

Chapter 1

Functional integrals *(Last version: 11 June 2009)*

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The aim of this chapter is to introduce the general framework for the study of macroscopic quantum systems. The formalism is based on the functional integral, an extension of Feynman's path integral to systems with an infinite number of degrees of freedom. It enables to derive standard results, such as perturbation expansions, in an economical way and set up non-perturbative approaches. It also provides a unified view of many concepts and theoretical methods that can be found in various fields of physics: condensed-matter physics, quantum optics, nuclear physics or field theory.

We first derive the functional integral representation of the partition function of a system of interacting quantum particles (bosons or fermions) (Secs. 1.2-1.4). This representation is based on second-quantized fields and coherent states. We discuss the perturbative calculation of the partition function and the correlation functions (Green functions), and its representation in terms of Feynman diagrams (Secs. 1.5 and 1.6). These diagrams provide an intuitive picture of perturbation theory in terms of elementary interaction processes taking place in the system. They are also a very efficient tool to partially resum the perturbation series to infinite order. We show how the perturbation expansion should be organized about a broken-symmetry state when a symmetry is spontaneously broken (Sec. 1.7). We also discuss the quantization of the electromagnetic field in the functional integral formalism and the coherent state representation of the partition function of quantum spin systems (Secs. 1.9 and 1.10).

Although Feynman diagrams play an essential role in many-body physics, both as a pictorial representation of perturbation expansions and an efficient computational tool, they also suffer serious drawbacks. On the one hand they often lead to uncontrolled approximations. On the other hand diagrammatic resummations are usually restricted to systems with weak interactions. In many cases, however, one is interested in strongly-correlated systems where the interactions are strong and perturbative expansions likely to fail. We shall see in chapters 7 and ?? how the generating functionals of one-particle and two-particles irreducible vertices introduced in section 1.6 can be used to set up non-perturbative approaches. The effective action (Sec. 1.6.2) is at the basis of the formulation of the non-perturbative renormalization-group approach while the Luttinger-Ward functional (Sec. 1.6.3) is the starting point of various cluster expansions.

This chapter is somewhat formal but constitutes the backbone of the book. The prerequisite knowledge of classical, quantum and statistical mechanics is summarized in Appendices 1.A-1.C. Other Appendices provide technical details on functional calculus, Gaussian integrals and Matsubara sums.

1.1 Introduction

Elementary quantum mechanics is usually formulated in the framework of canonical quantization where observables of the classical theory become quantum mechanical operators acting on state vectors in a Hilbert space (Appendix 1.B). In this introductory section, we discuss an alternative formulation of quantum mechanics based on the Feynman path integral. As in classical mechanics, the concept of trajectories (or paths) plays a central role and the Feynman path integral yields a very intuitive picture of quantum mechanics. For a single quantum particle, there is no real advantage to use the path integral formalism, except for pedagogical purposes, the usual approach based on the Schrödinger equation being often very efficient. However, for systems with a large number of degrees of freedom and in particular in statistical physics, the path integral formalism – or, more precisely, the functional integral formalism – is much more appropriate.

We start our discussion with the study of a quantum particle moving in a static potential (Sec. 1.1.1). Then we consider the functional integral formalism for the quantum harmonic string (Sec. 1.1.2). This example already exhibits many key aspects of the functional integral formalism of quantum many-particle systems that will be introduced in the following sections and used throughout the book.

1.1.1 Path integral in quantum mechanics

To introduce the concept of path integral in quantum mechanics, we consider a particle of mass m in a one-dimensional space. Its classical dynamics is governed by the Lagrangian

$$L(q, \dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q), \quad (1.1)$$

assuming that the particle moves in a time-independent potential $V(q)$. q denotes the position of the particle and $\dot{q} = \partial_t q$. The trajectory of the particle is obtained from

the Euler-Lagrange equation (Appendix 1.A)

$$\frac{d}{dt} \frac{\partial L(q, \dot{q})}{\partial \dot{q}} = \frac{\partial L(q, \dot{q})}{\partial q}, \quad \text{i.e.} \quad m\ddot{q} = -\frac{\partial V(q)}{\partial q}. \quad (1.2)$$

