar}. \quad (1.28)$$

They satisfy the Heisenberg EOM, which read in this case

$$\dot{\mathbf{q}}_H(t) = \frac{1}{m} \mathbf{p}_H(t), \quad \dot{\mathbf{p}}_H(t) = -m\omega^2 \mathbf{q}_H(t), \quad (1.29)$$

and can be integrated to give

$$\begin{aligned} \mathbf{q}_H(t) &= \cos(\omega t) \mathbf{q}_H(0) + \frac{1}{m\omega} \sin(\omega t) \mathbf{p}_H(0), \\ \mathbf{p}_H(t) &= -m\omega \sin(\omega t) \mathbf{q}_H(0) + \cos(\omega t) \mathbf{p}_H(0). \end{aligned} \quad (1.30)$$

We remind that $\mathbf{q}_H(0) = \mathbf{q}$, $\mathbf{p}_H(0) = \mathbf{p}$ are the operators in the Schrödinger representation. Let us also denote

$$|q_0(t)\rangle = e^{-iHt/\hbar} |q_0\rangle. \quad (1.31)$$

We want to calculate

$$K(q_f, q_0; t, 0) = \langle q_f | q_0(t) \rangle. \quad (1.32)$$

We first note that

$$\langle q_f | \mathbf{q}_H(-t) | q_0(t) \rangle = \langle q_f | e^{-iHt/\hbar} \mathbf{q} e^{iHt/\hbar} e^{-iHt/\hbar} | q_0 \rangle = q_0 K(q_f, q_0; t, 0). \quad (1.33)$$

On the other hand, by using the explicit solution to $\mathbf{q}_H(-t)$, we find

$$\begin{aligned} \langle q_f | \mathbf{q}_H(-t) | q_0(t) \rangle &= \cos(\omega t) \langle q_f | \mathbf{q}_H(0) | q_0(t) \rangle - \frac{1}{m\omega} \sin(\omega t) \langle q_f | \mathbf{p}_H(0) | q_0(t) \rangle \\ &= \cos(\omega t) q_f K(q_f, q_0; t, 0) + \frac{i\hbar}{m\omega} \sin(\omega t) \frac{\partial}{\partial q_f} K(q_f, q_0; t, 0). \end{aligned} \quad (1.34)$$

Putting both results together, we obtain the following differential equation for the propagator,

$$\frac{\partial}{\partial q_f} K(q_f, q_0; t, 0) = \frac{m\omega}{i\hbar \sin(\omega t)} (q_0 - q_f \cos(\omega t)) K(q_f, q_0; t, 0), \quad (1.35)$$

whose solution is

$$K(q_f, q_0; t, 0) = \mathcal{N}(t) \exp \left[\frac{im\omega}{\hbar \sin(\omega t)} \left(\frac{1}{2} q_f^2 \cos(\omega t) - q_f q_0 \right) \right]. \quad (1.36)$$

Here, $\mathcal{H}(t)$ is an undetermined function of t . To determine $\mathcal{N}(t)$, we use that

$$i\hbar \frac{\partial}{\partial t} K(q_f, q_0; t, 0) = \langle q_f | \mathbf{H} | q_0(t) \rangle = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q_f^2} + \frac{m\omega^2}{2} q_f^2 \right) K(q_f, q_0; t, 0). \quad (1.37)$$

Plugging (1.36) in this equation, we obtain

$$\frac{\partial \mathcal{N}}{\partial t} = \left(-\frac{\omega}{2} \cot(\omega t) - \frac{im\omega^2}{2\hbar \sin^2(\omega t)} q_0^2 \right) \mathcal{N}(t), \quad (1.38)$$

which is easily integrated to

$$\mathcal{N}(t) = \frac{C}{\sqrt{\sin(\omega t)}} \exp\left(\frac{im\omega}{2\hbar} \cot(\omega t) q_0^2 \right). \quad (1.39)$$

The quantum propagator reads then,

$$K(q_f, q_0; t, 0) = \frac{C}{\sqrt{\sin(\omega t)}} \exp\left[\frac{im\omega}{2\hbar \sin(\omega t)} \left((q_f^2 + q_0^2) \cos(\omega t) - 2q_f q_0 \right) \right]. \quad (1.40)$$

The constant C can be determined by considering the free particle limit $\omega \rightarrow 0$. In this limit, we should recover the result (1.22). This fixes

$$C = \sqrt{\frac{m\omega}{2\pi i \hbar}}, \quad (1.41)$$

and we finally obtain

$$K(q_f, q_0; t_f, t_0) = \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega T)}} \exp\left[\frac{im\omega}{2\hbar \sin(\omega T)} \left((q_f^2 + q_0^2) \cos(\omega T) - 2q_f q_0 \right) \right], \quad (1.42)$$

where we use time translation invariance and T is given in (1.8). \square

Example 1.3. *Propagator for the linear potential.* Let us consider now the quantum Hamiltonian

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} - F\mathbf{q}, \quad (1.43)$$

which corresponds to a linear potential in one dimension. We can compute the QM propagator by using a method similar to the one in the previous example. The Heisenberg EOM are

$$\dot{\mathbf{q}}(t) = \frac{\mathbf{p}(t)}{m}, \quad \dot{\mathbf{p}}(t) = F, \quad (1.44)$$

which can be integrated immediately to

$$\begin{aligned} \mathbf{q}(t) &= \frac{Ft^2}{2m} + \frac{t}{m} \mathbf{p} + \mathbf{q}, \\ \mathbf{p}(t) &= Ft + \mathbf{p}, \end{aligned} \quad (1.45)$$

where $\mathbf{q} = \mathbf{q}(0)$, $\mathbf{p} = \mathbf{p}(0)$. Using this explicit solution we obtain

$$\langle q_f | \mathbf{q}(-t) | q_0(t) \rangle = \left(\frac{Ft^2}{2m} + \frac{i\hbar t}{m} \frac{\partial}{\partial q_f} + q_f \right) K(q_f, q_0; t, 0), \quad (1.46)$$

and we find the equation

$$\frac{\partial}{\partial q_f} \log K(q_f, q_0; t, 0) = \frac{im}{t\hbar} \left(q_f - q_0 + \frac{Ft^2}{2m} \right). \quad (1.47)$$

This can be integrated as

$$K(q_f, q_0; t, 0) = \mathcal{N}(t) \exp \left[\frac{im}{t\hbar} \left(\frac{q_f^2}{2} - q_f q_0 \right) + \frac{iFq_f t}{2\hbar} \right]. \quad (1.48)$$

To determine $\mathcal{N}(t)$, we use again the analogue of (1.37), which reads in this case

$$i\hbar \frac{\partial}{\partial t} K(q_f, q_0; t, 0) = \langle q_f | \mathbf{H} | q_0(t) \rangle = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q_f^2} - Fq_f \right) K(q_f, q_0; t, 0). \quad (1.49)$$

Plugging (1.48) in this equation, we find

$$\frac{\partial}{\partial t} \log \mathcal{N}(t) = -\frac{1}{2t} + \frac{iFq_0}{2\hbar} - \frac{imq_0^2}{2\hbar t^2} - \frac{iF^2 t^2}{8m\hbar}, \quad (1.50)$$

so that

$$\mathcal{N}(t) = \frac{C}{\sqrt{t}} \exp \left(\frac{imq_0^2}{2\hbar t} + \frac{iFq_0 t}{2\hbar} - \frac{iF^2 t^3}{24m\hbar} \right). \quad (1.51)$$

The integration constant can be obtained again by comparing to the free particle limit, when $F \rightarrow 0$. One finally finds,

$$K(q_f, q_0; t, 0) = \sqrt{\frac{m}{2\pi i\hbar t}} \exp \left[\frac{im}{2t\hbar} (q_f - q_0)^2 + \frac{iFt}{2\hbar} (q_f + q_0) - \frac{iF^2 t^3}{24m\hbar} \right]. \quad (1.52)$$

□

An interesting aspect of the examples we have just considered is both the exponent and the prefactor of the QM propagator are related to quantities in classical mechanics. Let us consider a classical path of trajectory, $q(t)$ satisfying the boundary conditions

$$\mathbf{q}(t_0) = \mathbf{q}_0, \quad \mathbf{q}(t_f) = \mathbf{q}_f. \quad (1.53)$$

The classical action is a functional of the trajectory obtained by integrating the Lagrangian,

$$S(\mathbf{q}(t)) = \int_{t_0}^{t_f} L(\mathbf{q}(t), \dot{\mathbf{q}}(t)) dt. \quad (1.54)$$

As it is well-known from classical mechanics, this functional has an extremum when the trajectory $\mathbf{q}(t)$ solves the EOM. Indeed, if we perform a variation $\delta\mathbf{q}(t)$ preserving the boundary conditions (1.53), one has

$$\frac{\delta S}{\delta \mathbf{q}(t)} = -\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\mathbf{q}}} \right) + \frac{\partial L}{\partial \mathbf{q}}. \quad (1.55)$$

Let us denote by $\mathbf{q}_c(t)$ the solution to the Lagrange EOM with the boundary conditions (1.53) (which we assume to exist and be unique, for simplicity). Then, we have

$$\left. \frac{\delta S}{\delta \mathbf{q}(t)} \right|_{\mathbf{q}(t)=\mathbf{q}_c(t)} = 0. \quad (1.56)$$

In the following, we will denote by S_c the value of the classical action on the classical trajectory:

$$S_c = S(\mathbf{q}_c(t)). \quad (1.57)$$

It is a function of the boundary data \mathbf{q}_f , \mathbf{q}_0 , t_f and t_0 .

In the case of the free particle in one dimension, the action reads

$$S(q(t)) = \frac{m}{2} \int_{t_0}^{t_f} (\dot{q}(t))^2 dt. \quad (1.58)$$

The classical trajectory has constant velocity, equal to

$$\dot{q}_c(t) = \frac{q_f - q_0}{t_f - t_0}. \quad (1.59)$$

The classical action is in this case,

$$S_c = \frac{m}{2} \frac{(q_f - q_0)^2}{t_f - t_0}. \quad (1.60)$$

We can then write (1.22) as

$$K(q_f, q_0; t_f, t_0) = \frac{1}{\sqrt{2\pi i \hbar}} \left(-\frac{\partial^2 S_c}{\partial q_f \partial q_0} \right)^{1/2} e^{iS_c/\hbar}. \quad (1.61)$$

This result also holds for the harmonic oscillator and for the particle in a linear potential. Let us verify it for the harmonic oscillator. The solution to the classical EOM which satisfies the boundary conditions is

$$q_c(t) = q_0 \cos(\omega(t - t_0)) + \frac{q_f - q_0 \cos(\omega T)}{\sin(\omega T)} \sin(\omega(t - t_0)). \quad (1.62)$$

The classical action evaluated at this path is:

$$\begin{aligned} S_c &= \int_{t_0}^{t_f} \left(\frac{m\dot{q}_c^2}{2} - \frac{m\omega^2 q_c^2}{2} \right) dt = \frac{m}{2} \dot{q}_c(t) q_c(t) \Big|_{t_0}^{t_f} - \frac{m}{2} \int_{t_0}^{t_f} q_c (\ddot{q}_c + \omega^2 q_c) dt \\ &= \frac{m}{2} (\dot{q}_c(t_f) q_c(t_f) - \dot{q}_c(t_0) q_c(t_0)) = \frac{m\omega}{2 \sin(\omega T)} ((q_f^2 + q_0^2) \cos(\omega T) - 2q_f q_0). \end{aligned} \quad (1.63)$$

It is now easy to verify that the quantum propagator (1.42) has also the structure (1.61).

In the conventional formulation of quantum mechanics, the result (1.61) is surprising. We will find an *a priori* explanation of this structure in Chapter ??, in the context of the path integral formulation of quantum mechanics.

1.3 Path integral representation of the quantum propagator

We will now see that the propagator (1.9) can be formulated in terms of a sum over classical paths. This is the famous path integral formulation of QM due to Feynman, which can be regarded as a self-contained approach to QM.

To calculate the QM propagator, let us divide the interval (t_0, t_f) into $N + 1$ small intervals

$$(t_0, t_1), \quad (t_1, t_2), \quad \dots \quad (t_N, t_f), \quad (1.64)$$

and let us denote

$$\Delta t_k = t_{k+1} - t_k. \quad (1.65)$$

Therefore, we have

$$\mathbf{U}(t_f, t_0) = \mathbf{U}(t_f, t_N) \cdots \mathbf{U}(t_1, t_0) = \prod_{k=0}^N \mathbf{U}(t_{k+1}, t_k). \quad (1.66)$$

Note that we have defined $t_{N+1} = t_f$. We can now introduce N resolutions of the identity,

$$\int_{\mathbb{R}} |q_i\rangle \langle q_i| dq_i = 1, \quad (1.67)$$

to obtain

$$K(q_f, q_0; t_f, t_0) = \int_{\mathbb{R}^N} \prod_{k=0}^N K(q_{k+1}, q_k; t_{k+1}, t_k) dq_N dq_{N-1} \cdots dq_1. \quad (1.68)$$

We are interested in taking the limit $N \rightarrow \infty$, $\Delta t_k \rightarrow 0$, as in the calculation of Riemann integrals. In this limit, we expect

$$K(q_{k+1}, q_k; t_{k+1}, t_k) = \langle q_{k+1} | e^{-\frac{i\Delta t_k}{\hbar} \mathbf{H}} | q_k \rangle \approx \langle q_{k+1} | 1 - \frac{i\Delta t_k}{\hbar} \mathbf{H} | q_k \rangle. \quad (1.69)$$

We calculate now

$$\langle q_{k+1} | \mathbf{H} | q_k \rangle = \int_{\mathbb{R}} \langle q_{k+1} | p_k \rangle \langle p_k | \mathbf{H} | q_k \rangle dp_k = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} e^{\frac{i}{\hbar} p_k q_{k+1}} \langle p_k | \mathbf{H} | q_k \rangle dp_k. \quad (1.70)$$

If we now assume that \mathbf{H} is the standard non-relativistic, time-independent Hamiltonian,

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}), \quad (1.71)$$

we have

$$\begin{aligned} \langle p_k | \mathbf{H} | q_k \rangle &= \left(\frac{p_k^2}{2m} + V(q_k) \right) \langle p_k | q_k \rangle = \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{p_k^2}{2m} + V(q_k) \right) e^{-\frac{i}{\hbar} p_k q_k} \\ &= \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar} p_k q_k} H(q_k, p_k). \end{aligned} \quad (1.72)$$

Therefore,

$$\langle q_{k+1} | \mathbf{H} | q_k \rangle = \int_{\mathbb{R}} \frac{dp_k}{2\pi\hbar} e^{\frac{i}{\hbar} p_k (q_{k+1} - q_k)} H(q_k, p_k), \quad (1.73)$$

and by using that

$$\langle q_{k+1} | q_k \rangle = \delta(q_{k+1} - q_k) = \int_{\mathbb{R}} \frac{dp_k}{2\pi\hbar} e^{\frac{i}{\hbar} p_k (q_{k+1} - q_k)}, \quad (1.74)$$

we find,

$$\begin{aligned} \langle q_{k+1} | 1 - \frac{i\Delta t_k}{\hbar} \mathbf{H} | q_k \rangle &= \int_{\mathbb{R}} \frac{dp_k}{2\pi\hbar} e^{\frac{i}{\hbar} p_k (q_{k+1} - q_k)} \left(1 - \frac{i\Delta t_k}{\hbar} H(q_k, p_k) \right) \\ &\approx \int_{\mathbb{R}} \frac{dp_k}{2\pi\hbar} \exp \left[\frac{i\Delta t_k}{\hbar} \left(p_k \frac{q_{k+1} - q_k}{\Delta t_k} - H(q_k, p_k) \right) \right]. \end{aligned} \quad (1.75)$$

We obtain,

$$K(q_f, q_0; t_f, t_0) \approx \int_{\mathbb{R}^{2N+1}} \left[\prod_{k=1}^N \frac{dp_k dq_k}{2\pi\hbar} \right] \frac{dp_0}{2\pi\hbar} \exp \left[\sum_{k=0}^N \frac{i\Delta t_k}{\hbar} \left(p_k \frac{q_{k+1} - q_k}{\Delta t_k} - H(q_k, p_k) \right) \right]. \quad (1.76)$$

Let us now assume that $\Delta t_k = \Delta t$ for all k . The approximation for the propagator in (1.76) becomes arbitrarily good in the limit in which $\Delta t \rightarrow 0$. Since

$$(N+1)\Delta t = t_f - t_0 \quad (1.77)$$

is fixed, N has to go to infinity simultaneously. The appropriate limit is then

$$N \rightarrow \infty, \quad \Delta t \rightarrow 0, \quad (1.78)$$

so that the product (1.77) is fixed by the condition (1.77). This type of limit is sometimes called a double-scaling limit, since we have to consider the limit of two different variables which are correlated. We then obtain the following formula for the propagator:

$$\begin{aligned} & K(q_f, q_0; t_f, t_0) \\ &= \lim_{N \rightarrow \infty} \int_{\mathbb{R}^{2N+1}} \left[\prod_{k=1}^N \frac{dp_k dq_k}{2\pi\hbar} \right] \frac{dp_0}{2\pi\hbar} \exp \left[\sum_{k=0}^N \frac{i\Delta t}{\hbar} \left(p_k \frac{q_{k+1} - q_k}{\Delta t_k} - H(q_k, p_k) \right) \right], \end{aligned} \quad (1.79)$$

where it is understood that we have to consider the double-scaling limit (1.78). The exponent in the r.h.s. of (1.79) can be interpreted as a standard approximation to the integral

$$\int_{t_0}^{t_f} (p\dot{q} - H(p, q)) dt, \quad (1.80)$$

which is recovered in the double-scaling limit. We can also interpret the limiting integral measure in (1.79) as an integration over all possible paths $q(t)$, $p(t)$ going from $q(t_0) = q_0$ to $q(t_f) = q_f$. We will then write the r.h.s. of (1.79) as a *path integral in phase space*:

$$K(q_f, q_0; t_f, t_0) = \int \mathcal{D}q(t) \mathcal{D}p(t) e^{\frac{i}{\hbar} \int_{t_0}^{t_f} (p\dot{q} - H(p, q)) dt}. \quad (1.81)$$

Here, $\mathcal{D}q(t) \mathcal{D}p(t)$ is a representation of the measure of the path integral, which is defined more precisely in (1.79).

We will now find an even more useful formula for the propagator by integrating over the momenta. Indeed, the integral over p_k in

$$K(q_{k+1}, q_k; t_{k+1}, t_k) \approx \int_{\mathbb{R}} \frac{dp_k}{2\pi\hbar} \exp \left[\frac{i\Delta t_k}{\hbar} \left(p_k \frac{q_{k+1} - q_k}{\Delta t_k} - \frac{p_k^2}{2m} - V(q_k) \right) \right] \quad (1.82)$$

is a Gaussian, and we can use (A.1) with

$$A = -\frac{\Delta t_k}{m\hbar}. \quad (1.83)$$

One finds,

$$K(q_{k+1}, q_k; t_{k+1}, t_k) = \sqrt{\frac{m}{2\pi i \hbar \Delta t_k}} \exp \left[\frac{i\Delta t_k}{\hbar} \left(\frac{m}{2} \left(\frac{q_{k+1} - q_k}{\Delta t_k} \right)^2 - V(q_k) \right) \right]. \quad (1.84)$$

We can now set $\Delta t_k = \Delta t$ for all k , as before, and take the double-scaling limit $N \rightarrow \infty$ and $\Delta t \rightarrow 0$. We obtain

$$K(q_f, q_0; t_f, t_0) = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N+1}{2}} \int_{\mathbb{R}^N} \prod_{k=1}^N dq_k \exp \left[\sum_{k=0}^N \frac{i\Delta t}{\hbar} \left(\frac{m}{2} \left(\frac{q_{k+1} - q_k}{\Delta t} \right)^2 - V(q_k) \right) \right]. \quad (1.85)$$

The exponent in the r.h.s. of (1.85) is a discretization of the classical action of the mechanical system (1.54). The integration can be interpreted again as being over all possible paths $q(t)$, with the appropriate boundary conditions

$$q(t_0) = q_0, \quad q(t_f) = q_f. \quad (1.86)$$

Like before, we can interpret (1.85) as an integral over all paths with the above boundary conditions, and we can write the following *path integral formula in position space*,

$$K(q_f, q_0; t_f, t_0) = \int \mathcal{D}q(t) e^{\frac{i}{\hbar} S(q(t))}, \quad (1.87)$$

where $\mathcal{D}q(t)$ is defined more precisely by the limit in (1.85). This formula is the basis for the path integral formulation of Quantum Mechanics pioneered by Feynman.

In the above derivation, we have assumed that our Hamiltonian is of the form (1.71). However, the expression (1.85) is also valid for a time-dependent Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}, t), \quad (1.88)$$

after replacing $V(q_k) \rightarrow V(q_k, t_k)$. The reason is that, for small times, the evolution operator is given by

$$U(t_{k+1}, t_k) \approx 1 - \frac{i\Delta t_k}{\hbar} H(t_k), \quad (1.89)$$

and the derivation of (1.85) with the replacement mentioned above remains valid.

1.4 Path integral representation of the density matrix

The QM propagator is closely related to the integral kernel of the canonical density matrix, as we saw in (1.17). Therefore, we should be able to compute $\rho(q_f, q_0; \beta)$ in a similar way. The analogue of $T = t_f - t_0$ is $u = \beta\hbar$, which should be regarded as an interval of ‘‘Euclidean’’ time. We will denote the density matrix by $\rho(q_f, q_0; u)$, since in this context u is a more appropriate variable than β . We will parametrize the interval of Euclidean time by the variable $0 \leq \tau \leq u$. To obtain a path integral representation of the density matrix, we split u into N intervals $\Delta\tau_k$. The analogue of formula (1.82) above is

$$\rho(q_{k+1}, q_k; \tau_{k+1}, \tau_k) \approx \int \frac{dp_k}{2\pi\hbar} \exp \left[\frac{i\Delta\tau_k}{\hbar} p_k \frac{q_{k+1} - q_k}{\Delta\tau_k} - \frac{\Delta\tau_k}{\hbar} \left(\frac{p_k^2}{2m} + V(q_k) \right) \right], \quad (1.90)$$

which can be integrated over p_k , this time with a *bone fide* Gaussian. One finds,

$$\rho(q_{k+1}, q_k; \tau_{k+1}, \tau_k) = \sqrt{\frac{m}{2\pi\hbar\Delta\tau_k}} \exp \left[-\frac{\Delta\tau_k}{\hbar} \left(\frac{m}{2} \left(\frac{q_{k+1} - q_k}{\Delta\tau_k} \right)^2 + V(q_k) \right) \right], \quad (1.91)$$

and due to the change of relative sign between the kinetic and the potential terms, we find a path integral representation for the density matrix

$$\rho(q_f, q_0; u) = \int \mathcal{D}q(t) e^{-\frac{1}{\hbar} S_E(q(\tau))} \quad (1.92)$$

in terms of the *Euclidean* action:

$$S_E = \int_0^u \left(\frac{m}{2} \dot{q}^2 + V(q) \right) d\tau, \quad u = \beta \hbar. \quad (1.93)$$

This is an integral over paths satisfying the boundary conditions

$$q(0) = q_0, \quad q(u) = q_f. \quad (1.94)$$

The calculation of the density matrix is formally equivalent to the one of the propagator, after performing a Wick rotation of the time variable,

$$t = -i\tau. \quad (1.95)$$

We can also obtain from this a path-integral representation of the canonical partition function of the system at inverse temperature β . Since we are taking a trace, paths have to finish and end at the same point, i.e. we have

$$q(0) = q(u) = q, \quad (1.96)$$

and in addition we have to integrate over all possible points q . This means that the thermal partition function can be written as a path integral with *periodic* boundary conditions, instead of Dirichlet boundary conditions:

$$Z(\beta) = \int_{q(0)=q(u)} \mathcal{D}q(\tau) e^{-\frac{1}{\hbar} S_E(q(\tau))}. \quad (1.97)$$

In particular, we have the following representation in terms of a limit of integrations,

$$Z(\beta) = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi\hbar\Delta\tau} \right)^{\frac{N+1}{2}} \int \prod_{k=1}^{N+1} dq_k \exp \left[- \sum_{k=0}^N \frac{\Delta\tau}{\hbar} \left(\frac{m}{2} \left(\frac{q_{k+1} - q_k}{\Delta\tau} \right)^2 + V(q_k) \right) \right], \quad (1.98)$$

where $q_0 = q_{N+1}$ due to the periodic boundary conditions. Note that there is an additional integration to perform, due to the trace.