Alternatively, one can consider the Hamiltonian $H(p, q)$ defined by

$$\begin{aligned} p &= \frac{\partial L(q, \dot{q})}{\partial \dot{q}} = m\dot{q}, \\ H(p, q) &= p\dot{q} - L(q, \dot{q}) = \frac{p^2}{2m} + V(q), \end{aligned} \quad (1.3)$$

where p is the momentum conjugated to the variable q . The classical dynamics of the particle then follows from Hamilton's equations of motion,

$$\begin{aligned} \dot{p} &= -\frac{\partial H(p, q)}{\partial q} = -\frac{\partial V(q)}{\partial q}, \\ \dot{q} &= \frac{\partial H(p, q)}{\partial p} = \frac{p}{m}. \end{aligned} \quad (1.4)$$

Canonical quantization

Canonical quantization is achieved by promoting the canonical variables p and q of the classical theory to operators \hat{p} and \hat{q} satisfying the commutation relations

$$[\hat{q}, \hat{p}] = i\hbar. \quad (1.5)$$

A classical variable $A(p, q)$ becomes an operator $\hat{A} \equiv A(\hat{p}, \hat{q})$. In particular, the quantum Hamiltonian reads

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}). \quad (1.6)$$

A physical state of the system is described by a state vector $|\psi(t)\rangle$ of a Hilbert space \mathcal{H} . The time evolution of $|\psi(t)\rangle$ is given by the Schrödinger equation

$$\hat{H}|\psi\rangle = i\hbar\partial_t|\psi(t)\rangle, \quad (1.7)$$

the solution of which can be written in terms of the evolution operator \hat{U} ,

$$|\psi(t)\rangle = \hat{U}(t)|\psi(t=0)\rangle, \quad i\hbar\partial_t\hat{U}(t) = \hat{H}\hat{U}(t). \quad (1.8)$$

The Hamiltonian being time independent, one simply has

$$\hat{U}(t) = \exp\left(-\frac{i}{\hbar}\hat{H}t\right). \quad (1.9)$$

The probability amplitude to find the particle at position q_f at time t_f is given by

$$\psi(q_f, t_f) = \langle q_f | \psi(t_f) \rangle = \langle q_f | \hat{U}(t_f - t_i) | \psi(t_i) \rangle = \int dq_i U(q_f, q_i; t_f - t_i) \psi(q_i, t_i). \quad (1.10)$$

$U(q_f, q_i; t_f - t_i) = \langle q_f | \hat{U}(t_f - t_i) | q_i \rangle$ is sometimes referred to as the propagator, since it expresses the probability amplitude for the particle to propagate from point q_i to

point q_f in a time $t_f - t_i$. If we know a basis $\{|n\rangle, \epsilon_n\}$ of eigenstates of the Hamiltonian \hat{H} , we can write the propagator as

$$\begin{aligned} U(q_f, q_i; t_f - t_i) &= \langle q_f | e^{-\frac{i}{\hbar} \hat{H}(t_f - t_i)} | q_i \rangle = \sum_n \langle q_f | n \rangle e^{-\frac{i}{\hbar} \epsilon_n (t_f - t_i)} \langle n | q_i \rangle \\ &= \sum_n e^{-\frac{i}{\hbar} \epsilon_n (t_f - t_i)} \varphi_n(q_f) \varphi_n^*(q_i) \end{aligned} \quad (1.11)$$

(using the closure relation $\sum_n |n\rangle \langle n| = 1$), where $\varphi_n(q) = \langle q | n \rangle$ denotes the wave function in the coordinate representation. $U(q_f, q_i; t_f - t_i)$ provides information about wavefunctions and energy levels of the Hamiltonian.

Path integral

The propagator $U(q_f, q_i; t)$ can also be represented as a “path integral”. We first consider an infinitesimal time ϵ . To leading order in ϵ , one has¹

$$U(q_f, q_i; \epsilon) = \langle q_f | e^{-i\hat{H}\epsilon} | q_i \rangle \approx \langle q_f | e^{-i\epsilon \frac{\hat{p}^2}{2m}} e^{-i\epsilon V(\hat{q})} | q_i \rangle \quad (1.12)$$

(we now set $\hbar = 1$). The propagator is then calculated by inserting the closure relation $\sum_p |p\rangle \langle p| = 1$,²

$$\begin{aligned} U(q_f, q_i; \epsilon) &= \sum_p \langle q_f | e^{-i\epsilon \frac{\hat{p}^2}{2m}} | p \rangle \langle p | e^{-i\epsilon V(\hat{q})} | q_i \rangle \\ &= \int \frac{dp}{2\pi} \exp \left\{ -i\epsilon \left[\frac{p^2}{2m} + V(q) \right] + ip(q_f - q_i) \right\} \\ &= \left(\frac{m}{2\pi i\epsilon} \right)^{1/2} \exp \left\{ i\epsilon \left[\frac{m}{2} \frac{(q_f - q_i)^2}{\epsilon^2} - V(q_i) \right] \right\}. \end{aligned} \quad (1.13)$$