1.5 The free particle

There are some simple examples where the path integral can be computed *exactly*. The free particle is of course one of them. Let us now calculate the path integral in the case $V(q) = 0$, by starting from the definition given in (1.85). We write

$$\sum_{k=0}^N (q_{k+1} - q_k)^2 = \mathbf{q}^T P_N \mathbf{q} - 2\mathbf{v} \cdot \mathbf{q} + q_0^2 + q_f^2, \quad (1.99)$$

where the $N \times N$ matrix P_N is given by¹

$$P_N = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 2 \end{pmatrix}, \quad (1.100)$$

and the N -dimensional vectors \mathbf{q} , \mathbf{v} are given by

$$\mathbf{q} = (q_1, \dots, q_N), \quad \mathbf{v} = (q_0, 0, \dots, 0, q_f). \quad (1.101)$$

Let us now use the basic formula of Gaussian integration (A.1), with

$$A = \frac{m}{\hbar\Delta t} P_N, \quad \mathbf{p} = -\frac{m}{\hbar\Delta t} \mathbf{v}. \quad (1.102)$$

To write down the result of this integration, we need various properties of the matrix P_N , like for example the number of its positive and negative eigenvalues. It turns out that it is possible to calculate the eigenvalues of P_N explicitly. More generally, let us consider an $N \times N$ matrix $C^{(\alpha,\beta)}$ with entries

$$C_{jk}^{(\alpha,\beta)} = \alpha\delta_{jk} - \beta(\delta_{j,k+1} + \delta_{j,k-1}), \quad j, k = 1, \dots, N. \quad (1.103)$$

Then, it is immediate to check that the N -dimensional vectors $\chi^{(p)}$, $p = 1, \dots, N$, with entries

$$\chi_j^{(p)} = \sqrt{\frac{2}{N+1}} \sin \frac{\pi pj}{N+1}, \quad j = 1, \dots, N, \quad (1.104)$$

are eigenvectors of $C^{(\alpha,\beta)}$ with eigenvalues

$$\alpha - 2\beta \cos \frac{\pi p}{N+1}, \quad p = 1, \dots, N. \quad (1.105)$$

The matrix P_N corresponds to $\alpha = 2$, $\beta = 1$, so that its eigenvalues are of the form

$$2 \left(1 - \cos \frac{\pi p}{N+1} \right), \quad p = 1, \dots, N, \quad (1.106)$$

which are all positive. We then find,

$$\begin{aligned} & \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N+1}{2}} \int \prod_{k=1}^N dq_k \exp \left[\frac{im\Delta t}{2\hbar} \sum_{k=0}^N \left(\frac{q_{k+1} - q_k}{\Delta t} \right)^2 \right] \\ &= \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N+1}{2}} \left(\frac{m}{\hbar \Delta t} \right)^{-N/2} \frac{(2\pi i)^{N/2}}{\sqrt{\det(P_N)}} \exp \left[\frac{im}{2\hbar \Delta t} (q_0^2 + q_f^2 - \mathbf{v}^T P_N^{-1} \mathbf{v}) \right] \\ &= \sqrt{\frac{m}{2\pi i \hbar \Delta t \det(P_N)}} \exp \left[\frac{im}{2\hbar \Delta t} (q_0^2 + q_f^2 - \mathbf{v}^T P_N^{-1} \mathbf{v}) \right]. \end{aligned} \quad (1.107)$$

¹This turns out to be the Cartan matrix of the Lie algebra \mathfrak{a}_{N+1} .

Note that, if we denote $B = P_N^{-1}$, we have

$$\mathbf{v}^T P_N^{-1} \mathbf{v} = B_{11}q_0^2 + B_{NN}q_f^2 + q_0q_f(B_{1N} + B_{N1}). \quad (1.108)$$

Therefore, we have to compute these matrix entries as well as $p_N = \det(P_N)$. By developing the determinant with respect to the last row, we easily find the recurrence relation

$$p_N = 2p_{N-1} + \det \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 \end{pmatrix} = 2p_{N-1} - p_{N-2}, \quad N \geq 3. \quad (1.109)$$

We can regard this relation as a second order difference equations, with initial conditions

$$p_1 = 2, \quad p_2 = 3. \quad (1.110)$$

Its solution is given by

$$p_N = N + 1. \quad (1.111)$$

In order to calculate the inverse matrix, we also use the minors of P_N . We find,

$$p_N B_{11} = p_N B_{NN} = p_{N-1}, \quad (1.112)$$

while for the other entry,

$$p_N B_{1N} = (-1)^{N+1} \det \begin{pmatrix} -1 & 2 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ 0 & 0 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -1 \end{pmatrix} = 1. \quad (1.113)$$

By symmetry, we have $B_{N1} = B_{1N}$. We then obtain,

$$B_{11} = B_{NN} = \frac{p_{N-1}}{p_N} = \frac{N}{N+1} \quad (1.114)$$

and

$$B_{1N} = B_{N1} = \frac{1}{p_N} = \frac{1}{N+1}. \quad (1.115)$$

It follows that

$$\begin{aligned} q_0^2 + q_f^2 - \mathbf{v}^T P_N^{-1} \mathbf{v} &= q_0^2 + q_f^2 - B_{11}q_0^2 - B_{NN}q_f^2 - q_0q_f(B_{1N} + B_{N1}) \\ &= q_0^2 + q_f^2 - \frac{N}{N+1}(q_0^2 + q_f^2) - \frac{2q_0q_f}{N+1} = \frac{1}{N+1}(q_0 - q_f)^2. \end{aligned} \quad (1.116)$$

Therefore, we find that (1.107) is given by

$$K(q_f, q_0; t_f, t_0) = \sqrt{\frac{m}{2\pi i \hbar T}} \exp \left[\frac{im}{2\hbar T} (q_0 - q_f)^2 \right], \quad (1.117)$$

where

$$T = (N+1)\Delta t = t_f - t_0. \quad (1.118)$$

This is in agreement with the result obtained in (1.22).

1.6 Gaussian theories

The main reason that we were able to calculate (1.85) explicitly in the case of the free particle is that all the integrals were Gaussian. In order to find solvable models, we should then consider theories defined by a quadratic Lagrangian, of the form

$$L = \frac{m}{2}\dot{q}^2 - \frac{c(t)}{2}q^2 + f(t)q. \quad (1.119)$$

Let us denote by $q_c(t)$ the solution to the Lagrange EOM, with boundary conditions

$$q_c(t_0) = q_0, \quad q_c(t_f) = q_f. \quad (1.120)$$

An arbitrary path contributing to the path integral expression for $K(q_f, q_0; t_f, t_0)$ can be written as

$$q(t) = q_c(t) + y(t), \quad (1.121)$$

where

$$y(t_0) = y(t_f) = 0. \quad (1.122)$$

We can now expand the action around $q_c(t)$ as

$$S(q(t)) = S_c + \frac{1}{2} \int_{t_0}^{t_f} \int_{t_0}^{t_f} \frac{\delta^2 S}{\delta q(t) \delta q(t')} \Big|_{q(t)=q_c(t)} y(t)y(t') dt dt', \quad (1.123)$$

where S_c , introduced in (1.57), is the action evaluated at $q_c(t)$. We note that, in the functional Taylor expansion in (1.123), the term involving the first functional derivative vanishes, since $q_c(t)$ is an extremum of the action and one has (1.56). Since S is quadratic, the expansion in (1.123) stops at second order (in particular, the dependence on the linear term in (1.119) will only enter through the classical action S_c). By using (1.55), we obtain

$$\frac{\delta S}{\delta q(t)} = -m\ddot{q}(t) - c(t)q(t) + f(t), \quad (1.124)$$

therefore,

$$\frac{\delta^2 S}{\delta q(t) \delta q(t')} = \left[-m \left(\frac{d}{dt} \right)^2 - c(t) \right] \delta(t - t'), \quad (1.125)$$

The double integral involving the second derivative of the delta function can be simplified as follows:

$$\begin{aligned} \int_{t_0}^{t_f} \left(\int_{t_0}^{t_f} \frac{d^2}{dt^2} \delta(t - t') y(t) dt \right) y(t') dt' &= - \int_{t_0}^{t_f} \left(\int_{t_0}^{t_f} \frac{d}{dt} \delta(t - t') \dot{y}(t) dt \right) y(t') dt' \\ &= \int_{t_0}^{t_f} \left(\int_{t_0}^{t_f} \frac{d}{dt'} \delta(t - t') y(t') dt' \right) \dot{y}(t) dt \\ &= - \int_{t_0}^{t_f} (\dot{y}(t))^2 dt. \end{aligned} \quad (1.126)$$

In the first line we integrated by parts w.r.t. t , and in going from the second to the third line, we integrated by parts w.r.t. t' . In both cases we took into account the boundary conditions (1.122), which set to zero the boundary terms. We conclude that

$$S(q(t)) = S_c + \mathcal{S}(y(t)), \quad (1.127)$$

where

$$\mathcal{S}(y) = \frac{1}{2} \int_{t_0}^{t_f} (my^2 - c(t)y^2) dt. \quad (1.128)$$

The propagator is then given by

$$K(q_f, q_0; t_f, t_0) = e^{\frac{i}{\hbar} S_c(q_f, q_0; t_f, t_0)} \int \mathcal{D}y(t) e^{\frac{i}{\hbar} \mathcal{S}(y(t))}, \quad (1.129)$$

where we have explicitly indicated that the action evaluated at the classical trajectory, S_c , is a function of the boundary data q_f, q_0, t_f, t_0 . Note that, in doing the integration over paths, the decomposition (1.121) can be regarded as a change of variables, which is a translation by a “constant” (i.e. fixed) path. Therefore, the Jacobian of the change of variables is just one. The path integral over the path $y(t)$ is defined as above, by the limit

$$\begin{aligned} & \int \mathcal{D}y(t) e^{\frac{i}{\hbar} \mathcal{S}(y(t))} \\ &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N+1}{2}} \int \prod_{k=1}^N dy_k \exp \left[\frac{im}{2\hbar \Delta t} \sum_{k=0}^N \left((y_{k+1} - y_k)^2 - \frac{(\Delta t)^2 c_k}{m} y_k^2 \right) \right], \end{aligned} \quad (1.130)$$

where $c_k = c(t_k)$, and we recall that in this case the boundary conditions are $y_0 = y_{N+1} = 0$. We can now generalize the calculation in the case of the free particle. The sum in the exponent of (1.130) can be written as

$$\mathbf{y}^T P_N \mathbf{y}, \quad \mathbf{y}^T = (y_1, \dots, y_N), \quad (1.131)$$

where the $N \times N$ matrix P_N is now given by

$$P_N = \begin{pmatrix} 2 - \rho_1 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 - \rho_2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 - \rho_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 - \rho_{N-1} & -1 \\ 0 & 0 & 0 & \cdots & -1 & 2 - \rho_N \end{pmatrix}, \quad (1.132)$$

and

$$\rho_j = \frac{(\Delta t)^2 c_j}{m}. \quad (1.133)$$

For any N , the integral (1.130) is then a Gaussian, and it can be evaluated explicitly by using (A.1). We obtain,

$$\begin{aligned} & \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N+1}{2}} \int \prod_{k=1}^N dy_k \exp \left[\frac{im}{2\hbar \Delta t} \sum_{k=0}^N \left((y_{k+1} - y_k)^2 - \frac{(\Delta t)^2 c_k}{m} y_k^2 \right) \right] \\ &= \sqrt{\frac{m}{2\pi i \hbar \Delta t \det(P_N)}}. \end{aligned} \quad (1.134)$$

In this formula, it has to be understood that

$$\frac{1}{\sqrt{\det(P_N)}} = e^{-\pi i \nu_N / 2} \frac{1}{\sqrt{|\det(P_N)|}}, \quad (1.135)$$

where ν_N is the number of negative eigenvalues of the matrix P_N . In some simple cases, like the harmonic oscillator, ν_N this can be calculated in detail, as we will see below. It is easy to find the recursion relation satisfied by the determinant $p_N = \det(P_N)$, by generalizing (1.109) for the free particle:

$$p_N = (2 - \rho_N)p_{N-1} - p_{N-2}, \quad N \geq 3. \quad (1.136)$$

This can be extended to $N = 2$ by setting $p_0 = 1$. This recursion can be also written as

$$\frac{p_{j+1} + p_{j-1} - 2p_j}{(\Delta t)^2} = -\frac{c_{j+1}p_j}{m}. \quad (1.137)$$

We want to regard p_j as the discretization of a function $\phi(t)$, defined as follows

$$\phi(t_j) = (\Delta t) p_j. \quad (1.138)$$

The recursion (1.137) can now be regarded as the discretization of a second order differential equation satisfied by $\phi(t)$, namely

$$m \frac{d^2 \phi}{dt^2} + c(t)\phi(t) = 0. \quad (1.139)$$

Indeed, let us multiply both sides of (1.137) by Δt . Then,

$$\lim_{\Delta t \rightarrow 0} \frac{\phi(t_{j+1}) + \phi(t_{j-1}) - 2\phi(t_j)}{(\Delta t)^2} = \frac{d^2 \phi}{dt^2}, \quad (1.140)$$

where we identify $t_j = t$, and

$$\lim_{\Delta t \rightarrow 0} c(t_{j+1})\phi(t_j) = \lim_{\Delta t \rightarrow 0} c(t + \Delta t)\phi(t) = c(t)\phi(t). \quad (1.141)$$

The ODE (1.139) is the EOM for the action (1.128). The initial conditions for this ODE are as follows: in the continuum limit

$$\phi(t_0) = \lim_{\Delta t \rightarrow 0} (\Delta t) p_0 = 0. \quad (1.142)$$

The first derivative is given by

$$\left. \frac{d\phi}{dt} \right|_{t=t_0} = \lim_{\Delta t \rightarrow 0} \frac{\Delta t(p_1 - p_0)}{\Delta t} = \lim_{\Delta t \rightarrow 0} \left(1 - \frac{(\Delta t)^2 c_1}{m} \right) = 1. \quad (1.143)$$

Therefore, we find that

$$\lim_{\Delta t \rightarrow 0} (\Delta t) p_N = \lim_{\Delta t \rightarrow 0} \phi(t_{N+1} - \Delta t) = \phi(t_f). \quad (1.144)$$

In order to keep track of the dependence on t_0 , we will denote

$$f(t; t_0) = \phi(t), \quad (1.145)$$

which satisfies the ODE

$$m \frac{d^2 f(t; t_0)}{dt^2} + c(t)f(t; t_0) = 0, \quad (1.146)$$

with the boundary conditions

$$f(t_0; t_0) = 0, \quad \dot{f}(t_0; t_0) = 1. \quad (1.147)$$

We conclude that

$$\int \mathcal{D}y(t) e^{\frac{i}{\hbar} S(y(t))} = \sqrt{\frac{m}{2\pi i \hbar f(t_f; t_0)}}, \quad (1.148)$$

so that the propagator is given by

$$K(q_f, q_0; t_f, t_0) = \sqrt{\frac{m}{2\pi i \hbar f(t_f; t_0)}} e^{i S_c(q_f, q_0; t_f, t_0)/\hbar}. \quad (1.149)$$

This is a remarkable formula. It states that, in a theory with a quadratic Lagrangian, the propagator has an interpretation in terms of classical paths: its phase is given by the classical action, and the prefactor is determined by a particular solution to the EOM. As a consequence of (1.135), we have to remember that

$$\frac{1}{\sqrt{f(t_f; t_0)}} = e^{-\pi i \nu/2} \frac{1}{\sqrt{|f(t_f; t_0)|}}, \quad (1.150)$$

where ν is the appropriate limit of the ν_N appearing in (1.135), and it depends on the value of t_f and t_0 . It is sometimes called the *Maslov index*.

Example 1.4. *The free particle redux.* Let us recover the result for the free particle from (1.149). The classical trajectory is

$$q_c(t) = q_0 + \frac{q_f - q_0}{T} t, \quad (1.151)$$

and the classical action is

$$S_c = \frac{m}{2} \int_{t_0}^{t_f} \dot{q}_{\text{cl}}^2(t) dt = \frac{m}{2T} (q_f - q_0)^2. \quad (1.152)$$

The ODE (1.146) when $c(t) = 0$ is solved by

$$f(t; t_0) = at + b, \quad (1.153)$$

and the boundary conditions require

$$f(t_0; t_0) = at_0 + b = 0, \quad \dot{f}(t_0; t_0) = a = 1, \quad (1.154)$$

so that

$$f(t; t_0) = t - t_0, \quad (1.155)$$

and

$$f(t_f; t_0) = T. \quad (1.156)$$

By plugging (1.152) and (1.156) in (1.149), we recover (1.117). \square

Example 1.5. *The harmonic oscillator.* Let us set, like before, $T = t_f - t_0$. In the case of the harmonic oscillator, we have that $c(t) = m\omega^2$, and

$$\rho_j = (\Delta t)^2 \omega^2, \quad j = 1, \dots, N. \quad (1.157)$$

The matrix P_N is of the form (1.103) with $\beta = 1$ and

$$\alpha = 2 - (\Delta t)^2 \omega^2. \quad (1.158)$$

When Δt is very small we can write

$$\alpha = 2 \cos \theta, \quad \theta \approx \omega \Delta t = \frac{\omega T}{N+1}. \quad (1.159)$$

The eigenvalues of the matrix P_N are then of the form,

$$2 \left(\cos \frac{\omega T}{N+1} - \cos \frac{\pi p}{N+1} \right), \quad p = 1, \dots, N+1, \quad (1.160)$$

for N sufficiently large. We conclude that, if

$$T_\nu < T < T_{\nu+1}, \quad (1.161)$$

where

$$T_\nu = \frac{\pi \nu}{\omega}, \quad (1.162)$$

there are exactly ν negative eigenvalues. This determines the Maslov index in the case of the harmonic oscillator. Let us now compute the function $f(t; t_0)$. It satisfies the EOM

$$\ddot{f}(t; t_0) + \omega^2 f(t; t_0) = 0, \quad (1.163)$$

therefore

$$f(t; t_0) = A \cos \omega(t - t_0) + B \sin \omega(t - t_0). \quad (1.164)$$

Imposing the boundary conditions (1.147) leads to $A = 0$, $B = 1/\omega$, so that we find

$$f(t; t_0) = \frac{1}{\omega} \sin \omega(t - t_0), \quad (1.165)$$

and we conclude that

$$f(t_f; t_0) = \frac{1}{\omega} \sin \omega T. \quad (1.166)$$

In this case, it is easy to verify directly that the determinant of the matrix P_N behaves as

$$(\Delta t) p_N \approx f(t_f; t_0) \quad (1.167)$$

in the limit $N \rightarrow \infty$, $\Delta t \rightarrow 0$, $(N+1)\Delta t = T$. To see this, let us consider the recursion (1.136), which we write as

$$p_N = (z + z^{-1})p_{N-1} - p_{N-2}. \quad (1.168)$$

This recursion has two general solutions, z^N and z^{-N} . The initial conditions are $p_1 = z + z^{-1}$ and $p_2 = z^2 + z^{-2} + 1$. This fixes the solution to the recursion to be

$$p_N = \frac{z^{N+1} - z^{-N-1}}{z - z^{-1}}. \quad (1.169)$$

In our case, as we have seen,

$$z + z^{-1} \approx 2 \cos \theta, \quad (1.170)$$

where $\theta = \omega \Delta t$. Therefore, $z = e^{i\theta}$ and we conclude that

$$p_N \approx \frac{\sin(N+1)\theta}{\sin \theta} \approx \frac{\sin \omega T}{\omega \Delta t}, \quad (1.171)$$

as we found above. \square

In order to calculate corrections to this leading order approximation, we expand the path around the classical path as in (1.121). Then, we find

$$S(q(t)) = S_c + \frac{1}{2} \int dt dt' y(t) y(t') \frac{\delta^2 S}{\delta q(t) \delta q(t')} \Big|_{q(t)=q_c(t)} + \dots \quad (1.176)$$

When the Lagrangian is of the standard form

$$L = \frac{m}{2} \dot{q}^2 - V(q), \quad (1.177)$$

the second functional derivative reads

$$\frac{\delta^2 S}{\delta q(t) \delta q(t')} \Big|_{q(t)=q_c(t)} = \left[-m \left(\frac{d}{dt} \right)^2 - V''(q_c(t)) \right] \delta(t - t'), \quad (1.178)$$

and we conclude that

$$S(q(t)) = S_c + \mathcal{S}_2(y(t)) + \dots, \quad (1.179)$$

where the quadratic functional is

$$\mathcal{S}_2(y(t)) = \frac{1}{2} \int_{t_0}^{t_f} dt (m \dot{y}^2 - V''(q_c(t)) y^2). \quad (1.180)$$

The next correction to the leading order result is obtained by doing the path integral over the path $y(t)$ with the action $\mathcal{S}_2(y(t))$. This is exactly of the form considered in the previous section, where now

$$c(t) = V''(q_c(t)), \quad (1.181)$$

so we find the answer

$$K(q_f, q_0; t_f, t_0) \approx \sqrt{\frac{m}{2\pi i \hbar f(t_f; t_0)}} e^{\frac{i}{\hbar} S_c(q_f, q_0; t_f, t_0)}, \quad (1.182)$$

where $f(t; t_0)$ satisfies (1.146) with the boundary conditions (1.147). It turns out that this function can be written in terms of the action evaluated at the classical trajectory. To understand this, we consider a family of classical trajectories $q(t; q_0, p)$, parametrized by the initial position q_0 and the initial momentum p , so that they verify

$$q(t_0; q_0, p) = q_0, \quad \dot{q}(t_0; q_0, p) = \frac{p}{m}. \quad (1.183)$$

They also satisfy Newton's equation

$$m \ddot{q}(t; q_0, p) + V'(q(t; q_0, p)) = 0. \quad (1.184)$$

Let us consider now the function

$$\xi(t; q_0, p) = m \frac{\partial q}{\partial p}. \quad (1.185)$$

Then, by taking a derivative w.r.t. p in Newton's equation, we find

$$m \ddot{\xi}(t; q_0, p) + V''(q(t; q_0, p)) \xi(t; q_0, p) = 0. \quad (1.186)$$

At the same time, by taking derivatives w.r.t. p in the initial conditions (1.183) for the family of paths, we find

$$\xi(t_0; q_0, p) = 0, \quad \dot{\xi}(t_0; q_0, p) = 1. \quad (1.187)$$

We conclude that

$$f(t; t_0) = \xi(t; q_0, p). \quad (1.188)$$

To calculate $f(t_f; t_0)$, we first note that

$$q_f = q(t_f; q_0, p). \quad (1.189)$$

This gives p , the initial momentum, implicitly as a function of the final position q_f . Using chain's rule, we have that

$$\frac{\partial q(t_f; q_0, p)}{\partial p} \frac{\partial p}{\partial q_f} = 1. \quad (1.190)$$

But

$$f(t_f; t_0) = m \frac{\partial q(t_f; q_0, p)}{\partial p} = m \left(\frac{\partial p}{\partial q_f} \right)^{-1}. \quad (1.191)$$

As it is well-known, the initial momentum can be obtained from the value of the action at the classical trajectory as

$$p = -\frac{\partial S_c}{\partial q_0}. \quad (1.192)$$

We conclude that

$$f(t_f; t_0) = -m \left(\frac{\partial^2 S_c}{\partial q_f \partial q_0} \right)^{-1}. \quad (1.193)$$

When we put all together, we end up with the following formula for the semiclassical quantum propagator,

$$K(q_f, q_0; t_f, t_0) \approx \frac{1}{\sqrt{2\pi i \hbar}} \sqrt{-\frac{\partial^2 S_c}{\partial q_f \partial q_0}} e^{\frac{i}{\hbar} S_c(q_f, q_0; t_f, t_0)}. \quad (1.194)$$

This is sometimes called *Van Vleck's formula*.

1.8 Semiclassical approximation to the partition function

When we study the canonical partition function, there are two different semiclassical regimes that one can consider. In the first one, we take

$$\beta \hbar \rightarrow 0, \quad (1.195)$$

which corresponds to either \hbar small or high temperature. In this case, the Euclidean time interval u is very small, and we can approximate

$$S_E \approx uV(q) + \frac{m}{2} \int_0^u \dot{q}^2(\tau) d\tau, \quad (1.196)$$

where we consider periodic trajectories $q(u) = q(0) = q$. Therefore, the path integral computing the thermal partition function can be written as

$$\begin{aligned} Z(\beta) &= \int dq \int_{q(0)=q(u)=q} \mathcal{D}q(\tau) e^{-\frac{1}{\hbar} S_E(q(\tau))} \\ &\approx \int dq e^{-\beta V(q)} \int_{q(0)=q(u)=q} \mathcal{D}q(\tau) e^{-\frac{m}{2\hbar} \int_0^u \dot{q}^2(\tau) d\tau} \\ &= \sqrt{\frac{m}{2\pi\hbar^2\beta}} \int dq e^{-\beta V(q)}. \end{aligned} \quad (1.197)$$

This is precisely the classical answer, displaying the Boltzmann factor.

Another limit consists in taking \hbar small, but keeping $\beta\hbar$ finite. This is exactly like the semiclassical limit studied in section 1.7, and the analysis proceeds exactly in the same way. First of all, we consider stationary, periodic paths for the Euclidean action, which we denote by $q_c(\tau)$. Note that these are not the classical solutions of the EOM for the original theory, but for a theory with an *inverted* potential:

$$m\ddot{q}_c(\tau) - V'(q_c(\tau)) = 0, \quad (1.198)$$

since the Euclidean action differs from the original action in the sign of the potential. These are sometimes called the Euclidean EOM. We then expand the action around this path as

$$q(\tau) = q_c(\tau) + y(\tau). \quad (1.199)$$

Note that $y(\tau)$ is also a periodic path: $y(0) = y(u)$. We find,

$$S_E(q(\tau)) = S_E(q_c(\tau)) + \mathcal{S}_E(y(\tau)) + \dots, \quad (1.200)$$

where the quadratic functional is

$$\mathcal{S}_E(y(\tau)) = \frac{1}{2} \int_0^u d\tau (m\dot{y}^2 + V''(q_c(\tau))y^2). \quad (1.201)$$

We conclude that, in the semiclassical approximation

$$Z(\beta) \approx e^{-\frac{1}{\hbar} S_E(q_c(\tau))} \int_{y(0)=y(u)} \mathcal{D}y(\tau) e^{-\frac{1}{\hbar} \mathcal{S}_E(y(\tau))}. \quad (1.202)$$

We have to evaluate now this Euclidean, Gaussian path integral with periodic boundary conditions. In principle, we can evaluate it by first computing the propagator for the corresponding Gaussian theory, performing a Wick rotation, and finally integrating over $q = q_0 = q_f$. However, it is useful to have a general formula for the Gaussian path integral with periodic boundary conditions, instead of Dirichlet boundary conditions. As we will see, the answer is very elegant, as in the Dirichlet case, and it can be expressed in terms of classical solutions to the Euclidean EOM.

Let us first consider the Euclidean, quadratic functional

$$\mathcal{S}_E(y) = \frac{1}{2} \int_0^u d\tau (m\dot{y}^2 + c(\tau)y^2). \quad (1.203)$$

We consider trajectories $y(t)$ which are periodic:

$$y(0) = y(u), \quad (1.204)$$

and we want to perform an Euclidean path integral over all possible periodic paths $y(t)$. This path integral is defined as

$$\int_{y(0)=y(u)} \mathcal{D}y(\tau) e^{-\frac{1}{\hbar} S_E(y(\tau))} = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi\hbar\Delta\tau} \right)^{\frac{N+1}{2}} \int \prod_{k=1}^{N+1} dy_k \exp \left[-\frac{m}{2\hbar\Delta\tau} \sum_{k=0}^N \left((y_{k+1} - y_k)^2 + \frac{(\Delta\tau)^2 c_k}{m} y_k^2 \right) \right], \quad (1.205)$$

where $c_k = c(\tau_k)$, and periodicity implies that

$$y_0 = y_{N+1}. \quad (1.206)$$

The calculation is similar to the case of the free particle. The exponent in (1.205) can be written as

$$-\frac{m}{2\hbar\Delta\tau} \mathbf{y}^T \mathbf{a}_{N+1} \mathbf{y}, \quad (1.207)$$

where

$$\mathbf{y}^T = (y_0, y_1, \dots, y_N). \quad (1.208)$$

The matrix \mathbf{a}_{N+1} is given by

$$\mathbf{a}_{N+1} = \begin{pmatrix} 2 + \rho_0 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 + \rho_1 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 + \rho_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 + \rho_{N-1} & -1 \\ -1 & 0 & 0 & \cdots & -1 & 2 + \rho_N \end{pmatrix}, \quad (1.209)$$

where

$$\rho_j = \frac{(\Delta\tau)^2 c_j}{m}. \quad (1.210)$$

The N -th approximation to the path integral is now given by

$$\begin{aligned} & \left(\frac{m}{2\pi\hbar\Delta\tau} \right)^{\frac{N+1}{2}} \int \prod_{k=1}^{N+1} dy_k \exp \left[-\frac{m}{2\hbar\Delta\tau} \sum_{k=0}^N \left((y_{k+1} - y_k)^2 + \rho_k y_k^2 \right) \right] \\ &= \sqrt{\frac{1}{\det(\mathbf{a}_{N+1})}}. \end{aligned} \quad (1.211)$$

To calculate the large N limit of this determinant, we consider the eigenvalue problem for the matrix \mathbf{a}_{N+1} . A vector \mathbf{y} will be an eigenvector with eigenvalue λ if

$$\mathbf{a}_k y_k - y_{k+1} - y_{k-1} = \lambda y_k, \quad (1.212)$$

where we set

$$\mathbf{a}_k = 2 + \rho_k, \quad (1.213)$$

and in addition we have the periodicity condition (1.206). We can think about (1.212) as the discretization of the second order differential equation

$$-y'' + \frac{c(\tau)}{m}y = \lambda y. \quad (1.214)$$

In addition, we can regard the y_i as variables associated to a periodic lattice. We will write the eigenvalue equations in the form

$$\begin{pmatrix} y_i \\ y_{i+1} \end{pmatrix} = t_i(\lambda) \begin{pmatrix} y_{i-1} \\ y_i \end{pmatrix}, \quad (1.215)$$

where

$$t_i(\lambda) = \begin{pmatrix} 0 & 1 \\ -1 & \mathbf{a}_i - \lambda \end{pmatrix}. \quad (1.216)$$

In other words, to each site of the lattice we associate a vector with two coordinates y_{i-1} , y_i . Two consecutive sites are related by the “transfer matrix” $t_i(\lambda)$. Note that

$$\det(t_i(\lambda)) = 1. \quad (1.217)$$

Given an initial condition y_{-1} , y_0 , we can find a solution to (1.212) at all discretized times by acting with products of the $t_i(\lambda)$:

$$\begin{pmatrix} y_{i-1} \\ y_i \end{pmatrix} = t_{i-1}(\lambda) \cdots t_0(\lambda) \begin{pmatrix} y_{-1} \\ y_0 \end{pmatrix}. \quad (1.218)$$

The *monodromy matrix* is defined by

$$T_{N+1} = t_N(\lambda) \cdots t_0(\lambda), \quad (1.219)$$

and we have

$$\begin{pmatrix} y_N \\ y_{N+1} \end{pmatrix} = T_{N+1}(\lambda) \begin{pmatrix} y_{-1} \\ y_0 \end{pmatrix}. \quad (1.220)$$

Existence of a periodic solution to the discretized equation (1.212) is equivalent to the existence of an eigenvector of the monodromy matrix of eigenvalue 1. Therefore, λ is an eigenvalue of \mathbf{a}_{N+1} if and only if it satisfies

$$\det(T_{N+1}(\lambda) - 1) = 0. \quad (1.221)$$

If we write

$$T_{N+1}(\lambda) = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad (1.222)$$

we find that

$$p(\lambda) \equiv \det(T_{N+1}(\lambda) - 1) = 2 - \text{Tr } T_{N+1}, \quad (1.223)$$

since $\det(T_{N+1}) = 1$. It is easy to see that d has degree $N + 1$ in λ , and it goes like

$$d \approx (-\lambda)^{N+1}, \quad \lambda \gg 1. \quad (1.224)$$

One can also see that a is of degree $N - 2$ in λ , for $N \geq 2$. It follows that $p(\lambda)$ is a polynomial in λ which has the same degree than the characteristic polynomial of \mathbf{a}_{N+1} , and the same roots.

In addition, its leading coefficient $-(-\lambda)^{N+1}$ is minus the leading coefficient of the characteristic polynomial. We conclude that

$$\det(T_{N+1}(\lambda) - 1) = -\det(\mathbf{a}_{N+1} - \lambda). \quad (1.225)$$

Let us now compute the diagonal entries of $T_{N+1}(\lambda)$. To do this, we note the following. Let us consider a basis for the vector at the initial site:

$$\begin{pmatrix} v_{-1}^{(1)} \\ v_0^{(1)} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} v_{-1}^{(2)} \\ v_0^{(2)} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (1.226)$$

Then,

$$\begin{pmatrix} v_N^{(1)} \\ v_{N+1}^{(1)} \end{pmatrix} = T_{N+1}(\lambda) \begin{pmatrix} v_{-1}^{(1)} \\ v_0^{(1)} \end{pmatrix}, \quad \begin{pmatrix} v_N^{(2)} \\ v_{N+1}^{(2)} \end{pmatrix} = T_{N+1}(\lambda) \begin{pmatrix} v_{-1}^{(2)} \\ v_0^{(2)} \end{pmatrix}. \quad (1.227)$$

It follows that

$$T_{N+1}(\lambda) = \begin{pmatrix} v_N^{(1)} & v_N^{(2)} \\ v_{N+1}^{(1)} & v_{N+1}^{(2)} \end{pmatrix}. \quad (1.228)$$

Let us now consider a solution to (1.212) with initial conditions

$$y_{-1}^{(1)} = y_0^{(1)} = 1, \quad (1.229)$$

and another one with

$$y_{-1}^{(2)} = 0, \quad y_0^{(2)} = \Delta t. \quad (1.230)$$

This leads to another basis of solutions, so the previous basis can be expressed as a linear combination of this one. One quickly finds,

$$v_k^{(1)} = y_k^{(1)} - \frac{1}{\Delta t} y_k^{(2)}, \quad v_k^{(2)} = \frac{1}{\Delta t} y_k^{(2)}. \quad (1.231)$$

Therefore,

$$\det(\mathbf{a}_{N+1} - \lambda) = v_N^{(1)} + v_{N+1}^{(1)} - 2 = y_N^{(1)} + \frac{y_{N+1}^{(2)} - y_N^{(2)}}{\Delta t} - 2. \quad (1.232)$$

In the continuum limit $N \rightarrow \infty$, $y_k^{(1)}$ becomes a solution $y_1(\tau; \lambda)$ of (1.214) with boundary conditions

$$y_1(0; \lambda) = 1, \quad y_1'(0; \lambda) = 0, \quad (1.233)$$

while $y_k^{(2)}$ becomes a solution $y_2(\tau; \lambda)$ with boundary conditions

$$y_2(0; \lambda) = 0, \quad y_2'(0; \lambda) = 1. \quad (1.234)$$

Given such a solution, we have that

$$\lim_{N \rightarrow \infty} \det(\mathbf{a}_{N+1} - \lambda) = y_1(u; \lambda) + y_2'(u; \lambda) - 2. \quad (1.235)$$

This makes it possible to compute the path integral from a basis of solutions to the EOM (1.214).

Example 1.6. Let us consider the (Euclidean) harmonic oscillator. In this case, the function $c(\tau)$ in (1.203) is given by

$$c(\tau) = \omega^2 \quad (1.236)$$

We will also set $m = 1$. The path integral (1.205) computes the canonical partition function of the harmonic oscillator, which we will denote by $Z_G(\beta)$ (here, G stands for Gaussian). The differential equation (1.214) is in this case,

$$-y'' + \omega^2 y = 0. \quad (1.237)$$

We have already set $\lambda = 0$. The solutions $y_1(\tau)$, $y_2(\tau)$ with the above boundary conditions are

$$y_1(\tau) = \cosh(\omega\tau), \quad y_2(\tau) = \frac{\sinh(\omega\tau)}{\omega}. \quad (1.238)$$

Then,

$$y_1(u) + y_2'(u) - 2 = 2 \cosh(\beta\hbar\omega) - 2 = 4 \sinh^2\left(\frac{\beta\omega\hbar}{2}\right). \quad (1.239)$$

We conclude that

$$Z_G(\beta) = \frac{1}{2 \sinh\left(\frac{\beta\omega\hbar}{2}\right)}, \quad (1.240)$$

which is the standard partition function for the harmonic oscillator at finite temperature. \square

1.9 Functional determinants

In the Gaussian approximation, the calculation of path integrals involves taking the limit as $N \rightarrow \infty$ of the determinant of a matrix of size $N \times N$. It is natural to interpret this limit as the *determinant of an operator*. To be concrete, let us reconsider the case of the free particle, as an example of a Gaussian integration. The propagator takes the form in (1.129),

$$K(q_f, q_0; t_f, t_0) = e^{\frac{i}{\hbar} S_c(q_f, q_0; t_f, t_0)} \int e^{\frac{im}{2\hbar} \int_{t_0}^{t_f} \dot{y}^2 dt} \mathcal{D}y(t) \quad (1.241)$$

Let us focus on the path integral over $y(t)$. Let

$$\mathbf{A} = -\frac{d^2}{dt^2} \quad (1.242)$$

be the second order differential operator on the interval $[t_0, t_f]$ with Dirichlet boundary conditions $y(t_0) = y(t_f) = 0$. Then,

$$\langle y | \mathbf{A} | y \rangle = - \int_{t_0}^{t_f} y(t) \ddot{y}(t) dt = \int_{t_0}^{t_f} \dot{y}^2(t) dt. \quad (1.243)$$

Therefore, the path integral can be written as

$$\int e^{\frac{im}{2\hbar} \langle y | \mathbf{A} | y \rangle} \mathcal{D}y(t). \quad (1.244)$$

We can think about this integral as an infinite-dimensional version of a Gaussian integral. Therefore, we would expect the answer to be proportional to

$$\frac{1}{\sqrt{\det(\mathbf{A})}}. \quad (1.245)$$

However, this determinant should be appropriately defined, since the naive infinite product

$$\prod_{n=1}^{\infty} \lambda_n, \quad (1.246)$$

where λ_n are the eigenvalues of the operator A , does not make sense. Indeed, the spectral problem of A is easy to solve: the eigenfunctions are

$$\psi_n(t) = \sin\left(\frac{n\pi t}{T}\right), \quad n = 1, 2, \dots, \quad (1.247)$$

and the corresponding eigenvalues are

$$\lambda_n = \left(\frac{\pi n}{T}\right)^2, \quad n = 1, 2, \dots. \quad (1.248)$$

The product over the eigenvalues is clearly divergent. There is however a natural way for defining a *regularized* determinant, which is as follows. Let us assume that A has a discrete and positive spectrum $\lambda_n > 0$, $n = 0, 1, \dots$. The *zeta function* of the operator A is defined by

$$\zeta_A(s) = \sum_{n \geq 0} \frac{1}{\lambda_n^s}. \quad (1.249)$$

If s is real and sufficiently large, this sum converges. For example, in the case of the operator (1.242), the sum converges if $\text{Re}(s) > 1/2$. Let us now suppose that $\zeta_A(s)$ can be analytically continued to a larger domain containing $s = 0$, where it is regular. Then, the regularized determinant of A is defined as

$$\det A = \exp(-\zeta'_A(0)). \quad (1.250)$$

The rationale for this definition is that, if the infinite product (1.246) converges, one has

$$\zeta'_A(0) = \sum_{n \geq 0} \frac{d}{ds} \left(e^{-s \log \lambda_n} \right)_{s=0} = - \sum_{n \geq 0} \log(\lambda_n). \quad (1.251)$$

The classical example for this procedure is Riemann's zeta function, which is defined as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}. \quad (1.252)$$

Clearly, this converges when $\text{Re}(s) > 1$. It can be shown that $\zeta(s)$ can be extended to the whole complex plane, and the only singularity in this extension is a simple pole at $s = 1$.

In the case of the operator (1.242), its zeta function is closely related to Riemann's zeta function, since

$$\zeta_A(s) = \left(\frac{T}{\pi}\right)^{2s} \sum_{n=1}^{\infty} \frac{1}{n^{2s}} = \left(\frac{T}{\pi}\right)^{2s} \zeta(2s). \quad (1.253)$$

In this case, the fact that Riemann's zeta function has an analytic extension to $s = 0$ makes it possible to define and calculate the regularized determinant of A . One finds,

$$\zeta'_A(0) = 2 \log\left(\frac{T}{\pi}\right) \zeta(0) + 2\zeta'(0). \quad (1.254)$$

We can now use the values

$$\zeta(0) = -\frac{1}{2}, \quad \zeta'(0) = -\frac{1}{2} \log(2\pi), \quad (1.255)$$

to obtain

$$\zeta'_A(0) = -\log(2T), \quad (1.256)$$

therefore

$$\det A = 2T. \quad (1.257)$$

We have found in the analysis of the free particle that (we set $m = 1$ for convenience)

$$\int e^{\frac{i}{2\hbar} \int_{t_0}^{t_f} \dot{y}^2 dt} \mathcal{D}y(t) = \frac{1}{\sqrt{2\pi i \hbar T}}, \quad (1.258)$$

so indeed the result is indeed proportional to $1/\sqrt{\det(A)}$:

$$\int e^{\frac{i}{2\hbar} \int_{t_0}^{t_f} \dot{y}^2 dt} \mathcal{D}y(t) = \frac{1}{\sqrt{\pi i \hbar \det(A)}}. \quad (1.259)$$

The result (1.257) can be generalized to operators which appear naturally in path integrals. Let us first consider the operator

$$A = -\frac{d^2}{dt^2} - c(t) \quad (1.260)$$

with Dirichlet boundary conditions in the interval $[t_0, t_f]$. Let us assume that this operator does not have a zero eigenvalue (one usually says that it has no zero modes). By using the zeta function regularization defined above, one can show that

$$\det A = 2f(t_f; t_0), \quad (1.261)$$

where the function $f(t_f; t_0)$ is defined by the ODE (1.146) with boundary conditions (1.147) (and we set again $m = 1$). Therefore, the result (1.148) can be written as

$$\int e^{\frac{i}{2\hbar} \int_{t_0}^{t_f} (\dot{y}^2 - c(t)y^2) dt} \mathcal{D}y(t) = \frac{1}{\sqrt{\pi i \hbar \det(A)}}. \quad (1.262)$$

We also have the Euclidean version,

$$\int e^{-\frac{1}{2\hbar} \int_{\tau_0}^{\tau_f} (\dot{y}^2 + c(\tau)y^2) d\tau} \mathcal{D}y(\tau) = \frac{1}{\sqrt{\pi i \hbar \det(A)}}, \quad (1.263)$$

where the operator A is now given by

$$A = -\frac{d^2}{dt^2} + c(t). \quad (1.264)$$

When the operator A in (1.260) has zero modes one has to be more careful, since the standard determinant vanishes. To take into account this more general case, it is useful to consider the operator

$$A_\lambda = A - \lambda, \quad (1.265)$$

associated to the eigenvalue problem

$$-y''(t) - c(t)y(t) = \lambda y(t). \quad (1.266)$$

One has in this case the following result. Let $y(t; \lambda)$ a solution of (1.266) with the boundary conditions

$$y(t_0; \lambda) = 0, \quad y'(t_0; \lambda) = 1. \quad (1.267)$$

Then,

$$\det(\mathbf{A} - \lambda) = 2y(t_f; \lambda). \quad (1.268)$$

When \mathbf{A} has no zero mode, we recover (1.261) by setting $\lambda = 0$. When \mathbf{A} has a zero mode, we can extract it as follows. The effect of subtracting $-\lambda$ in (1.265) is to shifting all eigenvalues by $-\lambda$. We can then define

$$\det'(\mathbf{A}) = -\left. \frac{\partial}{\partial \lambda} \det(\mathbf{A} - \lambda) \right|_{\lambda=0}. \quad (1.269)$$

If \mathbf{A} has a discrete spectrum of eigenvalues λ_n , $n = 0, 1, \dots$, with $0 = \lambda_0 < \lambda_1 < \dots$, the primed determinant (1.269) is the regularized version of

$$\prod_{n \geq 1} \lambda_n. \quad (1.270)$$

It is also possible to consider the operator (1.260) acting on the space of *periodic* functions in the interval $[t_0, t_f]$, as we had to do in the evaluation of the path integral (1.205). In this case we have the result

$$\det(\mathbf{A} - \lambda) = 2y_1(t_f; \lambda) + 2y_2'(t_f; \lambda) - 2, \quad (1.271)$$

where $y_{1,2}(t; \lambda)$ are solutions of (1.266) with the boundary conditions (1.233) and (1.234), respectively. This can be proved as well with zeta function techniques.