In order for the integral over p to converge, we assume ϵ to contain a small negative imaginary part. The argument in the exponential is nothing but i times the infinitesimal action $S(q_f, q_i; \epsilon)$ corresponding to the straight line trajectory (at constant velocity) between q_i and q_f in the infinitesimal time ϵ ,

$$U(q_f, q_i; \epsilon) = \left(\frac{m}{2\pi i\epsilon} \right)^{1/2} \exp [iS(q_f, q_i; \epsilon) + \mathcal{O}(\epsilon^2)] \quad (1.14)$$

(writting explicitly that the error in the exponential is of order ϵ^2).

To calculate the propagator $U(q_f, q_i; t_f - t_i)$ for an arbitrary time $t_f - t_i$, we split $t_f - t_i$ into N equal steps of size $\epsilon = (t_f - t_i)/N$; we shall eventually take the limit

¹To first order in ϵ , one has $e^{\epsilon \hat{A} + \epsilon \hat{B}} = 1 + \epsilon(\hat{A} + \hat{B}) + \mathcal{O}(\epsilon^2) = e^{\epsilon \hat{A}} e^{\epsilon \hat{B}} e^{\mathcal{O}(\epsilon^2)}$ for two operators \hat{A} and \hat{B} , where the $\mathcal{O}(\epsilon^2)$ term is given by the commutator $-\frac{\epsilon^2}{2} [\hat{A}, \hat{B}]$. This follows from the Campbell-Baker-Hausdorff formula: $e^{\hat{A} + \hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2} [\hat{A}, \hat{B}]}$ for two operators \hat{A} and \hat{B} which commute with their commutator $[\hat{A}, \hat{B}]$.

²We use the normalization conventions $\langle q | p \rangle = L^{-1/2} e^{ipq}$, $\int dq |q\rangle \langle q| = 1$, and $\sum_p = |p\rangle \langle p| = 1$. $q \in [0, L]$ is a continuous position variable and $p = n \frac{2\pi}{L}$ (n integer) a discrete momentum variable corresponding to periodic boundary conditions ($e^{ipL} = 1$). In the thermodynamic limit $L \rightarrow \infty$, one has $\frac{1}{L} \sum_p \rightarrow \int_{-\infty}^{\infty} \frac{dp}{2\pi}$ (appendix 1.B).

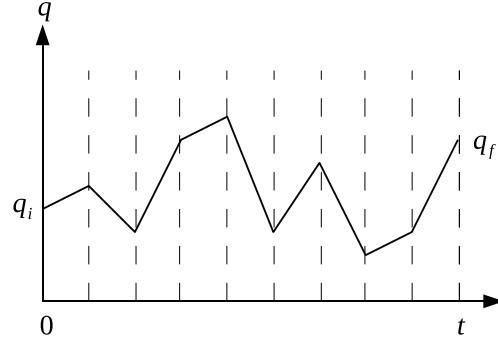


Figure 1.1: A typical discrete trajectory contributing to the action $S[q]$.

$N \rightarrow \infty$ ($\epsilon \rightarrow 0$). Inserting the closure relation $\int dq|q\rangle\langle q| = 1$ at each intermediate time, we obtain

$$\begin{aligned}
 U(q_f, q_i; t_f - t_i) &= \langle q_f | e^{-i\hat{H}\epsilon} \dots e^{-i\hat{H}\epsilon} | q_i \rangle \\
 &= \int \prod_{k=1}^{N-1} dq_k \langle q_f | e^{-i\hat{H}\epsilon} | q_{N-1} \rangle \langle q_{N-1} | e^{-i\hat{H}\epsilon} | q_{N-2} \rangle \dots \langle q_1 | e^{-i\hat{H}\epsilon} | q_i \rangle \\
 &= \int \prod_{k=1}^{N-1} dq_k \prod_{k=1}^N U(q_k, q_{k-1}; \epsilon),
 \end{aligned} \tag{1.15}$$