1.10 Correlation functions and Wick's theorem

So far we have used the Feynman path integral to calculate propagators, but it can be also used to compute correlation functions. To do this, we work in the Heisenberg picture. The Heisenberg operator associated to \mathbf{q} is given in (1.28). The eigenvector of this operator is

$$|q, t\rangle = e^{iHt/\hbar}|q\rangle, \quad (1.272)$$

since

$$\mathbf{q}_H(t)|q, t\rangle = q|q, t\rangle. \quad (1.273)$$

We are interested in computing *correlation functions*, i.e. averages of operators in the Heisenberg picture, like for example

$$\langle q_f, t_f | \mathbf{q}_H(t) | q_0, t_0 \rangle. \quad (1.274)$$

In order to give a path integral representation for this function, we write it as

$$\begin{aligned} \langle q_f, t_f | \mathbf{q}_H(t) | q_0, t_0 \rangle &= \int_{\mathbb{R}} dq \langle q_f, t_f | \mathbf{q}_H(t) e^{iHt/\hbar} | q \rangle \langle q | e^{-iHt/\hbar} | q_0, t_0 \rangle \\ &= \int_{\mathbb{R}} dq \langle q_f, t_f | \mathbf{q}_H(t) | q, t \rangle \langle q, t | q_0, t_0 \rangle = \int_{\mathbb{R}} dq \langle q_f, t_f | q, t \rangle q \langle q, t | q_0, t_0 \rangle \\ &= \int_{\mathbb{R}} dq K(q_f, q; t_f, t) q K(q, q_0; t, t_0) \end{aligned} \quad (1.275)$$

If we now use the path integral expression for the propagator, we obtain

$$\langle q_f, t_f | \mathbf{q}_H(t) | q_0, t_0 \rangle = \int \mathcal{D}q(s) e^{\frac{i}{\hbar} S(q(s))} q(t). \quad (1.276)$$

To derive this equality, let us consider a $t \in [t_0, t_f]$. Any path $q(s)$ going from q_0 at $s = t_0$ to q_f at $s = t_f$ can be regarded as the union of two paths: the first one, which we will denote as $q_1(s)$ goes from q_0 at $s = t_0$, to q at $s = t$; the second one goes, which we will denote as $q_2(s)$, goes from q at t , to q_f at $s = t_f$. The integration over all paths going from q_0 to q_f can then be written as

$$\int_{q(t_0)=q_0, q(t_f)=q_f} \mathcal{D}q(s) = \int_{\mathbb{R}} dq \int_{q_1(t_0)=q_0, q_1(t)=q} \mathcal{D}q_1(s) \int_{q_2(t)=q, q_2(t_f)=q_f} \mathcal{D}q_2(s). \quad (1.277)$$

Then, taking into account that

$$S(q(s)) = S(q_1(s)) + S(q_2(s)), \quad (1.278)$$

we find

$$\begin{aligned} & \int \mathcal{D}q(s) e^{\frac{i}{\hbar} S(q(s))} q(t) \\ &= \int_{\mathbb{R}} dq q \int_{q_1(t_0)=q_0, q_1(t)=q} \mathcal{D}q_1(s) e^{\frac{i}{\hbar} S(q_1(s))} \int_{q_2(t)=q, q_2(t_f)=q_f} \mathcal{D}q_2(s) e^{\frac{i}{\hbar} S(q_2(s))}, \end{aligned} \quad (1.279)$$

which is precisely the last line in (1.275).

Let us now consider

$$\int \mathcal{D}q(s) e^{\frac{i}{\hbar} S(q(s))} q(t_1) q(t_2). \quad (1.280)$$

The result of this path integral depends on the order of the times: if $t_1 > t_2$, this computes

$$\int_{\mathbb{R}^2} dq_1 dq_2 K(q_f, q_1; t_f, t_1) q_1 K(q_1, q_2; t_1, t_2) q_2 K(q_2, q_0; t_2, t_0), \quad (1.281)$$

and if $t_2 > t_1$, it computes

$$\int_{\mathbb{R}^2} dq_1 dq_2 K(q_f, q_2; t_f, t_2) q_2 K(q_2, q_1; t_2, t_1) q_1 K(q_1, q_0; t_1, t_0). \quad (1.282)$$

We conclude that

$$\langle q_f, t_f | T(\mathbf{q}_H(t_1) \mathbf{q}_H(t_2)) | q_0, t_0 \rangle = \int \mathcal{D}q(s) e^{\frac{i}{\hbar} S(q(s))} q(t_1) q(t_2), \quad (1.283)$$

where T denotes time-ordering, i.e.

$$T(\mathbf{q}_H(t_1) \mathbf{q}_H(t_2)) = \begin{cases} \mathbf{q}_H(t_1) \mathbf{q}_H(t_2), & \text{if } t_1 > t_2, \\ \mathbf{q}_H(t_2) \mathbf{q}_H(t_1), & \text{if } t_2 > t_1. \end{cases} \quad (1.284)$$

In the Euclidean theory, “time” evolution is implemented by

$$\mathbf{q}_H(\tau) = e^{\tau H/\hbar} \mathbf{q} e^{-\tau H/\hbar}, \quad (1.285)$$

and we define

$$|q, \tau\rangle = e^{\tau H/\hbar}|q\rangle, \quad \langle q, \tau| = \langle q|e^{-\tau H/\hbar}. \quad (1.286)$$

Note that $|q, \tau\rangle$ and $\langle q, \tau|$ are no longer related by Hermitian conjugation. In the Euclidean path integral with periodic boundary conditions, as in (1.97), the natural correlation functions are of the form

$$\int_{q(0)=q(u)} \mathcal{D}q(\tau) e^{-S_E(q(\tau))/\hbar} q(\tau_1) \cdots q(\tau_\ell), \quad (1.287)$$

where $u = \beta\hbar$. This path integral calculates

$$\begin{aligned} \int_{\mathbb{R}} dq \langle q, u|T(\mathbf{q}_H(\tau_1) \cdots \mathbf{q}_H(\tau_\ell))|q, 0\rangle &= \int_{\mathbb{R}} dq \langle q|e^{-\beta H}T(\mathbf{q}_H(\tau_1) \cdots \mathbf{q}_H(\tau_\ell))|q\rangle \\ &= \text{Tr} \left\{ e^{-\beta H}T(\mathbf{q}_H(\tau_1) \cdots \mathbf{q}_H(\tau_\ell)) \right\}. \end{aligned} \quad (1.288)$$

The normalized correlator will be defined as

$$\begin{aligned} \langle q(\tau_1) \cdots q(\tau_\ell) \rangle &= \frac{1}{Z(\beta)} \int_{q(0)=q(u)} \mathcal{D}q(\tau) e^{-S_E(q(\tau))/\hbar} q(\tau_1) \cdots q(\tau_\ell) \\ &= \frac{1}{Z(\beta)} \text{Tr} \left\{ e^{-\beta H}T(\mathbf{q}_H(\tau_1) \cdots \mathbf{q}_H(\tau_\ell)) \right\}. \end{aligned} \quad (1.289)$$

We will focus on the correlators of the Euclidean theory. They have the following important property. Let us suppose that the Hamiltonian H has a discrete spectrum, with eigenstates $|n\rangle$ and eigenvalues E_n , $n = 0, 1, 2, \dots$, and such that

$$E_0 < E_1 < \dots. \quad (1.290)$$

This means in particular that there is an energy gap between the ground state and the excited states. Let us now consider the low temperature limit

$$\beta \rightarrow \infty. \quad (1.291)$$

We note that,

$$\begin{aligned} \text{Tr} \left\{ e^{-\beta H}T(\mathbf{q}_H(\tau_1) \cdots \mathbf{q}_H(\tau_\ell)) \right\} &= \sum_{n \geq 0} e^{-\beta E_n} \langle n|T(\mathbf{q}_H(\tau_1) \cdots \mathbf{q}_H(\tau_\ell))|n\rangle \\ &= e^{-\beta E_0} \langle 0|T(\mathbf{q}_H(\tau_1) \cdots \mathbf{q}_H(\tau_\ell))|0\rangle + \mathcal{O}\left(e^{-\beta(E_1-E_0)}\right). \end{aligned} \quad (1.292)$$

Similarly,

$$Z(\beta) = e^{-\beta E_0} + \mathcal{O}\left(e^{-\beta(E_1-E_0)}\right). \quad (1.293)$$

Therefore, in the limit (1.291) only the ground state survives, and we have

$$\lim_{\beta \rightarrow \infty} \langle q(\tau_1) \cdots q(\tau_\ell) \rangle = \langle 0|T(\mathbf{q}_H(\tau_1) \cdots \mathbf{q}_H(\tau_\ell))|0\rangle, \quad (1.294)$$

i.e. this limit computes correlation functions in the vacuum state.

Correlation functions can be easily obtained from the generating functional

$$Z[j] = \int_{q(0)=q(u)} \mathcal{D}q(\tau) e^{-\frac{1}{\hbar}S_E(q(\tau)) + \int q(\tau)j(\tau)d\tau}, \quad (1.295)$$

which is the partition function in a theory with a modified action depending on an arbitrary source $j(\tau)$. Note that $Z[0]$ is the standard partition function. Then, by functional differentiation we find

$$\langle q(\tau_1) \cdots q(\tau_\ell) \rangle = \frac{1}{Z[0]} \frac{\delta^\ell Z[j]}{\delta j(\tau_1) \cdots \delta j(\tau_\ell)} \Big|_{j=0}. \quad (1.296)$$

The path integral $Z[j]$ can be computed exactly in the case of a Gaussian theory. Let us consider the Euclidean action

$$S_E(q; j) = \int_0^u \left(\frac{1}{2} \dot{q}^2 + \frac{\omega^2}{2} q^2 - \hbar j q \right) d\tau. \quad (1.297)$$

The classical EOM is given by

$$(-\partial_\tau^2 + \omega^2) q(\tau) = \hbar j(\tau), \quad (1.298)$$

with periodic boundary conditions. To solve this equation, let us introduce the Green's function or propagator satisfying

$$(-\partial_\tau^2 + \omega^2) G(\tau, \tau') = \delta(\tau - \tau'). \quad (1.299)$$

We impose periodic boundary conditions both for this function and its first derivative. It follows from time translation invariance that in this case

$$G(\tau, \tau') = G(\tau - \tau', 0) \equiv G(\tau - \tau'). \quad (1.300)$$

We also have, by time reversal symmetry, that

$$G(\tau, \tau') = G(\tau', \tau). \quad (1.301)$$

Then, the solution of (1.298) is given by

$$q_c(\tau) = \hbar \int_0^u G(\tau, \tau') j(\tau') d\tau'. \quad (1.302)$$

Let us use bra and ket notation and write this as

$$|q_c\rangle = \hbar \mathbf{G} |j\rangle, \quad (1.303)$$

where G is the operator whose integral kernel is the Green's function $G(\tau, \tau')$. It follows that the classical action is given by

$$\frac{1}{\hbar} S_E(q_c, j) = \frac{1}{2\hbar} \langle q_c | \mathbf{G}^{-1} | q_c \rangle - \langle j | q_c \rangle = -\frac{\hbar}{2} \langle j | \mathbf{G} | j \rangle = -\frac{\hbar}{2} \int j(\tau) G(\tau - \tau') j(\tau') d\tau d\tau'. \quad (1.304)$$

We can now expand the action around the classical trajectory, as we did above, to obtain

$$Z[j] = e^{-S_E(q_c, j)/\hbar} \int \mathcal{D}y e^{-\frac{1}{\hbar} S_G(y)}, \quad (1.305)$$

where

$$S_G(y) = \int_0^u \left(\frac{1}{2} \dot{y}^2 + \frac{\omega^2}{2} y^2 \right) d\tau. \quad (1.306)$$

In other words, we find that

$$Z[j] = Z[0] \exp \left(\frac{\hbar}{2} \int j(\tau) G(\tau - \tau') j(\tau') d\tau d\tau' \right). \quad (1.307)$$

We can now use this explicit formula for $Z[j]$, together with (1.296), to calculate correlation functions for the harmonic oscillator. For the correlation function of two variables or *two-point function* we find

$$\langle q(\tau)q(\tau') \rangle = \hbar G(\tau - \tau'). \quad (1.308)$$

To calculate a generic correlation function, let us expand the exponential in (1.307)

$$\begin{aligned} \exp\left(\frac{\hbar}{2} \int d\tau d\tau' j(\tau)G(\tau - \tau')j(\tau')\right) &= \sum_{n=0}^{\infty} \frac{\hbar^n}{2^n n!} \left(\int d\tau d\tau' j(\tau)G(\tau - \tau')j(\tau') \right)^n \\ &= \sum_{n=0}^{\infty} \frac{\hbar^n}{2^n n!} \int d\tau_1 \cdots d\tau_{2n} j(\tau_1) \cdots j(\tau_{2n}) G(\tau_1, \tau_2) \cdots G(\tau_{2n-1}, \tau_{2n}) \\ &= \sum_{n=0}^{\infty} \frac{\hbar^n}{2^n n!} \int d\tau_1 \cdots d\tau_{2n} j(\tau_1) \cdots j(\tau_{2n}) \frac{1}{(2n)!} \sum_{\sigma \in S_{2n}} G(\tau_{\sigma(1)}, \tau_{\sigma(2)}) \cdots G(\tau_{\sigma(2n-1)}, \tau_{\sigma(2n)}). \end{aligned} \quad (1.309)$$

In going to the last line, we have used the fact that $G(\tau_1, \tau_2) \cdots G(\tau_{2n-1}, \tau_{2n})$ can be symmetrized w.r.t. the indices $1, \dots, 2n$, since it multiplies a symmetric function and is integrated with the symmetric measure $d\tau_1 \cdots d\tau_{2n}$. Therefore, we sum over all possible permutations σ of the indices in the permutation group of $2n$ elements S_{2n} . On the other hand, (1.309) is computing the generating functional (1.295),

$$Z[j] = Z[0] \sum_{M=0}^{\infty} \frac{1}{M!} \int d\tau_1 \cdots d\tau_M j(\tau_1) \cdots j(\tau_M) \langle q(\tau_1) \cdots q(\tau_M) \rangle. \quad (1.310)$$

Since (1.309) with (1.310) are equal, and since the source $j(\tau)$ is arbitrary, we conclude first of all that the correlation functions with an odd number of terms vanish, as expected from the symmetry $q(\tau) \leftrightarrow -q(\tau)$ of the theory. When $M = 2n$ is even, we find that

$$\langle q(\tau_1) \cdots q(\tau_{2n}) \rangle = \frac{\hbar^n}{2^n n!} \sum_{\sigma \in S_{2n}} G(\tau_{\sigma(1)}, \tau_{\sigma(2)}) \cdots G(\tau_{\sigma(2n-1)}, \tau_{\sigma(2n)}). \quad (1.311)$$

We notice however that in the r.h.s. many terms are equal, namely, terms which differ by a permutation of the two labels inside $G(\tau, \tau')$ (recall (1.301)), or by a permutations of the n groups of paired indices. For example, if $n = 2$, the terms $G(\tau_1, \tau_2)G(\tau_3, \tau_4)$ and $G(\tau_2, \tau_1)G(\tau_3, \tau_4)$ give the same contribution in the sum, as does the term $G(\tau_3, \tau_4)G(\tau_1, \tau_2)$. We will say that two permutations of $2n$ elements are equivalent if they give the same contribution in the r.h.s. of (1.311). An equivalence class of permutations is called a *pairing*. Each pairing corresponds to $2^n n!$ different permutations, which is precisely the factor in front of the sum in (1.311). The different pairings are obtained by grouping the $2n$ labels in groups of 2, irrespectively of the ordering of the groups and the order of the labels inside each pair. We conclude that (1.311) can be written as a sum over pairings, as follows:

$$\langle q(\tau_1) \cdots q(\tau_{2n}) \rangle = \hbar^n \sum_{\text{pairings } P} G(\tau_{P(1)}, \tau_{P(2)}) \cdots G(\tau_{P(2n-1)}, \tau_{P(2n)}). \quad (1.312)$$

This important result is *Wick's theorem*. Let us note that there are

$$\frac{(2n)!}{2^n n!} \quad (1.313)$$

inequivalent pairings contributing to the r.h.s. of (1.312). For example, when $n = 2$ there are $4!/4 \cdot 2! = 3$ different pairings, and one finds

$$\begin{aligned} \langle q(\tau_1)q(\tau_2)q(\tau_3)q(\tau_4) \rangle &= \langle q(\tau_1)q(\tau_2) \rangle \langle q(\tau_3)q(\tau_4) \rangle + \langle q(\tau_1)q(\tau_3) \rangle \langle q(\tau_2)q(\tau_4) \rangle \\ &+ \langle q(\tau_1)q(\tau_4) \rangle \langle q(\tau_2)q(\tau_3) \rangle. \end{aligned} \quad (1.314)$$

Wick's theorem applies to any Gaussian probability measure and it is the basis of the perturbation theory of path integrals, as we will see in the next section.

Finally, it is useful to have an explicit expression for the propagator $G(\tau)$. This can be obtained in various ways, but it is easy to check by direct substitution that

$$G(\tau) = \frac{1}{2\omega} \frac{\cosh\left(\omega\left(|\tau| - \frac{u}{2}\right)\right)}{\sinh\left(\frac{\omega u}{2}\right)}, \quad 0 \leq \tau \leq u, \quad (1.315)$$

satisfies (1.299). It is also possible to work in the interval

$$-\frac{u}{2} \leq \tau \leq \frac{u}{2}. \quad (1.316)$$

In this interval, the propagator (1.315) can be approximated as $u \rightarrow \infty$ by

$$G_{\mathbb{R}}(\tau) = \frac{e^{-\omega|\tau|}}{2\omega}. \quad (1.317)$$

Example 1.7. According to the path integral arguments presented above, the quantity

$$\langle q(\tau)q(0) \rangle = \frac{1}{Z(\beta)} \text{Tr} \left\{ e^{-\frac{u\mathbf{H}}{\hbar}} T(\mathbf{q}_H(\tau)\mathbf{q}_H(0)) \right\} \quad (1.318)$$

is given by \hbar , times the propagator (1.315). Let us verify this with a calculation in conventional Quantum Mechanics. By taking into account the two possible cases for the time ordering, $\tau > 0$ or $\tau < 0$, we can write

$$\langle q(\tau)q(0) \rangle = \frac{1}{Z(\beta)} \text{Tr} \left\{ e^{\left(\frac{|\tau|}{\hbar} - \beta\right)\mathbf{H}} \mathbf{q} e^{-\frac{|\tau|}{\hbar}\mathbf{H}} \right\}. \quad (1.319)$$

We evaluate this trace in the basis of eigenvectors of \mathbf{H} , which we denote by $|n\rangle$, $n = 0, 1, 2, \dots$, which satisfy

$$\mathbf{H}|n\rangle = \hbar\omega \left(n + \frac{1}{2}\right) |n\rangle. \quad (1.320)$$

We obtain in this way

$$\langle q(\tau)q(0) \rangle = \frac{1}{Z(\beta)} \sum_{m,n=0}^{\infty} \exp\left(\left(|\tau| - \beta\hbar\right)\omega \left(n + \frac{1}{2}\right) - |\tau|\omega \left(m + \frac{1}{2}\right)\right) |\langle n|\mathbf{q}|m \rangle|^2. \quad (1.321)$$

It is an elementary result in Quantum Mechanics that

$$|\langle n|\mathbf{q}|m \rangle|^2 = \frac{\hbar}{2\omega} (m\delta_{n,m-1} + (m+1)\delta_{n,m+1}), \quad (1.322)$$

where we have set the mass equal to unity, as in (1.297). We conclude that

$$\begin{aligned}
\langle q(\tau)q(0) \rangle &= \frac{\hbar}{2\omega Z(\beta)} e^{-\beta\hbar\omega/2} \left\{ \sum_{n=0}^{\infty} (n+1) e^{-|\tau|\omega - \beta\hbar\omega n} + \sum_{m=0}^{\infty} (m+1) e^{|\tau|\omega - \beta\hbar\omega(m+1)} \right\} \\
&= \frac{\hbar}{2\omega Z(\beta)} \left\{ \frac{e^{-\omega|\tau|}}{(1 - e^{-\beta\hbar\omega})^2} + \frac{e^{\omega|\tau| - \beta\hbar\omega}}{(1 - e^{-\beta\hbar\omega})^2} \right\} \\
&= \frac{\hbar}{2\omega} \frac{\cosh\left(\omega\left(|\tau| - \frac{\beta\hbar}{2}\right)\right)}{\sinh\left(\frac{\omega\beta\hbar}{2}\right)},
\end{aligned} \tag{1.323}$$

where we have used the standard expression for $Z(\beta)$. This confirms the result obtained in (1.315) with path integral methods.

2 Second quantization

2.1 Identical particles

So far we have presented the path-integral formalism for a single particle. In the case of N identical particles, we have to take into account the symmetrization postulate of Quantum Mechanics. Let us first review this postulate.

Let \mathcal{H} be the Hilbert space of a single particle, and let

$$\{|\lambda\rangle\}_{\lambda \in \Lambda} \tag{2.1}$$

be an orthonormal basis of \mathcal{H} , where λ is an appropriate label. To construct the Hilbert space for N identical particles, we first consider the N -th tensor product

$$\mathcal{H}_N = \mathcal{H} \otimes \cdots \otimes \mathcal{H}. \tag{2.2}$$

An orthonormal basis for \mathcal{H}_N is given by the states of the form

$$|\lambda_1 \cdots \lambda_N\rangle = |\lambda_1\rangle \otimes \cdots \otimes |\lambda_N\rangle. \tag{2.3}$$

They satisfy the completeness relation

$$\sum_{\lambda_1, \dots, \lambda_N} |\lambda_1 \cdots \lambda_N\rangle \langle \lambda_1 \cdots \lambda_N| = \mathbf{1}. \tag{2.4}$$

Let us introduce the projection operator on totally (anti)symmetric states

$$P_\zeta = \frac{1}{N!} \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \hat{\sigma}, \tag{2.5}$$

where $\hat{\sigma}$ is the operator

$$\hat{\sigma} |\lambda_1 \cdots \lambda_N\rangle = |\lambda_{\sigma(1)} \cdots \lambda_{\sigma(N)}\rangle, \tag{2.6}$$

and

$$\zeta = \pm 1 \tag{2.7}$$

for bosons and fermions, respectively. This operator satisfies

$$P_\zeta^2 = P_\zeta. \quad (2.8)$$

(the proof of this property will be done in the exercise section). Then, the Hilbert space for a system of N bosons (respectively, fermions) is given by

$$\mathcal{B}_N = P_+ \mathcal{H}_N, \quad \mathcal{F}_N = P_- \mathcal{H}_N. \quad (2.9)$$

The appropriately (anti)symmetrized states

$$|\lambda_1 \cdots \lambda_N\rangle = \sqrt{N!} P_\zeta |\lambda_1 \cdots \lambda_N\rangle = \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} |\lambda_{\sigma(1)} \cdots \lambda_{\sigma(N)}\rangle \quad (2.10)$$

are a basis of the Hilbert space of bosons/fermions $\mathcal{B}_N, \mathcal{F}_N$. By applying P_ζ to (2.4), we find the resolution of the identity in $\mathcal{B}_N/\mathcal{F}_N$:

$$\frac{1}{N!} \sum_{\lambda_1, \dots, \lambda_N} |\lambda_1 \cdots \lambda_N\rangle \langle \lambda_1 \cdots \lambda_N| = \mathbf{1}. \quad (2.11)$$

A state $|\lambda_1 \cdots \lambda_N\rangle$ in \mathcal{B}/\mathcal{F} can be represented by a set of occupation numbers n_λ , indicating the number of particles which are in the state $\lambda \in \Lambda$. Clearly, in the case of fermions, we must have $n_\lambda = 0$ or 1.

Example 2.1. We now compute the overlap

$$\begin{aligned} \langle \lambda_1 \cdots \lambda_N | \mu_1 \cdots \mu_N \rangle &= \langle \lambda_1 \cdots \lambda_N | P_\zeta | \mu_1 \cdots \mu_N \rangle \\ &= \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \langle \lambda_1 | \mu_{\sigma(1)} \rangle \cdots \langle \lambda_N | \mu_{\sigma(N)} \rangle, \end{aligned} \quad (2.12)$$

where we used (2.8). Therefore, the overlap is different from zero only when μ_1, \dots, μ_N is a permutation σ of $\lambda_1, \dots, \lambda_N$, and one has

$$\langle \lambda_1 \cdots \lambda_N | \mu_1 \cdots \mu_N \rangle = \zeta^{\epsilon(\sigma)} \prod_{\lambda} n_\lambda!. \quad (2.13)$$

□

A *many-body operator* \mathbf{O} is an operator which is invariant under any permutation of the particles:

$$\langle \lambda_{\sigma(1)} \cdots \lambda_{\sigma(N)} | \mathbf{O} | \mu_{\sigma(1)} \cdots \mu_{\sigma(N)} \rangle = \langle \lambda_1 \cdots \lambda_N | \mathbf{O} | \mu_1 \cdots \mu_N \rangle. \quad (2.14)$$

In terms of the operator $\hat{\sigma}$ defined in (2.6), we have

$$\hat{\sigma} \mathbf{O} \hat{\sigma} = \mathbf{O}. \quad (2.15)$$

This implies that

$$P_\zeta \mathbf{O} = \mathbf{O} P_\zeta, \quad (2.16)$$

i.e.

$$[P_\zeta, \mathbf{O}] = 0. \quad (2.17)$$

To verify this, we show that their matrix elements agree:

$$\begin{aligned}
\langle \lambda_1 \cdots \lambda_N | \mathbf{O} \mathbf{P}_\zeta | \mu_1 \cdots \mu_N \rangle &= \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \langle \lambda_1 \cdots \lambda_N | \mathbf{O} \hat{\sigma} | \mu_1 \cdots \mu_N \rangle \\
&= \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \langle \lambda_1 \cdots \lambda_N | \hat{\sigma}^{-1} \mathbf{O} | \mu_1 \cdots \mu_N \rangle \\
&= \frac{1}{\sqrt{N!}} \sum_{\sigma^{-1} \in S_N} \zeta^{\epsilon(\sigma^{-1})} \langle \lambda_1 \cdots \lambda_N | \hat{\sigma}^{-1} \mathbf{O} | \mu_1 \cdots \mu_N \rangle \\
&= \langle \lambda_1 \cdots \lambda_N | \mathbf{P}_\zeta \mathbf{O} | \mu_1 \cdots \mu_N \rangle,
\end{aligned} \tag{2.18}$$

where we used that $\epsilon(\sigma^{-1}) = \epsilon(\sigma)$. The matrix elements of many-body operators in \mathcal{B}_N (or \mathcal{F}_N) can be computed as follows:

$$\begin{aligned}
\{ \lambda_1 \cdots \lambda_N | \mathbf{O} | \mu_1 \cdots \mu_N \} &= N! \langle \lambda_1 \cdots \lambda_N | \mathbf{P}_\zeta \mathbf{O} \mathbf{P}_\zeta | \mu_1 \cdots \mu_N \rangle \\
&= N! \langle \lambda_1 \cdots \lambda_N | \mathbf{P}_\zeta \mathbf{O} | \mu_1 \cdots \mu_N \rangle \\
&= \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \langle \lambda_{\sigma(1)} \cdots \lambda_{\sigma(N)} | \mathbf{O} | \mu_1 \cdots \mu_N \rangle,
\end{aligned} \tag{2.19}$$

where in going from the first to the second line we have used (2.16) and (2.8). We note that the Hamiltonian of a many-particle system \mathbf{H} should be a many-body operator.

In principle, one can use the above results to calculate the thermal properties of a many-particle system. Let us now compute e.g. the thermal partition function. Let $\{|n\rangle\}$ be an orthonormal basis of $\mathcal{B}_N, \mathcal{F}_N$. Then,

$$Z(\beta) = \text{Tr}_{\mathcal{B}_N, \mathcal{F}_N} e^{-\beta \mathbf{H}} = \sum_n \langle n | e^{-\beta \mathbf{H}} | n \rangle. \tag{2.20}$$

By using the resolution of the identity (2.11), we obtain

$$\begin{aligned}
Z(\beta) &= \frac{1}{N!} \sum_{\lambda_1, \dots, \lambda_N} \sum_n \langle n | \lambda_1 \cdots \lambda_N \rangle \{ \lambda_1 \cdots \lambda_N | e^{-\beta \mathbf{H}} | n \rangle \\
&= \frac{1}{N!} \sum_{\lambda_1 \cdots \lambda_N} \{ \lambda_1 \cdots \lambda_N | e^{-\beta \mathbf{H}} \sum_n | n \rangle \langle n | \lambda_1 \cdots \lambda_N \} \\
&= \frac{1}{N!} \sum_{\lambda_1 \cdots \lambda_N} \{ \lambda_1 \cdots \lambda_N | e^{-\beta \mathbf{H}} | \lambda_1 \cdots \lambda_N \} \\
&= \frac{1}{N!} \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \sum_{\lambda_1, \dots, \lambda_N} \langle \lambda_{\sigma(1)} \cdots \lambda_{\sigma(N)} | e^{-\beta \mathbf{H}} | \lambda_1 \cdots \lambda_N \rangle,
\end{aligned} \tag{2.21}$$

where we used (2.19) in the last line. In the position basis, and assuming that the Hamiltonian is of the standard form

$$\mathbf{H} = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} V(\mathbf{q}_i - \mathbf{q}_j), \tag{2.22}$$

this leads to the representation

$$Z(\beta) = \frac{1}{N!} \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \int_{\mathbf{q}_k(\beta) = \mathbf{q}_{\sigma(k)}(0)} \mathcal{D}\mathbf{q}_1 \cdots \mathcal{D}\mathbf{q}_N \cdot \exp \left\{ - \int_0^\beta d\tau \left[\sum_{i=1}^N \frac{m}{2} \dot{\mathbf{q}}_i^2(\tau) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{q}_i - \mathbf{q}_j) \right] \right\}. \quad (2.23)$$

Note that we integrate over trajectories where the endpoints are permutations of the initial points.

This is a nice formula but it is of little practical use. The sum over permutations makes the problem very complicated, and as we already know from elementary statistical mechanics, it is often more practical to consider a grand canonical ensemble where the number of particles is not fixed. To obtain a path integral formulation which incorporates these features, we need to introduce the formalism of second quantization and coherent states.

2.2 Second quantization

The basic idea of second quantization is to represent states in terms of occupation numbers. Different states can then be related to each other by creation and annihilation operators, which increase (respectively, decrease) the occupation number. One immediate consequence of this perspective is that the total number of particles can not be fixed, and we have to work in the total Hilbert space

$$\mathcal{B} = \bigoplus_{N=0}^{\infty} \mathcal{B}_N, \quad \mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{F}_N. \quad (2.24)$$

The resolution of identity in this space is now

$$\sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1, \dots, \lambda_N} |\lambda_1, \dots, \lambda_N\rangle \langle \lambda_1, \dots, \lambda_N| = \mathbf{1}. \quad (2.25)$$

Let us now introduce the creation operators \mathbf{a}_λ associated to the basis $\{|\lambda\rangle\}_{\lambda \in \Lambda}$. They act as follows,

$$\mathbf{a}_\lambda^\dagger |\lambda_1 \cdots \lambda_N\rangle = |\lambda \lambda_1 \cdots \lambda_N\rangle. \quad (2.26)$$

We have that

$$\begin{aligned} \mathbf{a}_\lambda^\dagger \mathbf{a}_\mu^\dagger |\lambda_1 \cdots \lambda_N\rangle &= |\lambda \mu \lambda_1 \cdots \lambda_N\rangle \\ &= \zeta |\mu \lambda \lambda_1 \cdots \lambda_N\rangle \\ &= \zeta \mathbf{a}_\mu^\dagger \mathbf{a}_\lambda^\dagger |\lambda_1 \cdots \lambda_N\rangle. \end{aligned} \quad (2.27)$$

We conclude that creation operators satisfy the (anti)commutation relations

$$[\mathbf{a}_\lambda^\dagger, \mathbf{a}_\mu^\dagger]_\zeta = 0, \quad (2.28)$$

where the subscript ζ denotes commutator for $\zeta = 1$ and anti-commutator for $\zeta = -1$.

The annihilation operators \mathbf{a}_λ are simply the adjoints of the creation operators. Their action can be obtained as follows,

$$\begin{aligned} \mathbf{a}_\lambda |\lambda_1 \cdots \lambda_N\rangle &= \sum_{M=0}^{\infty} \frac{1}{M!} \sum_{\mu_1, \dots, \mu_M} \{\mu_1 \cdots \mu_M | \mathbf{a}_\lambda |\lambda_1 \cdots \lambda_N\rangle | \mu_1 \cdots \mu_M\rangle \\ &= \sum_{M=0}^{\infty} \frac{1}{M!} \sum_{\mu_1, \dots, \mu_M} \{\lambda \mu_1 \cdots \mu_M | \lambda_1 \cdots \lambda_N\rangle | \mu_1 \cdots \mu_M\rangle. \end{aligned} \quad (2.29)$$

This can be evaluated with (2.12). In the sum over M , only the states where $M = N - 1$ contribute, and in addition $\lambda, \mu_1, \dots, \mu_{N-1}$ should be a permutation of the $\lambda_1, \dots, \lambda_N$:

$$\begin{aligned} \mathbf{a}_\lambda |\lambda_1 \cdots \lambda_N\rangle &= \frac{1}{(N-1)!} \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \langle \lambda | \lambda_{\sigma(1)} \rangle \langle \mu_1 | \lambda_{\sigma(2)} \rangle \cdots \langle \mu_{N-1} | \lambda_{\sigma(N)} \rangle |\mu_1 \cdots \mu_{N-1}\rangle \\ &= \frac{1}{(N-1)!} \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} |\lambda_{\sigma(2)} \cdots \lambda_{\sigma(N)}\rangle. \end{aligned} \quad (2.30)$$

To evaluate this, we use the fact that

$$|\lambda_{\sigma(2)} \cdots \lambda_{\sigma(N)}\rangle = \zeta^{\epsilon(\tau)} \left| \lambda_1 \cdots \hat{\lambda}_i \cdots \lambda_{\sigma(N)} \right\rangle, \quad (2.31)$$

where $i = \sigma(1)$ and, as usual, the hat indicates that the element is not there. Here, τ is the permutation of $N - 1$ elements

$$\tau = \begin{pmatrix} \sigma(2) & \cdots & \sigma(i) & \sigma(i+1) & \cdots & \sigma(N) \\ 1 & \cdots & i-1 & i+1 & \cdots & N \end{pmatrix}. \quad (2.32)$$

The signature of this permutation is identical to the signature of the permutation

$$\sigma' = \begin{pmatrix} \sigma(1) & \sigma(2) & \cdots & \sigma(i) & \sigma(i+1) & \cdots & \sigma(N) \\ \sigma(1) & 1 & \cdots & i-1 & i+1 & \cdots & N \end{pmatrix}, \quad (2.33)$$

which can be obtained as the composition of the permutation

$$\sigma^{-1} = \begin{pmatrix} \sigma(1) & \sigma(2) & \cdots & \sigma(i) & \sigma(i+1) & \cdots & \sigma(N) \\ 1 & 2 & \cdots & \sigma(1) & i+1 & \cdots & N \end{pmatrix} \quad (2.34)$$

and the permutation

$$\begin{pmatrix} 1 & 2 & \cdots & \sigma(1) & i+1 & \cdots & N \\ \sigma(1) & 1 & \cdots & i-1 & i+1 & \cdots & N \end{pmatrix}. \quad (2.35)$$

This last permutation can be decomposed in $i - 1$ transpositions, so its signature is

$$\zeta^{i-1}. \quad (2.36)$$

It follows that

$$\zeta^{\epsilon(\sigma)+\sigma(\tau)} = \zeta^{i-1} \quad (2.37)$$

and finally

$$\mathbf{a}_\lambda |\lambda_1 \cdots \lambda_N\rangle = \sum_{i=1}^N \zeta^{i-1} \delta_{\lambda\lambda_i} \left| \lambda_1 \cdots \hat{\lambda}_i \cdots \lambda_N \right\rangle. \quad (2.38)$$

Let us now evaluate the (anti)commutator of \mathbf{a}_λ and \mathbf{a}_μ^\dagger . We have

$$\mathbf{a}_\lambda \mathbf{a}_\mu^\dagger |\alpha_1 \cdots \alpha_N\rangle = \mathbf{a}_\lambda |\mu\alpha_1 \cdots \alpha_N\rangle = \delta_{\lambda\mu} |\alpha_1 \cdots \alpha_N\rangle + \sum_{i=1}^N \zeta^i \delta_{\lambda\alpha_i} |\mu\alpha_1 \cdots \hat{\alpha}_i \cdots \alpha_N\rangle. \quad (2.39)$$

On the other hand,

$$\mathbf{a}_\mu^\dagger \mathbf{a}_\lambda |\alpha_1 \cdots \alpha_N\rangle = \mathbf{a}_\mu^\dagger \sum_{i=1}^N \zeta^{i-1} \delta_{\lambda\alpha_i} |\alpha_1 \cdots \hat{\alpha}_i \cdots \alpha_N\rangle = \sum_{i=1}^N \zeta^{i-1} \delta_{\lambda\alpha_i} |\mu\alpha_1 \cdots \hat{\alpha}_i \cdots \alpha_N\rangle. \quad (2.40)$$

We conclude that

$$\mathbf{a}_\lambda \mathbf{a}_\mu^\dagger |\alpha_1 \cdots \alpha_N\rangle = (\delta_{\lambda\mu} + \zeta \mathbf{a}_\mu^\dagger \mathbf{a}_\lambda) |\alpha_1 \cdots \alpha_N\rangle. \quad (2.41)$$

Therefore,

$$[\mathbf{a}_\lambda, \mathbf{a}_\mu^\dagger]_{-\zeta} = \delta_{\lambda\mu}. \quad (2.42)$$

Example 2.2. The *number operator* n_λ is defined by

$$\mathbf{n}_\lambda = \mathbf{a}_\lambda^\dagger \mathbf{a}_\lambda. \quad (2.43)$$

It acts as follows:

$$\begin{aligned} n_\lambda |\lambda_1 \cdots \lambda_N\rangle &= \mathbf{a}_\lambda^\dagger \mathbf{a}_\lambda |\lambda_1 \cdots \lambda_N\rangle = \sum_{i=1}^N \zeta^{i-1} \delta_{\lambda\alpha_i} |\lambda\alpha_1 \cdots \hat{\alpha}_i \cdots \alpha_N\rangle \\ &= \sum_{i=1}^N \delta_{\lambda\alpha_i} |\alpha_1 \cdots \alpha_i \cdots \alpha_N\rangle, \end{aligned} \quad (2.44)$$

where we used (2.40). The eigenvalue of n_λ ,

$$n_\lambda = \sum_{i=1}^N \delta_{\lambda\alpha_i}, \quad (2.45)$$

is the number of particles in the state λ in the multi-particle state $|\alpha_1 \cdots \alpha_i \cdots \alpha_N\rangle$.

Example 2.3. We will define normalized states in the occupation number representation as

$$|n_{\lambda_1} n_{\lambda_2} \cdots\rangle = \frac{1}{\prod_{\lambda_i} \sqrt{n_{\lambda_i}!}} |\lambda_1 \cdots\rangle, \quad (2.46)$$

where n_{λ_i} is the number of particles in the state λ_i . For bosons, we have

$$\begin{aligned} \mathbf{a}_\lambda^\dagger |n_{\lambda_1} n_{\lambda_2} \cdots\rangle &= \sqrt{n_\lambda + 1} |n_{\lambda_1} n_{\lambda_2} \cdots n_\lambda + 1 \cdots\rangle, \\ \mathbf{a}_\lambda |n_{\lambda_1} n_{\lambda_2} \cdots\rangle &= \sqrt{n_\lambda} |n_{\lambda_1} n_{\lambda_2} \cdots n_\lambda - 1 \cdots\rangle. \end{aligned} \quad (2.47)$$

□

We finally study the behavior of the creation and annihilation operators under a change of basis. Let $\{|\tilde{\lambda}\rangle\}_{\tilde{\lambda} \in \tilde{\Lambda}}$ a different orthonormal basis of \mathcal{H} , which is related to the basis $\{|\lambda\rangle\}_{\lambda \in \Lambda}$ by the usual formula

$$|\tilde{\lambda}\rangle = \sum_{\lambda} \langle \lambda | \tilde{\lambda} \rangle |\lambda\rangle. \quad (2.48)$$

Let $\mathbf{a}_\lambda^\dagger$ the corresponding creation operator. We have

$$\begin{aligned} \mathbf{a}_\lambda^\dagger |\tilde{\lambda}_1 \cdots \tilde{\lambda}_N\rangle &= |\tilde{\lambda} \tilde{\lambda}_1 \cdots \tilde{\lambda}_N\rangle \\ &= \sum_{\lambda} \langle \lambda | \tilde{\lambda} \rangle |\lambda \tilde{\lambda}_1 \cdots \tilde{\lambda}_N\rangle \\ &= \sum_{\lambda} \langle \lambda | \tilde{\lambda} \rangle \mathbf{a}_\lambda^\dagger |\tilde{\lambda}_1 \cdots \tilde{\lambda}_N\rangle, \end{aligned} \quad (2.49)$$

so we conclude that

$$\mathbf{a}_\lambda^\dagger = \sum_\lambda \langle \lambda | \tilde{\lambda} \rangle \mathbf{a}_\lambda^\dagger. \quad (2.50)$$

By taking the hermitian conjugate, we deduce that

$$\mathbf{a}_{\tilde{\lambda}} = \sum_\lambda \langle \tilde{\lambda} | \lambda \rangle \mathbf{a}_\lambda. \quad (2.51)$$

Example 2.4. An important basis of delta-orthonormal states for a particle in d dimensions is $|\mathbf{x}\rangle$, and the corresponding creation/annihilation operators are denoted by

$$\hat{\psi}^\dagger(\mathbf{x}), \quad \hat{\psi}(\mathbf{x}). \quad (2.52)$$

satisfying the (anti)commutation relation,

$$[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})]_\zeta = \delta(\mathbf{x} - \mathbf{y}). \quad (2.53)$$

Let us now consider a basis $\{|\lambda\rangle\}$ (this can be e.g. eigenstates of a one-particle Hamiltonian). Then, we have

$$\begin{aligned} \hat{\psi}^\dagger(\mathbf{x}) &= \sum_\lambda \langle \lambda | \mathbf{x} \rangle \mathbf{a}_\lambda^\dagger = \sum_\lambda \psi_\lambda^*(\mathbf{x}) \mathbf{a}_\lambda^\dagger, \\ \hat{\psi}(\mathbf{x}) &= \sum_\lambda \langle \mathbf{x} | \lambda \rangle \mathbf{a}_\lambda = \sum_\lambda \psi_\lambda(\mathbf{x}) \mathbf{a}_\lambda. \end{aligned} \quad (2.54)$$

An important basis for translationally-invariant systems is the momentum basis. We have in this case

$$\begin{aligned} \hat{\psi}^\dagger(\mathbf{x}) &= \int_{\mathbb{R}^d} d\mathbf{k} \langle \mathbf{k} | \mathbf{x} \rangle \mathbf{a}_\mathbf{k}^\dagger = \int d\mathbf{k} \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{d/2}} \mathbf{a}_\mathbf{k}^\dagger, \\ \hat{\psi}(\mathbf{x}) &= \int_{\mathbb{R}^d} d\mathbf{k} \langle \mathbf{x} | \mathbf{k} \rangle \mathbf{a}_\mathbf{k} = \int_{\mathbb{R}^d} d\mathbf{k} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{d/2}} \mathbf{a}_\mathbf{k}. \end{aligned} \quad (2.55)$$

where we used

$$\langle \mathbf{x} | \mathbf{k} \rangle = \frac{1}{(2\pi)^{d/2}} e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (2.56)$$

As in [1], we will also introduce annihilation/creation operators in the momentum basis defined by

$$\psi(\mathbf{x}) = \int \frac{d^d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}\cdot\mathbf{x}} \mathbf{c}_\mathbf{k}, \quad \psi^\dagger(\mathbf{x}) = \int \frac{d^d\mathbf{k}}{(2\pi)^d} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathbf{c}_\mathbf{k}^\dagger, \quad (2.57)$$

i.e. we have

$$\mathbf{a}_\mathbf{k} = \frac{1}{(2\pi)^{d/2}} \mathbf{c}_\mathbf{k}. \quad (2.58)$$

It is often useful to discretize the momentum by putting the particles in a box. In that case, a useful basis is the momentum representation, with wavefunction

$$\langle \mathbf{x} | \mathbf{k} \rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (2.59)$$

and we have

$$\begin{aligned} \hat{\psi}^\dagger(\mathbf{x}) &= \sum_{\mathbf{k}} \langle \mathbf{k} | \mathbf{x} \rangle \mathbf{a}_\mathbf{k}^\dagger = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathbf{a}_\mathbf{k}^\dagger, \\ \hat{\psi}(\mathbf{x}) &= \sum_{\mathbf{k}} \langle \mathbf{x} | \mathbf{k} \rangle \mathbf{a}_\mathbf{k} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \mathbf{a}_\mathbf{k}. \end{aligned} \quad (2.60)$$

Example 2.5. The Schrödinger representation of a many-body state is defined by

$$\Psi(x_1, \dots, x_N, t) = \{x_1 \cdots x_N | \Psi(t)\rangle = \langle 0 | \psi(x_1) \cdots \psi(x_N) | \Psi(t)\rangle. \quad (2.61)$$

As an example, consider the state

$$|\Psi\rangle = \psi_{p_2}^\dagger \psi_{p_1}^\dagger |0\rangle. \quad (2.62)$$

Then,

$$\Psi(x_1, x_2) = \{x_1, x_2 | \Psi\rangle = \langle 0 | \psi(x_1) \psi(x_2) \psi_{p_2}^\dagger \psi_{p_1}^\dagger |0\rangle \quad (2.63)$$

To calculate this, we move the destruction operators to the right. When doing this, we pick anticommutators. We have

$$\{\psi(x), \psi_p^\dagger\} = \langle x | p \rangle. \quad (2.64)$$

This can be regarded as a contraction, and then we can calculate the vev above by using Wick's theorem,

$$\begin{aligned} \langle 0 | \psi(x_1) \psi(x_2) \psi_{p_2}^\dagger \psi_{p_1}^\dagger |0\rangle &= \overbrace{\psi(x_1) \psi(x_2) \psi_{p_2}^\dagger \psi_{p_1}^\dagger} - \overbrace{\psi(x_1) \psi(x_2) \psi_{p_2}^\dagger \psi_{p_1}^\dagger} \\ &= \langle x_1 | p_1 \rangle \langle x_2 | p_2 \rangle - \langle x_1 | p_2 \rangle \langle x_2 | p_1 \rangle. \end{aligned} \quad (2.65)$$

□

2.3 Operators in second-quantized form

A k -body operator is a many-body operator which acts on a state of \mathcal{H}_N as follows,

$$\mathcal{O} |\lambda_1 \cdots \lambda_N\rangle = \frac{1}{k!} \sum_{1 \leq i_1 \neq \dots \neq i_k \leq N} \mathcal{O}_{i_1 \dots i_k} |\lambda_1 \cdots \lambda_N\rangle \quad (2.66)$$

where the operator $\mathcal{O}_{i_1 \dots i_k}$ only acts on the particles i_1, \dots, i_k . For example, for a *one-body operator* we simply have

$$\mathcal{O} |\lambda_1 \cdots \lambda_N\rangle = \sum_{i=1}^N \mathcal{O}_i |\lambda_1 \cdots \lambda_N\rangle, \quad (2.67)$$

where

$$\mathcal{O}_i |\lambda_1 \cdots \lambda_N\rangle = |\lambda_1\rangle \otimes \cdots \otimes (\mathcal{O}_i |\lambda_i\rangle) \otimes \cdots \otimes |\lambda_N\rangle. \quad (2.68)$$

Indeed, a typical one-body operator is of the form

$$\mathcal{O} = \sum_{i=1}^N \mathcal{O}^{(i)}, \quad (2.69)$$

where $\mathcal{O}^{(i)}$ are copies of the same operator \mathcal{O}_1 but acting on the i -th factor of \mathcal{H}_N .