where $q_0 = q_i$ and $q_N = q_f$. The expression (1.14) introduces an error of order ϵ^2 at each time step, i.e. a total error of order ϵ . In the limit $N \rightarrow \infty$, one therefore finds³

$$U(q_f, q_i; t_f - t_i) = \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i t} \right)^{N/2} \int \prod_{k=1}^{N-1} dq_k \exp\{iS[q]\}, \tag{1.16}$$

where

$$S[q] = \sum_{k=1}^N S(q_k, q_{k-1}; \epsilon) = \epsilon \sum_{k=1}^N \left[\frac{m}{2} \frac{(q_k - q_{k-1})^2}{\epsilon^2} - V(q_{k-1}) \right] \tag{1.17}$$

is the action associated to the discrete trajectory (q_0, q_1, \dots, q_N) with $q_0 = q_i$ and $q_N = q_f$ (Fig. 1.1). In the limit $N \rightarrow \infty$, we may write symbolically

$$\begin{aligned}
 \epsilon \sum_{k=1}^N \frac{m}{2} \frac{(q_k - q_{k-1})^2}{\epsilon^2} &\rightarrow \int_{t_i}^{t_f} dt \frac{m}{2} \dot{q}^2, \\
 \epsilon \sum_{k=1}^N V(q_{k-1}) &\rightarrow \int_{t_i}^{t_f} dt V(q),
 \end{aligned} \tag{1.18}$$

and denote by $q(t)$ the “trajectory” (q_0, \dots, q_N) with $q(t_i) = q_i$ and $q(t_f) = q_f$. Note that this notation does not imply continuity or differentiability of the trajectory

³Note that the extension of (1.16,1.17) to three dimensions is straightforward. The variable q becomes a 3D vector \mathbf{q} and the factor $(mN/2\pi i t)^{N/2}$ should be replaced by $(mN/2\pi i t)^{3N/2}$.

(q_0, q_1, \dots, q_N) in the limit $N \rightarrow \infty$. If we define the integration measure as

$$\mathcal{D}[q] = \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i \hbar t} \right)^{N/2} \prod_{k=1}^{N-1} dq_k, \quad (1.19)$$

then the propagator reads

$$U(q_f, q_i; t_f - t_i) = \int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathcal{D}[q] \exp \left\{ \frac{i}{\hbar} S[q] \right\}, \quad (1.20)$$

where

$$S[q] = \int_{t_i}^{t_f} dt L(q, \dot{q}) \quad (1.21)$$

is the classical action corresponding to the trajectory $q(t)$. Note that the integration measure $\mathcal{D}[q]$ contains a factor that diverges in the limit $N \rightarrow \infty$. In (1.20), we have momentarily restored Planck constant \hbar since it plays an essential role in the discussion of the classical limit (see below). Thus the matrix element of the evolution operator $\hat{U}(t_f - t_i)$ can be represented as a sum over all possible paths going from $q(t_i) = q_i$ to $q(t_f) = q_f$ and weighted by the classical action $S[q]$ times i/\hbar . The Feynman path integral (1.20) provides a nice illustration of the superposition principle of quantum mechanics: when a process can take place in more than one way, its probability amplitude is given by the sum of the amplitudes for each way. Although no explicit reference to quantum mechanical operators is made, the Feynman path integral is an exact representation of the evolution operator $\hat{U}(t) = e^{-i\hat{H}t}$ and may be used as the starting point for the formulation of quantum mechanics [2].

The kinetic term selects sufficiently regular trajectories such that $[q(t+\epsilon) - q(t)]^2/\epsilon$ remains finite in the limit $\epsilon \rightarrow 0$. When this condition is not fulfilled, the kinetic energy is large and the exponential factor $e^{\frac{i}{\hbar} S[q]}$ strongly oscillates when considering nearby trajectories and therefore averages to zero. Thus typical paths are continuous but not necessarily differentiable, and reminiscent of Brownian motion ($|q(t+\epsilon) - q(t)| \sim \sqrt{\epsilon}$).⁴

Classical limit

The important trajectories are those for which the action varies weakly when the path $q(t)$ is slightly deformed, i.e. those which are near the classical trajectory $q_c(t)$ whose action is stationary,

$$\left. \frac{\delta S[q]}{\delta q(t)} \right|_{q_c} = 0. \quad (1.22)$$

Non stationary trajectories imply large oscillations of the action and therefore average to zero (the Feynman paths interfere destructively). More precisely, the propagator $U(q_f, q_i; t_f - t_i)$ is dominated by the trajectories $q(t)$ whose action $S[q]$ differs from the classical action $S_c = S[q_c]$ by a term of order \hbar : $|S - S_c| \lesssim \hbar$. When $|S_c| \gg \hbar$, these trajectories are very close to the classical trajectory and the particle behaves essentially classically. In the opposite limit, the condition $|S - S_c| \lesssim \hbar$ is fulfilled by trajectories very different from the classical one and a full quantum mechanical calculation is necessary. Formally, the classical limit corresponds to the limit $\hbar \rightarrow 0$.