For two-body operators we have

$$\mathcal{O} |\lambda_1 \cdots \lambda_N\rangle = \frac{1}{2} \sum_{i \neq j} \mathcal{O}_{ij} |\lambda_1 \cdots \lambda_N\rangle = \sum_{i < j} \mathcal{O}_{ij} |\lambda_1 \cdots \lambda_N\rangle. \quad (2.70)$$

We will assume, as we have done here, that two-body operators satisfy the symmetry property $\mathcal{O}_{ij} = \mathcal{O}_{ji}$.

Many-body operators can be always written as sums of products of creation/annihilation operators. Let us illustrate this in detail by considering one and two-body operators.

Let \mathbf{O} be a one-body operator. Let us consider the orthonormal basis of this operator (when $N = 1$):

$$\mathbf{O}|\lambda\rangle = O_\lambda|\lambda\rangle, \quad O_\lambda = \langle\lambda|\mathbf{O}|\lambda\rangle. \quad (2.71)$$

Let us consider an arbitrary matrix element of this operator. By using (2.19), we find

$$\begin{aligned} \{\lambda_1 \cdots \lambda_N | \mathbf{O} | \mu_1 \cdots \mu_N \} &= \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \langle \lambda_{\sigma(1)} \cdots \lambda_{\sigma(N)} | \mathbf{O} | \mu_1 \cdots \mu_N \rangle \\ &= \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \sum_{i=1}^N \prod_{k \neq i} \langle \lambda_{\sigma(k)} | \mu_k \rangle \langle \lambda_{\sigma(i)} | \mathbf{O} | \mu_i \rangle \\ &= \left(\sum_{i=1}^N O_{\mu_i} \right) \{\lambda_1 \cdots \lambda_N | \mu_1 \cdots \mu_N \} \end{aligned} \quad (2.72)$$

On the other hand,

$$\sum_{\lambda} O_\lambda n_\lambda | \mu_1 \cdots \mu_N \rangle = \sum_{\lambda} O_\lambda \sum_{i=1}^N \delta_{\lambda \mu_i} | \mu_1 \cdots \mu_N \rangle = \left(\sum_{i=1}^N O_{\mu_i} \right) | \mu_1 \cdots \mu_N \rangle. \quad (2.73)$$

We conclude that

$$\mathbf{O} = \sum_{\lambda} \langle \lambda | \mathbf{O} | \lambda \rangle a_\lambda^\dagger a_\lambda \quad (2.74)$$

since they have the same matrix elements. To transform to an arbitrary basis $\{|\alpha\rangle\}$, we use the transformation rules (2.50), (2.51) to write

$$\begin{aligned} \mathbf{O} &= \sum_{\lambda} \sum_{\alpha, \beta} \langle \lambda | \mathbf{O} | \lambda \rangle \langle \alpha | \lambda \rangle \langle \lambda | \beta \rangle a_\alpha^\dagger a_\beta \\ &= \sum_{\alpha, \beta} \langle \alpha | \mathbf{O} | \beta \rangle a_\alpha^\dagger a_\beta. \end{aligned} \quad (2.75)$$

We will now consider two-body operators. Let \mathbf{V} be a two-body operator. We consider again an orthonormal basis of this operator (when $N = 2$):

$$\mathbf{V}|\lambda\mu\rangle = V_{\lambda\mu}|\lambda\mu\rangle, \quad V_{\lambda\mu} = \langle\lambda\mu|\mathbf{V}|\lambda\mu\rangle. \quad (2.76)$$

Let us consider an arbitrary matrix element of this operator. By using (2.19), we find

$$\begin{aligned} \{\lambda_1 \cdots \lambda_N | \mathbf{V} | \mu_1 \cdots \mu_N \} &= \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \langle \lambda_{\sigma(1)} \cdots \lambda_{\sigma(N)} | \mathbf{V} | \mu_1 \cdots \mu_N \rangle \\ &= \sum_{\sigma \in S_N} \zeta^{\epsilon(\sigma)} \frac{1}{2} \sum_{i \neq j} \prod_{k \neq i, j} \langle \lambda_{\sigma(k)} | \mu_k \rangle \langle \lambda_{\sigma(i)} \lambda_{\sigma(j)} | \mathbf{V} | \mu_i \mu_j \rangle \\ &= \left(\frac{1}{2} \sum_{i \neq j} V_{\mu_i \mu_j} \right) \{\lambda_1 \cdots \lambda_N | \mu_1 \cdots \mu_N \} \end{aligned} \quad (2.77)$$

The overall factor is a sum over all different pairs of particles in the state $|\mu_1 \cdots \mu_N\rangle$. To reproduce this factor, we need an operator $\mathbf{P}_{\lambda\mu}$ which counts the number of pairs of particles in the states λ and μ . If $\lambda \neq \mu$, there are $n_\lambda n_\mu$ pairs, while if $\lambda = \mu$, there are $n_\lambda(n_\lambda - 1)$. Therefore,

$$\mathbf{P}_{\lambda\mu} = n_\lambda n_\mu - \delta_{\lambda\mu} n_\lambda. \quad (2.78)$$

This can be written as

$$P_{\lambda\mu} = a_\lambda^\dagger a_\lambda a_\mu^\dagger a_\mu - \delta_{\lambda\mu} a_\lambda^\dagger a_\lambda = \zeta a_\lambda^\dagger a_\mu^\dagger a_\lambda a_\mu = a_\lambda^\dagger a_\mu^\dagger a_\mu a_\lambda \quad (2.79)$$

We conclude that

$$V = \frac{1}{2} \sum_{\lambda\mu} \langle \lambda\mu | V | \lambda\mu \rangle P_{\lambda\mu} = \frac{1}{2} \sum_{\lambda\mu} \langle \lambda\mu | V | \lambda\mu \rangle a_\lambda^\dagger a_\mu^\dagger a_\mu a_\lambda \quad (2.80)$$

since they have the same matrix elements. To transform to an arbitrary basis $\{|\alpha\rangle\}$, we use the transformation rules (2.50), (2.51) to write

$$V = \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma. \quad (2.81)$$

Remark 2.6. These results can be generalized to a k -body operator, which is written, in terms of creation and annihilation operators, as

$$O = \frac{1}{k!} \sum_{\lambda_1 \dots \lambda_k} \sum_{\mu_1 \dots \mu_k} \langle \lambda_1 \dots \lambda_k | O | \mu_1 \dots \mu_k \rangle a_{\lambda_1}^\dagger \dots a_{\lambda_k}^\dagger a_{\mu_k} \dots a_{\mu_1}. \quad (2.82)$$

Example 2.7. *Kinetic energy.* An important one-body operator is the kinetic energy,

$$T = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m}. \quad (2.83)$$

In terms of the operators $\hat{\psi}(\mathbf{x})$, this is given by

$$T = -\frac{\hbar^2}{2m} \int_{\mathbb{R}^d} d\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \nabla^2 \hat{\psi}(\mathbf{x}). \quad (2.84)$$

In the momentum basis, this is

$$T = \int_{\mathbb{R}^d} d\mathbf{p} \frac{\mathbf{p}^2}{2m} a_{\mathbf{p}}^\dagger a_{\mathbf{p}}. \quad (2.85)$$

For particles with spin σ in a box, we have

$$T = \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2m} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}. \quad (2.86)$$

□

Example 2.8. *Two-body interaction.* We say that a two-body interaction U is *local*, or velocity independent, when it is diagonal in position space,

$$\langle \mathbf{x}_1 \mathbf{x}_2 | U | \mathbf{x}_3 \mathbf{x}_4 \rangle = \delta(\mathbf{x}_1 - \mathbf{x}_3) \delta(\mathbf{x}_2 - \mathbf{x}_4) U(\mathbf{x}_1 - \mathbf{x}_2). \quad (2.87)$$

We will also assume that U is spin-independent. Let us write a local two-body interaction in terms of creation and annihilation operators. We have

$$\begin{aligned} U &= \frac{1}{2} \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 d\mathbf{x}_4 \langle \mathbf{x}_1 \mathbf{x}_2 | V | \mathbf{x}_3 \mathbf{x}_4 \rangle \hat{\psi}^\dagger(\mathbf{x}_1) \hat{\psi}^\dagger(\mathbf{x}_2) \hat{\psi}(\mathbf{x}_4) \hat{\psi}(\mathbf{x}_3) \\ &= \frac{1}{2} \int d\mathbf{x} d\mathbf{x}' U(\mathbf{x} - \mathbf{x}') \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}') \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x}). \end{aligned} \quad (2.88)$$

It is useful to write the operator in momentum space. We find, after changing variables to center of mass and relative position,

$$\mathbf{R} = \frac{\mathbf{x} + \mathbf{x}'}{2}, \quad \mathbf{r} = \mathbf{x} - \mathbf{x}', \quad (2.89)$$

the following integral

$$\begin{aligned} & \frac{1}{2} \int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_3 d\mathbf{p}_4 \int d\mathbf{R} \exp[i\mathbf{R} \cdot (-\mathbf{p}_1 - \mathbf{p}_2 + \mathbf{p}_3 + \mathbf{p}_4)] \\ & \cdot \int \frac{d\mathbf{r}}{(2\pi)^{4d}} U(\mathbf{r}) \exp\left[i\mathbf{r} \cdot \frac{-\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3 + \mathbf{p}_4}{2}\right] c_{\mathbf{p}_1}^\dagger c_{\mathbf{p}_2}^\dagger c_{\mathbf{p}_3} c_{\mathbf{p}_4}, \end{aligned} \quad (2.90)$$

where the operators $c_{\mathbf{p}}$ were defined in (2.57). The integration over the center of mass leads to a delta function. It is useful to parametrize the independent momenta as

$$\mathbf{p}_1 = \mathbf{k}_1 + \mathbf{q}, \quad \mathbf{p}_2 = \mathbf{k}_2 - \mathbf{q}, \quad \mathbf{p}_3 = \mathbf{k}_2, \quad \mathbf{p}_4 = \mathbf{k}_1, \quad (2.91)$$

and we introduce

$$\widehat{U}(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{q} \cdot \mathbf{r}} U(\mathbf{r}), \quad (2.92)$$

with inverse

$$U(\mathbf{r}) = \int \frac{d\mathbf{q}}{(2\pi)^d} e^{i\mathbf{q} \cdot \mathbf{r}} \widehat{U}(\mathbf{q}), \quad (2.93)$$

so that the two-body interaction becomes

$$U = \frac{1}{2} \int \frac{d^d \mathbf{k}_1 d^d \mathbf{k}_2 d^d \mathbf{q}}{(2\pi)^{3d}} \widehat{U}(\mathbf{q}) c_{\mathbf{k}_1 + \mathbf{q}}^\dagger c_{\mathbf{k}_2 - \mathbf{q}}^\dagger c_{\mathbf{k}_2} c_{\mathbf{k}_1}. \quad (2.94)$$

It is also useful to add “spin” or “color” labels $\alpha = 1, \dots, N$:

$$U = \frac{1}{2} \int \frac{d^d \mathbf{k}_1 d^d \mathbf{k}_2 d^d \mathbf{q}}{(2\pi)^{3d}} \widehat{U}(\mathbf{q}) c_{\mathbf{k}_1 + \mathbf{q}\alpha}^\dagger c_{\mathbf{k}_2 - \mathbf{q}\beta}^\dagger c_{\mathbf{k}_2\beta} c_{\mathbf{k}_1\alpha}. \quad (2.95)$$

It is often convenient to work in finite volume. We can write the interaction directly in momentum space:

$$U = \frac{1}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \langle \mathbf{k}_1 \mathbf{k}_2 | U | \mathbf{k}_3 \mathbf{k}_4 \rangle a_{\mathbf{k}_1\sigma_1}^\dagger a_{\mathbf{k}_2\sigma_2}^\dagger a_{\mathbf{k}_4\sigma_2} a_{\mathbf{k}_3\sigma_1}, \quad (2.96)$$

where

$$\langle \mathbf{k}_1 \mathbf{k}_2 | U | \mathbf{k}_3 \mathbf{k}_4 \rangle = \frac{1}{V^2} \int d\mathbf{x} d\mathbf{y} e^{-i(\mathbf{x} \cdot \mathbf{k}_1 + \mathbf{y} \cdot \mathbf{k}_2)} U(\mathbf{x} - \mathbf{y}) e^{i(\mathbf{x} \cdot \mathbf{k}_3 + \mathbf{y} \cdot \mathbf{k}_4)}. \quad (2.97)$$

After the change of variables $\mathbf{z} = \mathbf{x} - \mathbf{y}$, $\mathbf{v} = \mathbf{y}$, we find

$$\begin{aligned} \langle \mathbf{k}_1 \mathbf{k}_2 | U | \mathbf{k}_3 \mathbf{k}_4 \rangle &= \frac{1}{V^2} \int d\mathbf{v} e^{i(\mathbf{k}_4 + \mathbf{k}_3 - \mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{v}} \int d\mathbf{z} U(\mathbf{z}) e^{i(\mathbf{k}_3 - \mathbf{k}_1) \cdot \mathbf{z}} \\ &= \frac{1}{V} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \widehat{U}(\mathbf{k}_1 - \mathbf{k}_3), \end{aligned} \quad (2.98)$$

where we have defined $\widehat{U}(\mathbf{q})$ as in (2.92). We now set $\mathbf{k}_1 - \mathbf{k}_3 = \mathbf{q}$ and relabel $\mathbf{k}_3 \rightarrow \mathbf{k}_1$, $\mathbf{k}_4 \rightarrow \mathbf{k}_2$, to obtain

$$U = \frac{1}{2V} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}} \widehat{V}(\mathbf{q}) a_{\mathbf{k}_1 + \mathbf{q}\alpha}^\dagger a_{\mathbf{k}_2 - \mathbf{q}\beta}^\dagger a_{\mathbf{k}_2\beta} a_{\mathbf{k}_1\alpha}. \quad (2.99)$$

□

Example 2.9. *Fourier transform of the Coulomb potential.* In the case of a potential with spherical symmetry in three dimensions, the Fourier transform reads

$$V(\mathbf{q}) = 2\pi \int_0^\infty r^2 dr V(r) \int_0^\pi e^{-iqr \cosh \theta} \sin \theta d\theta. \quad (2.100)$$

Since

$$\int_0^\pi e^{-iqr \cosh \theta} \sin \theta d\theta = \frac{2 \sin(qr)}{qr}, \quad (2.101)$$

we find

$$V(\mathbf{q}) = 4\pi \int_0^\infty r^2 V(r) \frac{\sin(qr)}{qr} dr. \quad (2.102)$$

We consider a Yukawa-type potential

$$V(r) = \frac{e^2}{4\pi\epsilon_0} \frac{e^{-\lambda r}}{r}. \quad (2.103)$$

Performing the above integral one finds,

$$V(r) = \frac{e^2}{\epsilon_0} \frac{1}{q^2 + \lambda^2}. \quad (2.104)$$

In the limit $\lambda \rightarrow 0$, we obtain the Fourier transform of the Coulomb potential

$$V(q) = \frac{e^2}{q^2 \epsilon_0}. \quad (2.105)$$

□

Example 2.10. Let us calculate

$$\hat{\psi}^\dagger(x) \hat{\psi}(y) |\lambda_1 \cdots \lambda_N\rangle, \quad (2.106)$$

where λ_i , $i = 1, 2, \dots$ label eigenstates of the one-particle Hamiltonian (we can for example consider fermions in a box or in a trapped potential). Let $\psi_i(x)$ be the corresponding eigenfunctions of the one-particle Hamiltonian. Using (2.29) we can write (2.106) as

$$\begin{aligned} \sum_{i=1}^{\infty} \sum_{j=1}^N \zeta^j \psi_i^*(x) \psi_j(y) |\lambda_i \lambda_1 \cdots \hat{\lambda}_j \cdots \lambda_N\rangle &= C(x, y) |\lambda_1 \cdots \lambda_N\rangle \\ + \sum_{i=N+1}^{\infty} \sum_{j=1}^N \zeta^{j+N-1} \psi_i^*(x) \psi_j(y) |\lambda_1 \cdots \hat{\lambda}_j \cdots \lambda_N \lambda_i\rangle, \end{aligned} \quad (2.107)$$

where

$$C(x, y) = \sum_{i=1}^N \psi_i^*(x) \psi_i(y). \quad (2.108)$$

We conclude that

$$\hat{\psi}^\dagger(x) \hat{\psi}(y) |\lambda_1 \cdots \lambda_N\rangle = C(x, y) |\lambda_1 \cdots \lambda_N\rangle + \sum_{i=N+1}^{\infty} \sum_{j=1}^N \zeta^{j+N-1} \psi_i^*(x) \psi_j(y) |\lambda_1 \cdots \hat{\lambda}_j \cdots \lambda_N \lambda_i\rangle. \quad (2.109)$$

In the first line of (2.107) we have used the fact that, if $1 \leq i \leq N$, then it must be equal to the index j . Using this result, we compute

$$\{\lambda_1 \cdots \lambda_N | \hat{\psi}^\dagger(x) \hat{\psi}(y) | \lambda_1 \cdots \lambda_N \} = C(x, y). \quad (2.110)$$

We can also compute vevs of products of the density operator in the ground state,

$$\hat{n}(x) = \hat{\psi}^\dagger(x) \hat{\psi}(x). \quad (2.111)$$

Clearly,

$$\langle \hat{n}(x) \rangle = C(x, x). \quad (2.112)$$

Let us now compute

$$\langle \hat{n}(x) \hat{n}(y) \rangle = \{\lambda_1 \cdots \lambda_N | \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}^\dagger(y) \hat{\psi}(y) | \lambda_1 \cdots \lambda_N \}. \quad (2.113)$$

Using (2.109) twice we find

$$\begin{aligned} \hat{\psi}^\dagger(y) \hat{\psi}(y) | \lambda_1 \cdots \lambda_N \} &= C(y, y) | \lambda_1 \cdots \lambda_N \} + \sum_{i=N+1}^{\infty} \sum_{j=1}^N \zeta^{j+N-1} \psi_i^*(y) \psi_j(y) | \lambda_1 \cdots \hat{\lambda}_j \cdots \lambda_N \lambda_i \}, \\ \{\lambda_1 \cdots \lambda_N | \hat{\psi}^\dagger(x) \hat{\psi}(x) &= C(x, x) \{\lambda_1 \cdots \lambda_N | + \sum_{k=N+1}^{\infty} \sum_{l=1}^N \zeta^{k+N-1} \psi_k(x) \psi_l^*(x) \{\lambda_1 \cdots \hat{\lambda}_l \cdots \lambda_N \lambda_k |, \end{aligned} \quad (2.114)$$

and

$$\langle \hat{n}(x) \hat{n}(y) \rangle = C(x, x) C(y, y) + \sum_{i=1}^{N+1} \psi_i^*(y) \psi_i(x) \sum_{j=1}^N \psi_j(y) \psi_j^*(x). \quad (2.115)$$

Let us now write

$$\sum_{i=1}^{N+1} \psi_i^*(y) \psi_i(x) = \left(\sum_{i=1}^{\infty} - \sum_{i=1}^N \right) \psi_i^*(y) \psi_i(x) = \delta(x - y) - C^*(x, y). \quad (2.116)$$

Therefore, we find finally

$$\langle \hat{n}(x) \hat{n}(y) \rangle = C(x, x) C(y, y) + \delta(x - y) C(x, y) - |C(x, y)|^2. \quad (2.117)$$

The connected vev is then,

$$\langle \hat{n}(x) \hat{n}(y) \rangle^{(c)} = \langle \hat{n}(x) \hat{n}(y) \rangle - \langle \hat{n}(x) \rangle \langle \hat{n}(y) \rangle = \delta(x - y) C(x, y) - |C(x, y)|^2. \quad (2.118)$$

□

3 Path integral formulation of quantum many-particle systems

Our goal is to find a representation of the path integral describing the thermal properties of the system which is more convenient than (2.23). In order to do this, we need the analogue of a representation basis for (anti)symmetrized particle states. This basis is provided by *coherent states*, which we now introduce. The construction of coherent states for fermions requires introducing anticommuting, or Grassmann, coordinates.

3.1 Bosonic coherent states

A bosonic coherent state is defined as an eigenstate of the annihilation operators \mathbf{a}_α , i.e.

$$\mathbf{a}_\alpha|\phi\rangle = \phi_\alpha|\phi\rangle, \quad (3.1)$$

where $\phi = \{\phi_\lambda\}_{\lambda \in \Lambda}$ and ϕ_α are complex numbers.