⁴For a detailed discussion of the relation between path integrals and Brownian motion, see Ref. [3].

To obtain the propagator in the limit $\hbar \rightarrow 0$, we write $q(t) = q_c(t) + r(t)$ (assuming there is only one classical trajectory) and expand the action to second order in $r(t)$,

$$U(q_f, q_i; t_f - t_i) \simeq e^{\frac{i}{\hbar} S[q_c]} \int_{r(t_i)=0}^{r(t_f)=0} \mathcal{D}[r] \exp \left\{ \frac{i}{2\hbar} \int_{t_i}^{t_f} dt dt' \frac{\delta^{(2)} S[q]}{\delta q(t) \delta q(t')} \bigg|_{q=q_c} r(t) r(t') \right\}. \quad (1.23)$$

The integral is Gaussian and can be done exactly (Appendix 1.E),

$$U(q_f, q_i; t_f - t_i) \simeq e^{\frac{i}{\hbar} S[q_c]} \det \left(\frac{1}{2\pi i \hbar} \frac{\delta^{(2)} S[q]}{\delta q(t) \delta q(t')} \bigg|_{q=q_c} \right)^{-1/2}. \quad (1.24)$$

The procedure we have followed to obtain (1.24) is known as the stationary phase approximation. It gives the leading term of an expansion in powers of \hbar that can be systematically carried out to higher-order (see Sec. 1.7).

Hamiltonian form of the path integral

Equations (1.20) and (1.21) define the Lagrangian form of the path integral, where the action is expressed in terms of the Lagrangian and the functional integral involves a sum over the paths $q(t)$. Alternatively, one can keep explicitly the p variable appearing in (1.13) and write the propagator as

$$\begin{aligned} U(q_f, q_i; t_f - t_i) &= \lim_{N \rightarrow \infty} \int \prod_{k=1}^{N-1} dq_k \int \prod_{k=1}^N \frac{dp_k}{2\pi} e^{\sum_{k=1}^N [ip_k(q_k - q_{k-1}) - i\epsilon \frac{p_k^2}{2m} - i\epsilon V(q_{k-1})]} \\ &\equiv \int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathcal{D}[p, q] \exp\{iS[p, q]\}, \end{aligned} \quad (1.25)$$

where

$$\begin{aligned} \mathcal{D}[p, q] &= \lim_{N \rightarrow \infty} \prod_{k=1}^{N-1} dq_k \prod_{k=1}^N \frac{dp_k}{2\pi}, \\ S[p, q] &= \lim_{N \rightarrow \infty} \sum_{k=1}^N \left[p_k(q_k - q_{k-1}) - \epsilon \frac{p_k^2}{2m} - \epsilon V(q_{k-1}) \right] \\ &\equiv \int_{t_i}^{t_f} dt [p\dot{q} - H(p, q)]. \end{aligned} \quad (1.26)$$

Equations (1.25) and (1.26) give the Hamiltonian form of the path integral, where the action $S[p, q]$ is a function of the position q as well as the momentum p of the particle. Note that q and p are independent variables in the functional integral (1.25) and only q is fixed at the initial (t_i) and final (t_f) times. When the particle travels from q_{k-1} to q_k , its momentum is given by p_k (which is independent of the velocity $(q_k - q_{k-1})/\epsilon$) so that the path is not a classical trajectory. The interpretation of the propagator as a sum over classical paths is therefore lost in the Hamiltonian form

of the path integral. Nevertheless, for $\hbar \rightarrow 0$, the path integral is dominated by the trajectories satisfying

$$\frac{\delta S}{\delta p(t)} = \frac{\delta S}{\delta q(t)} = 0, \quad (1.27)$$

and one recovers Hamilton's equations of motion.