It is useful to consider first the case of a single annihilation operator \mathbf{a} . The coherent state is defined by

$$\mathbf{a}|\phi\rangle = \phi|\phi\rangle. \quad (3.2)$$

To find the explicit form of this state, we write it in the orthonormal basis $\{|n\rangle\}$:

$$|\phi\rangle = \sum_{n \geq 0} c_n |n\rangle. \quad (3.3)$$

We have

$$\mathbf{a}|\phi\rangle = \sum_{n \geq 0} \sqrt{n} c_n |n-1\rangle = \sum_{n \geq 0} \phi c_n |n\rangle, \quad (3.4)$$

which leads to the equation

$$\sqrt{n+1} c_{n+1} = \phi c_n. \quad (3.5)$$

This leads to an explicit solution by recursion

$$c_n = \frac{\phi^n}{\sqrt{n!}} c_0. \quad (3.6)$$

We will set $c_0 = 1$. The coherent state is then given by

$$|\phi\rangle = \sum_{n=0}^{\infty} \frac{\phi^n}{\sqrt{n!}} |n\rangle = \sum_{n=0}^{\infty} \frac{\phi^n (\mathbf{a}^\dagger)^n}{n!} |0\rangle = e^{\phi \mathbf{a}^\dagger} |0\rangle. \quad (3.7)$$

It is straightforward to extend this to an arbitrary coherent state. We have

$$\begin{aligned} |\phi\rangle &= \sum_{n_{\alpha_1}, n_{\alpha_2}, \dots} \frac{\phi_{\alpha_1}^{n_{\alpha_1}}}{\sqrt{n_{\alpha_1}!}} \frac{\phi_{\alpha_2}^{n_{\alpha_2}}}{\sqrt{n_{\alpha_2}!}} \dots |n_{\alpha_1} n_{\alpha_2} \dots\rangle \\ &= \sum_{n_{\alpha_1}, n_{\alpha_2}, \dots} \frac{(\phi_{\alpha_1} \mathbf{a}_{\alpha_1}^\dagger)^{n_{\alpha_1}} (\phi_{\alpha_2} \mathbf{a}_{\alpha_2}^\dagger)^{n_{\alpha_2}}}{n_{\alpha_1}! n_{\alpha_2}!} \dots |0\rangle, \end{aligned} \quad (3.8)$$

or more compactly

$$|\phi\rangle = \exp\left(\sum_{\alpha} \phi_{\alpha} \mathbf{a}_{\alpha}^\dagger\right) |0\rangle, \quad (3.9)$$

On these states, the operator $\mathbf{a}_{\alpha}^\dagger$ acts as a derivative,

$$\mathbf{a}_{\alpha}^\dagger |\phi\rangle = \partial_{\phi_{\alpha}} |\phi\rangle. \quad (3.10)$$

The scalar product of two coherent states is

$$\begin{aligned}\langle\phi|\psi\rangle &= \sum_{n_{\alpha_1}, n_{\alpha_2}, \dots} \sum_{m_{\alpha_1}, m_{\alpha_2}, \dots} \frac{(\phi_{\alpha_1}^*)^{n_{\alpha_1}} (\phi_{\alpha_2}^*)^{n_{\alpha_2}} \dots \psi_{\alpha_1}^{m_{\alpha_1}} \psi_{\alpha_2}^{m_{\alpha_2}} \dots}{\sqrt{n_{\alpha_1}!} \sqrt{n_{\alpha_2}!} \dots \sqrt{m_{\alpha_1}!} \sqrt{m_{\alpha_2}!} \dots} \langle n_{\alpha_1} n_{\alpha_2} \dots | m_{\alpha_1} m_{\alpha_2} \dots \rangle \\ &= \sum_{n_{\alpha_1}, n_{\alpha_2}, \dots} \frac{(\phi_{\alpha_1}^* \psi_{\alpha_1})^{n_{\alpha_1}} (\phi_{\alpha_2}^* \psi_{\alpha_2})^{n_{\alpha_2}} \dots}{n_{\alpha_1}! n_{\alpha_2}! \dots} = \exp\left(\sum_{\alpha} \phi_{\alpha}^* \psi_{\alpha}\right).\end{aligned}\tag{3.11}$$

One of the most important properties of coherent states is the completeness relationship

$$\int \prod_{\alpha} \frac{d\phi_{\alpha} d\phi_{\alpha}^*}{2\pi i} e^{-\sum_{\alpha} \phi_{\alpha}^* \phi_{\alpha}} |\phi\rangle \langle\phi| = \mathbf{1},\tag{3.12}$$

where

$$\frac{d\phi d\phi^*}{2\pi i} = \frac{d(\operatorname{Re} \phi) d(\operatorname{Im} \phi)}{\pi}.\tag{3.13}$$

This is easily proved as follows. Let us consider the matrix elements of the operator in the l.h.s. of (3.12) between two arbitrary states in the Fock space:

$$\begin{aligned}& \int \prod_{\alpha} \frac{d\phi_{\alpha} d\phi_{\alpha}^*}{2\pi i} e^{-\sum_{\alpha} \phi_{\alpha}^* \phi_{\alpha}} \langle n_{\alpha_1} \dots | \phi \rangle \langle \phi | m_{\alpha_1} \dots \rangle \\ &= \int \prod_{\alpha} \frac{d\phi_{\alpha} d\phi_{\alpha}^*}{2\pi i} e^{-\sum_{\alpha} \phi_{\alpha}^* \phi_{\alpha}} \prod_{\alpha} \frac{\phi_{\alpha}^{n_{\alpha}} (\phi_{\alpha}^*)^{m_{\alpha}}}{\sqrt{n_{\alpha}! m_{\alpha}!}} \\ &= \prod_{\alpha} \frac{1}{\sqrt{n_{\alpha}! m_{\alpha}!}} \int \frac{d\phi_{\alpha} d\phi_{\alpha}^*}{2\pi i} e^{-\phi_{\alpha}^* \phi_{\alpha}} \phi_{\alpha}^{n_{\alpha}} (\phi_{\alpha}^*)^{m_{\alpha}}\end{aligned}\tag{3.14}$$

Let us then calculate the integral

$$\int \frac{d\phi d\phi^*}{2\pi i} e^{-\phi^* \phi} \phi^n (\phi^*)^m.\tag{3.15}$$

Clearly, it is convenient to do the calculation in polar coordinates, in which

$$\phi = \rho e^{i\theta}, \quad \phi^* = \rho e^{-i\theta},\tag{3.16}$$

and

$$\frac{d\phi d\phi^*}{2\pi i} = \frac{\rho d\rho d\theta}{\pi}.\tag{3.17}$$

The integral is calculated immediately,

$$\frac{1}{\pi} \int_0^{\infty} d\rho \int_0^{2\pi} d\theta e^{-\rho^2} e^{i\theta(n-m)} \rho^{n+m+1} = \delta_{nm} n!\tag{3.18}$$

and we conclude that

$$\langle n_{\alpha_1} \dots | \left(\int \prod_{\alpha} \frac{d\phi_{\alpha} d\phi_{\alpha}^*}{2\pi i} e^{-\sum_{\alpha} \phi_{\alpha}^* \phi_{\alpha}} |\phi\rangle \langle\phi| \right) | m_{\alpha_1} \dots \rangle = \prod_{\alpha} \delta_{n_{\alpha} m_{\alpha}} = \langle n_{\alpha_1} \dots | m_{\alpha_1} \dots \rangle.\tag{3.19}$$

Since this is the case for arbitrary matrix elements, we conclude that the operator must be the identity.

As a consequence of the completeness relation, we have the following result for the trace of an arbitrary operator A

$$\begin{aligned}
\text{Tr } A &= \sum_n \langle n|A|n \rangle = \int \prod_\alpha \frac{d\phi_\alpha d\phi_\alpha^*}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \sum_n \langle n|A|\phi_\alpha \rangle \langle \phi_\alpha|n \rangle \\
&= \int \prod_\alpha \frac{d\phi_\alpha d\phi_\alpha^*}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \sum_n \langle \phi_\alpha|n \rangle \langle n|A|\phi_\alpha \rangle \\
&= \int \prod_\alpha \frac{d\phi_\alpha d\phi_\alpha^*}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \langle \phi_\alpha|A|\phi_\alpha \rangle.
\end{aligned} \tag{3.20}$$

3.2 Bosonic path integrals

We will now show that bosonic coherent states make it possible to introduce a simple path integral formulation of bosonic many-particle systems.

As a warm-up example, we will consider a normal-ordered Hamiltonian involving a single degree of freedom, i.e. a pair of creation/annihilation operators \mathbf{a}^\dagger , \mathbf{a} :

$$\mathbf{H} = \mathbf{H}(\mathbf{a}^\dagger, \mathbf{a}). \tag{3.21}$$

We will assume that \mathbf{H} is in *normal-ordered* form, i.e. it is written as a sum of expressions in which all creation operators are to the left, and all annihilation operators are to the right. Clearly, we can always put an operator in this form by using the commutation relations. Then, we have

$$Z = \text{Tr} \left(e^{-\beta \mathbf{H}} \right) = \int \frac{d\phi d\phi^*}{2\pi i} e^{-\phi^* \phi} \langle \phi | e^{-\beta \mathbf{H}} | \phi \rangle. \tag{3.22}$$

We now divide β , regarded as an interval, in $N + 1$ segments of length

$$\Delta\tau = \frac{\beta}{N + 1}. \tag{3.23}$$

We also insert N resolutions of the identity and we identify

$$\phi = \phi_0 = \phi_{N+1}. \tag{3.24}$$

We obtain

$$Z = \int \prod_{j=0}^N \frac{d\phi_j d\phi_j^*}{2\pi i} e^{-\sum_{j=0}^N \phi_j^* \phi_j} \langle \phi_{N+1} | e^{-\Delta u \mathbf{H}} | \phi_N \rangle \langle \phi_N | e^{-\Delta u \mathbf{H}} | \phi_{N-1} \rangle \cdots \langle \phi_1 | e^{-\Delta u \mathbf{H}} | \phi_0 \rangle. \tag{3.25}$$

If $\Delta\tau$ is sufficiently small, we can write

$$\begin{aligned}
\langle \phi_j | e^{-\Delta\tau \mathbf{H}} | \phi_{j-1} \rangle &\approx \langle \phi_j | \mathbf{1} - \Delta\tau \mathbf{H} | \phi_{j-1} \rangle \\
&= e^{\phi_j^* \phi_{j-1}} (1 - \Delta\tau H(\phi_j^*, \phi_{j-1})) \\
&\approx e^{\phi_j^* \phi_{j-1} - \Delta\tau H(\phi_j^*, \phi_{j-1})}.
\end{aligned} \tag{3.26}$$

We then find

$$Z \approx Z_N, \tag{3.27}$$

where

$$Z_N = \int \prod_{j=0}^N \frac{d\phi_j d\phi_j^*}{2\pi i} \exp \left\{ - \sum_{j=1}^{N+1} (\phi_j^* (\phi_j - \phi_{j-1}) + \Delta\tau H(\phi_j^*, \phi_{j-1})) \right\}. \quad (3.28)$$

In the double-scaling limit

$$N \rightarrow \infty, \quad \Delta\tau \rightarrow 0, \quad \Delta\tau(N+1) = \beta, \quad (3.29)$$

Z_N should become equal to Z . Therefore, we obtain in this way the coherent path integral representation of the partition function,

$$Z = \lim_{N \rightarrow \infty} Z_N. \quad (3.30)$$

The term in the exponent of (3.116) is the discretization of the action

$$S = \int_0^\beta (\phi^* \partial_\tau \phi + H(\phi^*, \phi)) d\tau, \quad (3.31)$$

so we will also write

$$Z = \int \mathcal{D}\phi \mathcal{D}\phi^* \exp \left(- \int_0^\beta (\phi^* \partial_u \phi + H(\phi^*, \phi)) d\tau \right). \quad (3.32)$$

Example 3.1. *Gaussian theory.* As an example, let us consider the ‘‘Gaussian’’ case in which the Hamiltonian has the form

$$\mathbf{H} = \lambda \mathbf{a}^\dagger \mathbf{a} + c. \quad (3.33)$$

Note that, for

$$\lambda = \hbar\omega, \quad c = \frac{\hbar\omega}{2} \quad (3.34)$$

this is the Hamiltonian of the harmonic oscillator. In this case, the discretized path integral is a Gaussian integral. We will denote the corresponding partition function by

$$Z_G(\lambda, c; \beta). \quad (3.35)$$

The exponent of (3.116) reads in this case

$$\sum_{j=1}^{M+1} \left(\phi_j^* (\phi_j - \phi_{j-1}) + \tilde{\lambda} \phi_j^* \phi_{j-1} \right), \quad \tilde{\lambda} = \lambda \Delta u. \quad (3.36)$$

Let us introduce the vectors

$$\phi = (\phi_0, \phi_1, \dots, \phi_M), \quad \phi^* = (\phi_0^*, \phi_1^*, \dots, \phi_M^*). \quad (3.37)$$

Then, the exponent (3.124) can be written as

$$\phi^* \mathbf{A} \phi, \quad (3.38)$$

where the matrix A is given by

$$A = \begin{pmatrix} 1 & 0 & 0 \cdots & 0 & \tilde{\lambda} - 1 \\ \tilde{\lambda} - 1 & 1 & 0 \cdots & 0 & 0 \\ 0 & \tilde{\lambda} - 1 & 1 \cdots & 0 & 0 \\ \vdots & \vdots & \vdots \ddots & \vdots & \vdots \\ 0 & 0 & 0 \cdots & \tilde{\lambda} - 1 & 1 \end{pmatrix} \quad (3.39)$$

We can now use the Gaussian integration formula

$$\int \prod_{k=1}^n \frac{d\phi_k d\phi_k^*}{2\pi i} e^{-\phi^* A \phi} = \frac{1}{\det(A)}. \quad (3.40)$$

The determinant is easily calculated as

$$\det(A) = 1 - (1 - \tilde{\lambda})^{M+1}. \quad (3.41)$$

and we obtain

$$Z_M = \frac{e^{-\beta c}}{1 - \left(1 - \frac{\beta\lambda}{M+1}\right)^{M+1}}. \quad (3.42)$$

Since

$$\lim_{M \rightarrow \infty} \left(1 - \frac{\beta\lambda}{M+1}\right)^{M+1} = e^{-\beta\lambda}, \quad (3.43)$$

we find

$$Z_G(\lambda, c; \beta) = \frac{e^{-\beta c}}{1 - e^{-\beta\lambda}}. \quad (3.44)$$

On the other hand, a standard evaluation gives

$$Z_G(\lambda, c; \beta) = \sum_{n \geq 0} \langle n | e^{-\beta H} | n \rangle = \sum_{n \geq 0} e^{-\beta c - \beta\lambda n} = \frac{e^{-\beta c}}{1 - e^{-\beta\lambda}} \quad (3.45)$$

in agreement with the path integral evaluation. \square

It is now straightforward to obtain the path integral expression for the grand canonical partition function of a quantum many-particle system. We have

$$\Xi = \text{Tr} \left(e^{-\beta(H - \mu N)} \right), \quad (3.46)$$

where

$$N = \sum_{\lambda} n_{\lambda} = \sum_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} \quad (3.47)$$

is the total number of particles of the system. By using the trace formula (3.20), we obtain

$$\Xi = \int \prod_{\lambda} \frac{d\phi_{\lambda} d\phi_{\lambda}^*}{2\pi i} e^{-\sum_{\lambda} \phi_{\lambda}^* \phi_{\lambda}} \langle \phi_{\lambda} | e^{-\beta(H - \mu N)} | \phi_{\lambda} \rangle. \quad (3.48)$$

We repeat the procedure above: we introduce M resolutions of the identity and we integrate over the coordinates $\phi_{\lambda,j}$, $\lambda \in \Lambda$, $j = 0, \dots, M+1$. We also have the periodic boundary condition

$$\phi_\lambda = \phi_{\lambda,0} = \phi_{\lambda,M+1}. \quad (3.49)$$

We obtain

$$\Xi = \lim_{M \rightarrow \infty} \Xi_M \quad (3.50)$$

where

$$\Xi_M = \int \prod_\lambda \prod_{j=0}^M \frac{d\phi_{\lambda,j} d\phi_{\lambda,j}^*}{2\pi i} \exp \left\{ - \sum_{j=1}^{M+1} (\phi_{\lambda,j}^* (\phi_{\lambda,j} - \phi_{\lambda,j-1} - \Delta u \mu \phi_{\lambda,j-1}) + \Delta u H(\phi_{\lambda,j}^*, \phi_{\lambda,j-1})) \right\}. \quad (3.51)$$

The term in the exponent of (3.132) is the discretization of the action

$$S = \int_0^\beta \sum_\lambda \{ \phi_\lambda^* (\partial_\tau \phi_\lambda - \mu \phi_\lambda) + H(\phi_\lambda^*, \phi_\lambda) \} d\tau, \quad (3.52)$$

so we will also write

$$\Xi = \int \mathcal{D}\phi_\lambda \mathcal{D}\phi_\lambda^* \exp \left(- \int_0^\beta \sum_\lambda \{ \phi_\lambda^* (\partial_\tau \phi_\lambda - \mu \phi_\lambda) + H(\phi_\lambda^*, \phi_\lambda) \} d\tau \right). \quad (3.53)$$

The path integral is over trajectories which satisfy

$$\phi_\lambda(\beta) = \phi_\lambda(0), \quad \phi_\lambda^*(\beta) = \phi_\lambda^*(0). \quad (3.54)$$

This is the path integral formulation for a bosonic many-body system. Note that in this formulation we avoid the sum over permutations which appears in (2.23).

Example 3.2. *Non-interacting particles.* Let us assume that we have a system of non-interacting particles. The Hamiltonian is then of the form

$$\mathbf{H} = \sum_{i=1}^N \mathbf{h}^{(i)}, \quad (3.55)$$

where \mathbf{h} is the one-particle Hamiltonian and $\mathbf{h}^{(i)}$ is the copy of this operator acting on the i -th factor of \mathcal{H}_N . Let $\{|\lambda\rangle\}_{\lambda \in \Lambda}$ be an orthonormal basis of eigenstates of \mathbf{h} ,

$$\mathbf{h}|\lambda\rangle = \epsilon_\lambda |\lambda\rangle. \quad (3.56)$$

In the second-quantized formalism we have that

$$\mathbf{H} = \sum_\lambda \epsilon_\lambda a_\lambda^\dagger a_\lambda. \quad (3.57)$$

We see that the Hamiltonian is the sum of Hamiltonians of the form (3.122). We can now compute Ξ in the path integral formalism by extending the results of example 3.1. The path integral for Ξ factorizes as

$$\Xi = \prod_\lambda Z_G(\epsilon_\lambda - \mu, 0; \beta) = \prod_\lambda \left(1 - e^{-\beta(\epsilon_\lambda - \mu)} \right)^{-1}, \quad (3.58)$$

which is the standard result in statistical mechanics. \square

3.3 Grassmann variables

Let us try to construct a coherent state with fermions, satisfying

$$a_\lambda |\boldsymbol{\theta}\rangle = \theta_\lambda |\boldsymbol{\theta}\rangle. \quad (3.59)$$

Since

$$a_\mu a_\lambda |\boldsymbol{\theta}\rangle = -a_\lambda a_\mu |\boldsymbol{\theta}\rangle \quad (3.60)$$

the parameters $\theta_\lambda, \theta_\mu$ must *anticommute*:

$$\theta_\lambda \theta_\mu = -\theta_\mu \theta_\lambda \quad (3.61)$$

and cannot be ordinary complex numbers. These quantities are called *Grassmann variables* and we need them to construct the path integral for fermions. We will now develop their general theory.

A *Grassmann algebra* with n generators Gr_n is a \mathbb{C} -algebra where the generators $\theta_1, \dots, \theta_n$ satisfy the relations

$$\{\theta_i, \theta_j\} = 0, \quad i, j = 1, \dots, n \quad (3.62)$$

In particular, they are nilpotent.

Gr_n is a polynomial algebra in anticommuting variables. Its elements have a degree which is simply the number of generators. We will denote the degree of an element $\alpha \in \text{Gr}_n$ by $|\alpha|$. As a vector space, we can decompose

$$\text{Gr}_n = \bigoplus_{k=0}^n \text{Gr}_n^k, \quad (3.63)$$

where Gr_n^k are the elements of degree k . As a vector space, Gr_n^k has dimension $\binom{n}{k}$, and Gr_n has in total dimension 2^n . A general element of Gr_n can be written as

$$f(\boldsymbol{\theta}) = \sum_{k=0}^n \sum_{1 \leq i_1 < \dots < i_n \leq n} f^{i_1 \dots i_k} \theta_{i_1} \dots \theta_{i_k}, \quad f^{i_1 \dots i_k} \in \mathbb{C}. \quad (3.64)$$

We need to derive and to integrate in a Grassmann algebra. The derivatives

$$\frac{\partial}{\partial \theta_i} : \text{Gr}_n \rightarrow \text{Gr}_n \quad (3.65)$$

act as elementary derivatives but are antiderivations w.r.t. to the degree. Their action on a monomial is defined by

$$\frac{\partial}{\partial \theta_i} \theta_{i_1} \dots \theta_{i_n} = \sum_{l=1}^k (-1)^{l-1} \delta_{ii_l} \theta_{i_1} \dots \hat{\theta}_{i_l} \dots \theta_{i_k}, \quad (3.66)$$

where $\hat{\theta}_{i_l}$ means that we remove this generator.

Example 3.3. In the Grassmann algebra Gr_n , with $n \geq 2$, we have

$$\frac{\partial}{\partial \theta_1} (\theta_1 \theta_2) = \theta_2, \quad \frac{\partial}{\partial \theta_2} (\theta_1 \theta_2) = -\theta_1. \quad (3.67)$$

□

We want to define an integral over a Grassmann algebra. In the case of a single generator, integration is defined by

$$\int d\theta = 0, \quad \int d\theta\theta = 1. \quad (3.68)$$

More generally, the *Berezin integral* is a linear functional

$$\int d\theta_1 \cdots d\theta_n : \text{Gr}_n \rightarrow \mathbb{C} \quad (3.69)$$

defined as follows. Let $f(\boldsymbol{\theta})$ be of the form (3.64). Then

$$\int d\theta_1 \cdots d\theta_n f(\boldsymbol{\theta}) = f^{12 \cdots n}. \quad (3.70)$$

We will often denote

$$d\boldsymbol{\theta} = d\theta_1 \cdots d\theta_n. \quad (3.71)$$

Note that this integration acts as a differentiation. We also note that

$$\int d\theta_1 \cdots d\theta_n \theta_{\sigma(1)} \cdots \theta_{\sigma(n)} = (-1)^{\epsilon(\sigma)}, \quad (3.72)$$

where $\sigma \in S_n$ is a permutation of n elements and $\epsilon(\sigma)$ its signature.

Lemma 3.4. (*Change of variables in the Berezin integral*) Let $\{\theta_i\}_{i=1, \dots, n}$, $\{\tilde{\theta}_i\}_{i=1, \dots, n}$ two sets of generators of Gr_n , related by a linear change of variables:

$$\theta_i = \sum_{j=1}^n a_{ij} \tilde{\theta}_j. \quad (3.73)$$

Then,

$$\int d\theta_1 \cdots d\theta_n f(\boldsymbol{\theta}) = \frac{1}{\det(A)} \int d\tilde{\theta}_1 \cdots d\tilde{\theta}_n \tilde{f}(\tilde{\boldsymbol{\theta}}), \quad (3.74)$$

where

$$\tilde{f}(\tilde{\boldsymbol{\theta}}) = f(\boldsymbol{\theta}). \quad (3.75)$$

Proof: We have

$$\begin{aligned} f^{1 \cdots n} \theta_1 \cdots \theta_n &= f^{1 \cdots n} \sum_{j_1, \dots, j_n} a_{1j_1} \cdots a_{nj_n} \tilde{\theta}_{j_1} \cdots \tilde{\theta}_{j_n} \\ &= f^{1 \cdots n} \tilde{\theta}_1 \cdots \tilde{\theta}_n \sum_{\sigma \in S_n} (-1)^{\epsilon(\sigma)} a_{1\sigma(1)} \cdots a_{n\sigma(n)}, \end{aligned} \quad (3.76)$$

therefore

$$\tilde{f}^{12 \cdots n} = \det(A) f^{12 \cdots n}, \quad (3.77)$$

which proves the Lemma. \square

This lemma can be understood as a formula for the change of variables

$$d\boldsymbol{\theta} = \frac{1}{\det(A)} d\tilde{\boldsymbol{\theta}}. \quad (3.78)$$

After this, we can perform Gaussian integrations. A quadratic form in Grassmann variables is given by

$$\sum_{i,j=1}^n a_{ij}\theta_i\theta_j, \quad (3.79)$$

and we can take A to be an antisymmetric matrix. The exponential of such a quadratic form is defined by a power series expansion. However, this series terminates due to the nilpotency of θ_i :

$$\exp\left(\frac{1}{2}\sum_{i,j=1}^n a_{ij}\theta_i\theta_j\right) = \sum_{k=0}^m \frac{1}{2^k \cdot k!} \left(\sum_{i,j=1}^n a_{ij}\theta_i\theta_j\right)^k. \quad (3.80)$$

where

$$m = \left[\frac{n}{2}\right]. \quad (3.81)$$

We want to calculate now the Gaussian Berezin integral

$$\int d\theta_1 \cdots d\theta_n \exp\left(\frac{1}{2}\sum_{i,j=1}^n a_{ij}\theta_i\theta_j\right). \quad (3.82)$$

If n is odd, this integral vanishes. If $n = 2m$ is even, we have

$$\begin{aligned} \int d\theta_1 \cdots d\theta_n \exp\left(\frac{1}{2}\sum_{i,j=1}^n a_{ij}\theta_i\theta_j\right) &= \frac{1}{2^m \cdot m!} \int d\theta_1 \cdots d\theta_n \left(\sum_{i,j=1}^n a_{ij}\theta_i\theta_j\right)^m \\ &= \frac{1}{2^m \cdot m!} \sum_{\sigma \in S_n} (-1)^{\epsilon(\sigma)} a_{\sigma(1)\sigma(2)} \cdots a_{\sigma(n-1)\sigma(n)}. \end{aligned} \quad (3.83)$$

This is, by definition, the *Pfaffian* of the antisymmetric $2m \times 2m$ matrix A :

$$\text{Pf}(A) = \frac{1}{2^m \cdot m!} \sum_{\sigma \in S_n} (-1)^{\epsilon(\sigma)} a_{\sigma(1)\sigma(2)} \cdots a_{\sigma(n-1)\sigma(n)}. \quad (3.84)$$

Example 3.5. Let us consider the simple example of Pfaffian, for $n = 2$ and

$$A = \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix}. \quad (3.85)$$

We have

$$\text{Pf}(A) = \frac{1}{2}(a_{12} - a_{21}) = a. \quad (3.86)$$

Note that, in this example,

$$(\text{Pf}(A))^2 = \det(A), \quad (3.87)$$

which is true for general antisymmetric A . \square

In developing the path integral formulation of many-fermion systems, we need a *complex* Grassmann algebra with an even number of generators $\theta_1, \theta_1^*, \dots, \theta_n, \theta_n^*$. In such an algebra there is an involution, i.e. an antilinear map $f \rightarrow f^*$ satisfying

$$(f^*)^* = f, \quad (fg)^* = g^*f^*. \quad (3.88)$$

The Grassmann algebra $\mathbb{C}[\theta_1, \theta_1^*, \dots, \theta_n, \theta_n^*]$ has a natural involution $(\theta_i)^* = \theta_i^*$, $(\theta_i^*)^* = \theta_i$. We will denote

$$d\boldsymbol{\theta}^* d\boldsymbol{\theta} = d\theta_1^* d\theta_1 \cdots d\theta_n^* d\theta_n. \quad (3.89)$$

The basic result of complex Grassmann integration is

$$\int d\boldsymbol{\theta}^* d\boldsymbol{\theta} \exp \left\{ - \sum_{i,j=1}^n \theta_i^* a_{ij} \theta_j \right\} = \det(A). \quad (3.90)$$

3.4 Fermionic coherent states

We are now ready to construct fermionic coherent states. Given a set of fermionic creation and annihilation operators, $\mathbf{a}_\lambda, \mathbf{a}_\lambda^\dagger$, $\lambda \in \Lambda$, we associate to them the Grassmann variables $\xi_\lambda, \xi_\lambda^*$, respectively, and we consider the complex Grassmann algebra \mathcal{G} generated by them. We also consider a generalized fermionic Fock space $\mathcal{F}_{\mathcal{G}}$ with coefficients in the Grassmann algebra \mathcal{G} . We will assume that Grassmann variables *anticommute* with the creation/annihilation operators:

$$\{\xi, \mathbf{a}\} = 0, \quad (3.91)$$

where ξ is any Grassmann variable in $\{\xi_\lambda, \xi_\lambda^*\}_{\lambda \in \Lambda}$, and \mathbf{a} is any operator in $\{\xi_\lambda, \xi_\lambda^*\}_{\lambda \in \Lambda}$. We also have the Hermitian conjugate rule

$$(\xi \mathbf{a})^\dagger = \mathbf{a}^\dagger \xi^\dagger. \quad (3.92)$$

Let $\boldsymbol{\xi} = \{\xi_\lambda\}_{\lambda \in \Lambda}$ be a vector of Grassmann variables. A fermionic coherent state is defined, by analogy with the bosonic case, as

$$|\boldsymbol{\xi}\rangle = e^{-\sum_\lambda \xi_\lambda \mathbf{a}_\lambda} |0\rangle. \quad (3.93)$$

This can be also written as

$$|\boldsymbol{\xi}\rangle = \prod_\lambda e^{-\xi_\lambda \mathbf{a}_\lambda^\dagger} |0\rangle = \prod_\lambda (1 - \xi_\lambda \mathbf{a}_\lambda^\dagger) |0\rangle \quad (3.94)$$

due to the nilpotency of ξ_λ . Note that

$$\mathbf{a}_\mu (1 - \xi_\mu \mathbf{a}_\mu^\dagger) = \xi_\mu + (1 - \xi_\mu \mathbf{a}_\mu^\dagger) \mathbf{a}_\mu, \quad (3.95)$$

therefore

$$\begin{aligned} \mathbf{a}_\mu |\boldsymbol{\xi}\rangle &= \mathbf{a}_\mu \prod_\lambda (1 - \xi_\lambda \mathbf{a}_\lambda^\dagger) |0\rangle \\ &= \prod_{\lambda \neq \mu} (1 - \xi_\lambda \mathbf{a}_\lambda^\dagger) \xi_\mu |0\rangle \\ &= \xi_\mu |\boldsymbol{\xi}\rangle. \end{aligned} \quad (3.96)$$

We conclude that fermionic coherent states are indeed eigenstates of the annihilation operators.

We note that the adjoint of a coherent state is

$$\langle \boldsymbol{\xi} | = \langle 0 | e^{-\sum_\lambda \mathbf{a}_\lambda \xi_\lambda^*} = \langle 0 | e^{\sum_\lambda \xi_\lambda^* \mathbf{a}_\lambda}. \quad (3.97)$$

The overlap between two fermionic coherent states is

$$\langle \boldsymbol{\xi} | \boldsymbol{\eta} \rangle = \langle 0 | \prod_\lambda (1 - \mathbf{a}_\lambda \xi_\lambda^*) (1 - \eta_\lambda \mathbf{a}_\lambda^\dagger) |0\rangle. \quad (3.98)$$

To evaluate this, we normal order the operator as

$$(1 - \mathbf{a}_\lambda \xi_\lambda^*)(1 - \eta_\lambda \mathbf{a}_\lambda^\dagger) = 1 - \mathbf{a}_\lambda \xi_\lambda^* - \eta_\lambda \mathbf{a}_\lambda^\dagger + \xi_\lambda^* \eta_\lambda + \xi_\lambda^* \eta_\lambda \mathbf{a}_\lambda^\dagger \mathbf{a}_\lambda \quad (3.99)$$

Sandwiching this with the vacuum we get

$$1 + \xi_\lambda^* \eta_\lambda, \quad (3.100)$$

therefore

$$\langle \boldsymbol{\xi} | \boldsymbol{\eta} \rangle = \prod_{\lambda} (1 + \xi_\lambda^* \eta_\lambda) = e^{\sum_{\lambda} \xi_\lambda^* \eta_\lambda}. \quad (3.101)$$

The last ingredient we need is the completeness relation. We have,

$$\int d\boldsymbol{\xi}^* d\boldsymbol{\xi} e^{-\sum_{\lambda} \xi_\lambda^* \xi_\lambda} |\boldsymbol{\xi}\rangle \langle \boldsymbol{\xi}| = \mathbf{1}. \quad (3.102)$$

To prove this statement, we proceed as in the bosonic case, namely we show that the matrix elements of the operator in the l.h.s. are equal to the matrix elements of the identity, i.e. to inner products. Let us consider two arbitrary basis elements in \mathcal{F} , and let us compute

$$\begin{aligned} & \langle \alpha_1 \cdots \alpha_n | \left(\int d\boldsymbol{\xi}^* d\boldsymbol{\xi} e^{-\sum_{\lambda} \xi_\lambda^* \xi_\lambda} |\boldsymbol{\xi}\rangle \langle \boldsymbol{\xi}| \right) | \beta_1 \cdots \beta_m \rangle \\ &= \int d\boldsymbol{\xi}^* d\boldsymbol{\xi} e^{-\sum_{\lambda} \xi_\lambda^* \xi_\lambda} \langle \alpha_1 \cdots \alpha_n | \boldsymbol{\xi} \rangle \langle \boldsymbol{\xi} | \beta_1 \cdots \beta_m \rangle. \end{aligned} \quad (3.103)$$

We recall that, in the fermionic case,

$$|\alpha_1 \cdots \alpha_n\rangle = \mathbf{a}_{\alpha_1}^\dagger \cdots \mathbf{a}_{\alpha_n}^\dagger |0\rangle, \quad (3.104)$$

therefore

$$\langle \alpha_1 \cdots \alpha_n | \boldsymbol{\xi} \rangle = \langle 0 | \mathbf{a}_{\alpha_n} \cdots \mathbf{a}_{\alpha_1} | \boldsymbol{\xi} \rangle = \xi_{\alpha_n} \cdots \xi_{\alpha_1} \langle 0 | \boldsymbol{\xi} \rangle = \xi_{\alpha_n} \cdots \xi_{\alpha_1}. \quad (3.105)$$

We find that (3.103) is given by the Grassmann integral

$$\int d\boldsymbol{\xi}^* d\boldsymbol{\xi} e^{-\sum_{\lambda} \xi_\lambda^* \xi_\lambda} \xi_{\alpha_n} \cdots \xi_{\alpha_1} \xi_{\beta_1}^* \cdots \xi_{\beta_m}^*. \quad (3.106)$$

It is easy to see that this integral is non-vanishing unless the indices $\{\beta_i\}_{i=1, \dots, m}$ are a permutation of the indices $\{\alpha_i\}_{i=1, \dots, n}$, i.e. $n = m$ and $\beta_i = \alpha_{\sigma(i)}$ for some $\sigma \in S_n$. If we reorder the indices, we have

$$\xi_{\alpha_n} \cdots \xi_{\alpha_1} \xi_{\beta_1}^* \cdots \xi_{\beta_m}^* = (-1)^{\epsilon(\sigma)} \xi_{\alpha_n} \cdots \xi_{\alpha_1} \xi_{\alpha_1}^* \cdots \xi_{\alpha_n}^*, \quad (3.107)$$

and we end up with the integral

$$(-1)^{\epsilon(\sigma)} \int \prod_{i=1}^n d\xi_{\alpha_i}^* d\xi_{\alpha_i} e^{-\sum_{i=1}^n \xi_{\alpha_i}^* \xi_{\alpha_i}} \xi_{\alpha_1} \cdots \xi_{\alpha_n} \xi_{\alpha_1}^* \cdots \xi_{\alpha_n}^* = (-1)^{\epsilon(\sigma)}. \quad (3.108)$$

We can now use the completeness relation to obtain a convenient expression for the trace an operator. We have

$$\begin{aligned} \text{Tr } \mathbf{A} &= \sum_n \langle n | \mathbf{A} | n \rangle = \int \prod_{\lambda} d\xi_{\lambda}^* d\xi_{\lambda} e^{-\sum_{\lambda} \xi_{\lambda}^* \xi_{\lambda}} \sum_n \langle n | \mathbf{A} | \xi_{\lambda} \rangle \langle \xi_{\lambda} | n \rangle \\ &= \prod_{\lambda} d\xi_{\lambda}^* d\xi_{\lambda} e^{-\sum_{\lambda} \xi_{\lambda}^* \xi_{\lambda}} \sum_n \langle -\xi_{\lambda} | n \rangle \langle n | \mathbf{A} | \xi_{\lambda} \rangle \\ &= \prod_{\lambda} d\xi_{\lambda}^* d\xi_{\lambda} e^{-\sum_{\lambda} \xi_{\lambda}^* \xi_{\lambda}} \langle -\xi_{\lambda} | \mathbf{A} | \xi_{\lambda} \rangle. \end{aligned} \quad (3.109)$$

Here we have used the anticommutation relations

$$\langle n|\mathbf{A}|\xi_\lambda\rangle\langle\xi_\lambda|n\rangle = \langle-\xi_\lambda|n\rangle\langle n|\mathbf{A}|\xi_\lambda\rangle. \quad (3.110)$$

3.5 Fermionic path integrals

We now proceed as in the bosonic case. We first consider the simple case of a single degree of freedom.

$$Z = \text{Tr} \left(e^{-\beta\mathbf{H}} \right) = \int d\xi^* d\xi e^{-\xi^*\xi} \langle -\xi | e^{-\beta\mathbf{H}} | \xi \rangle. \quad (3.111)$$

We again divide β , regarded as an interval, in $M + 1$ segments of length $\Delta\tau$, given in (??), and we insert M resolutions of the identity. In the fermionic case, due to the minus sign in the bra, we have

$$\xi = \xi_0 = -\xi_{M+1}. \quad (3.112)$$

We obtain

$$Z = \int \prod_{j=0}^M d\xi_j^* d\xi_j e^{-\sum_{j=0}^M \xi_j^* \xi_j} \langle \xi_{M+1} | e^{-\Delta\tau\mathbf{H}} | \xi_M \rangle \langle \xi_M | e^{-\Delta\tau\mathbf{H}} | \xi_{M-1} \rangle \cdots \langle \xi_1 | e^{-\Delta\tau\mathbf{H}} | \xi_0 \rangle. \quad (3.113)$$

If $\Delta\tau$ is sufficiently small, we can write

$$\begin{aligned} \langle \xi_j | e^{-\Delta\tau\mathbf{H}} | \xi_{j-1} \rangle &\approx \langle \xi_j | \mathbf{1} - \Delta\tau\mathbf{H} | \xi_{j-1} \rangle \\ &= e^{\xi_j^* \xi_{j-1}} (1 - \Delta\tau H(\xi_j^*, \xi_{j-1})) \\ &\approx e^{\xi_j^* \xi_{j-1} - \Delta\tau H(\xi_j^*, \xi_{j-1})}. \end{aligned} \quad (3.114)$$

We then find

$$Z \approx Z_M, \quad (3.115)$$

where

$$Z_M = \int \prod_{j=0}^M d\xi_j^* d\xi_j \exp \left\{ - \sum_{j=1}^{M+1} (\xi_j^* (\xi_j - \xi_{j-1}) + \Delta\tau H(\xi_j^*, \xi_{j-1})) \right\}. \quad (3.116)$$

In the double-scaling limit

$$M \rightarrow \infty, \quad \Delta\tau \rightarrow 0, \quad \Delta\tau(N + 1) = \beta, \quad (3.117)$$

Z_M should become equal to Z . Therefore, we obtain in this way the coherent path integral representation of the fermionic partition function,

$$Z = \lim_{M \rightarrow \infty} Z_M. \quad (3.118)$$

The term in the exponent of (3.116) is the discretization of the action

$$S = \int_0^\beta (\xi^* \partial_\tau \xi + H(\xi^*, \xi)) d\tau, \quad (3.119)$$

so we will also write

$$Z = \int \mathcal{D}\xi^* \mathcal{D}\xi \exp \left(- \int_0^\beta (\xi^* \partial_\tau \xi + H(\xi^*, \xi)) d\tau \right). \quad (3.120)$$

This is formally identical to the bosonic case, with the only difference that the boundary conditions for the paths are *antiperiodic*:

$$\xi(\beta) = -\xi(0), \quad \xi^*(\beta) = -\xi^*(0). \quad (3.121)$$

Example 3.6. *Gaussian theory in the fermionic case.* As an example, let us consider the ‘‘Gaussian’’ case in which the Hamiltonian has the form

$$H = \lambda a^\dagger a + c. \quad (3.122)$$

This leads to a Gaussian Grassmann integral. We will denote the corresponding partition function by

$$Z_G^F(\lambda, c; \beta). \quad (3.123)$$

The exponent of (3.116) is given by

$$\sum_{j=1}^{M+1} \left(\xi_j^* (\xi_j - \xi_{j-1}) + \tilde{\lambda} \xi_j^* \xi_{j-1} \right) = \boldsymbol{\xi}^* \mathbf{A} \boldsymbol{\xi}, \quad (3.124)$$

where $\tilde{\lambda} = \lambda \Delta \tau$, we have introduced the vectors of Grassmann numbers

$$\boldsymbol{\xi} = (\xi_0, \xi_1, \dots, \xi_M), \quad \boldsymbol{\xi}^* = (\xi_0^*, \xi_1^*, \dots, \xi_M^*). \quad (3.125)$$

and the matrix \mathbf{A} is now given by

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 \cdots & 0 & 1 - \tilde{\lambda} \\ \tilde{\lambda} - 1 & 1 & 0 \cdots & 0 & 0 \\ 0 & \tilde{\lambda} - 1 & 1 \cdots & 0 & 0 \\ \vdots & \vdots & \vdots \ddots & \vdots & \vdots \\ 0 & 0 & 0 \cdots & \tilde{\lambda} - 1 & 1 \end{pmatrix} \quad (3.126)$$

The different sign in the entry $0N$ is due to the fact that $\xi_{M+1} = -\xi_0$. Therefore,

$$\det(\mathbf{A}) = 1 + (1 - \tilde{\lambda})^{M+1} \quad (3.127)$$

and from (3.90) we obtain

$$Z_M = e^{-\beta c} \left(1 + \left(1 - \frac{\beta \lambda}{M+1} \right)^{M+1} \right). \quad (3.128)$$

Therefore, in the limit $M \rightarrow \infty$ we find

$$Z_G^F(\lambda, c; \beta) = e^{-\beta c} \left(1 + e^{-\beta \lambda} \right). \quad (3.129)$$

On the other hand, a standard evaluation gives

$$Z_G^F(\lambda, c; \beta) = \sum_{n=0,1} \langle n | e^{-\beta H} | n \rangle = e^{-\beta c} + e^{-\beta c - \beta \lambda} = e^{-\beta c} \left(1 + e^{-\beta \lambda} \right), \quad (3.130)$$

in agreement with the path integral evaluation. \square

It is now straightforward to extend this analysis to obtain the path integral formulation of the grand canonical partition function for a system of fermions. One has

$$\Xi = \lim_{M \rightarrow \infty} \Xi_M \quad (3.131)$$

where

$$\Xi_M = \int \prod_{\lambda} \prod_{j=0}^M d\xi_{\lambda,j}^* d\xi_{\lambda,j} \exp \left\{ - \sum_{j=1}^{M+1} (\xi_{\lambda,j}^* (\xi_{\lambda,j} - \xi_{\lambda,j-1} - \Delta\tau \mu \xi_{\lambda,j-1}) + \Delta\tau H(\xi_{\lambda,j}^*, \xi_{\lambda,j-1})) \right\}. \quad (3.132)$$

The term in the exponent of (3.132) is the discretization of the action

$$S = \int_0^{\beta} \sum_{\lambda} \{ \xi_{\lambda}^* (\partial_{\tau} \xi_{\lambda} - \mu \xi_{\lambda}) + H(\xi_{\lambda}^*, \xi_{\lambda}) \} d\tau, \quad (3.133)$$

so we will also write

$$\Xi = \int \mathcal{D}\xi_{\lambda}^* \mathcal{D}\xi_{\lambda} \exp \left(- \int_0^{\beta} \sum_{\lambda} \{ \xi_{\lambda}^* (\partial_{\tau} \xi_{\lambda} - \mu \xi_{\lambda}) + H(\xi_{\lambda}^*, \xi_{\lambda}) \} d\tau \right). \quad (3.134)$$

The path integral is over trajectories which satisfy

$$\xi_{\lambda}(\beta) = -\xi_{\lambda}(0), \quad \xi_{\lambda}^*(\beta) = -\xi_{\lambda}^*(0). \quad (3.135)$$

In the case of a non-interacting system, we obtain

$$\Xi = \prod_{\lambda} Z_G^F(\epsilon_{\lambda} - \mu, 0; \beta) = \prod_{\lambda} \left(1 + e^{-\beta(\epsilon_{\lambda} - \mu)} \right). \quad (3.136)$$

3.6 Mode decomposition and Matsubara frequencies

In the path integral formulation of the grand canonical partition function, we have to integrate over (anti)periodic trajectories. It is then useful to introduce Fourier modes for the fields,

$$\eta_{\lambda}(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \eta_{\lambda n} e^{-i\omega_n \tau}, \quad \eta_{\lambda}^*(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \eta_{\lambda n}^* e^{i\omega_n \tau}. \quad (3.137)$$

Here,

$$\omega_n = \begin{cases} \frac{2\pi n}{\beta}, & \text{for bosons,} \\ \frac{\pi n(2n+1)}{\beta}, & \text{for fermions,} \end{cases} \quad (3.138)$$

are the so-called *Matsubara frequencies*. Let us split the Hamiltonian into a ‘‘Gaussian’’ and an interaction pieces

$$\mathbf{H} = \sum_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} + \mathbf{H}_I. \quad (3.139)$$

For the quadratic part of the action, we find

$$\sum_{\lambda} \int_0^{\beta} d\tau \eta_{\lambda}^* (\partial_{\tau} - \mu + \epsilon_{\lambda}) \eta_{\lambda} = \sum_{\lambda, n} \eta_{\lambda n}^* (-i\omega_n - \mu + \epsilon_{\lambda}) \eta_{\lambda n}. \quad (3.140)$$

This is sometimes called the *frequency representation of the action*. One advantage of this representation is that the integration over the trajectories can be translated into an integration over an infinite number of modes:

$$\prod_{\lambda} \mathcal{D}\eta_{\lambda}^*(\tau) \mathcal{D}\eta_{\lambda}(\tau) \rightarrow \frac{1}{\mathcal{N}} \prod_{n,\lambda} d\eta_{\lambda n}^* d\eta_{\lambda n}, \quad (3.141)$$

where \mathcal{N} is a normalization constant which takes into account possible differences of normalization.

3.7 Green functions

A Gaussian integration

In many calculations one needs the Gaussian integral

$$\int_{\mathbb{R}^n} e^{\frac{i}{2} \mathbf{q}^T A \mathbf{q} + i \mathbf{p} \cdot \mathbf{q}} = e^{\frac{\pi i (\nu_+ - \nu_-)}{4}} \frac{(2\pi)^{n/2}}{\sqrt{|\det(A)|}} e^{-\frac{i}{2} \mathbf{p}^T A^{-1} \mathbf{p}}, \quad (A.1)$$

where ν_{\pm} are the number of positive and negative eigenvalues of the matrix A , respectively. This formula can be obtained by starting from the basic Fresnel integral,

$$\int_{\mathbb{R}} e^{iax^2} dx = \exp\left(\frac{\pi i \operatorname{sgn}(a)}{4}\right) \sqrt{\frac{\pi}{|a|}}, \quad (A.2)$$

and diagonalizing A . Since $\nu_+ + \nu_- = n$, we can write the phase in (A.1) as

$$\exp\left[\frac{\pi i n}{4} - \frac{\pi i \nu_-}{2}\right]. \quad (A.3)$$

We will sometimes write the r.h.s of (A.1) as

$$\frac{(2\pi i)^{n/2}}{\sqrt{\det(A)}} e^{-\frac{i}{2} \mathbf{p}^T A^{-1} \mathbf{p}}, \quad (A.4)$$

where the i in the square root leads to the first phase in (A.3), while the square root of the determinant leads to the second phase.

References

- [1] P. Coleman, *Introduction to Many-Body Physics*. Cambridge University Press, 2015.
- [2] A. L. Fetter and J. D. Walecka, *Quantum theory of many-particle systems*. Dover, 2012.