Euclidean path integral

Suppose we want to calculate the partition function

$$Z = \text{Tr} e^{-\beta \hat{H}} = \int dq \langle q | e^{-\beta \hat{H}} | q \rangle \quad (1.28)$$

of the quantum particle considered above. Z can be obtained from the matrix elements of the evolution operator $e^{-i\hat{H}t}$ evaluated at the imaginary time $t = -i\beta$ (or $t = -i\beta\hbar$ if we restore \hbar). Real-time dynamics and quantum statistical mechanics are thus related by the transformation $t \rightarrow -i\tau$ known as a Wick rotation, i.e. a rotation of angle $\pi/2$ in the complex time plane. The concept of imaginary time plays an essential role in quantum statistical physics. The propagator in imaginary time, $U(q_i, q_f; -i\tau) = \langle q_f | e^{-\hat{H}\tau} | q_i \rangle$ is given by (1.11) with the replacement $t \rightarrow -i\tau$. It can be represented as a path integral following the same steps as before,⁵

$$\begin{aligned} U(q_f, q_i; -i\tau) &= \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi\tau} \right)^{N/2} \int \prod_{k=1}^{N-1} dq_k e^{-\epsilon \sum_{k=1}^N \left[\frac{m}{2} \frac{(q_k - q_{k-1})^2}{\epsilon^2} + V(q_{k-1}) \right]} \\ &= \int_{q(0)=q_i}^{q(\tau)=q_f} \mathcal{D}[q] \exp \{ -S_E[q] \}. \end{aligned} \quad (1.29)$$

The imaginary-time path integral is defined by a sum over trajectories from $q(0) = q_i$ to $q(\tau) = q_f$ weighted by the action

$$S_E[q] = \int_0^\tau d\tau' \left[\frac{m}{2} \dot{q}^2 + V(q) \right]. \quad (1.30)$$

$S_E[q]$ is referred to as the Euclidean action since (imaginary) time and space enter the action in a symmetric way.⁶ Note that the kinetic and potential terms have the same sign in the Euclidean Lagrangian, since the kinetic term changes sign under the Wick rotation $\tau = it$. As in the real-time formalism, the kinetic term selects trajectories such that $[q(\tau + \epsilon) - q(\tau)]^2/\epsilon$ remains finite in the limit $\epsilon \rightarrow 0$ – paths that do not fulfill this condition are exponentially suppressed – so that the paths contributing to the propagator are continuous (but not necessarily differentiable). The real-time action (1.21) can be recovered from S_E performing a Wick rotation,

$$S_E[q] \xrightarrow[\substack{\text{Wick rotation} \\ (\tau = it)}]{\quad} -i \int_0^t dt' \left[\frac{m}{2} \dot{q}^2 - V(q) \right] = -iS[q]. \quad (1.31)$$

⁵Contrary to the real-time propagator, there is no need here to add a small imaginary part to the infinitesimal time ϵ (see the remark after (1.13)). From a mathematical point of view, the Euclidean formalism is preferable to the real-time one.

⁶For example, $c^2 t^2 - x^2$ becomes $-c^2 \tau^2 - x^2$ in the Euclidean formalism.

Using the preceding results, we can express the partition function of the quantum particle,

$$Z = \int dq U(q, q, -i\beta) = \int_{q(\beta)=q(0)} \mathcal{D}[q] e^{-S_E[q]}, \quad (1.32)$$

as a path integral in imaginary time over all periodic trajectories of period β .

If $\beta \rightarrow 0$ (i.e. $T \rightarrow \infty$) or $\hbar \rightarrow 0$, the propagator $U(q, q; -i\beta\hbar)$ can be calculated with a single time step $N = 1$ (we restore \hbar in this paragraph). This leads to

$$\begin{aligned} Z_{\text{cl}} &= \frac{1}{\hbar} \sqrt{\frac{m}{2\pi\beta}} \int dq e^{-\beta V(q)} \\ &\equiv \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \int_{-\infty}^{\infty} dq \exp\left\{-\beta \left[\frac{p^2}{2m} + V(q)\right]\right\}, \end{aligned} \quad (1.33)$$

which is nothing but the classical partition function. In Sec. 1.1.2, we shall further discuss the connection between high-temperature limit and classical behavior of a quantum system.

Example: free particle and harmonic oscillator. Let us first consider the propagator of a free particle,

$$U(q_f, q_i; t) = \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i t}\right)^{N/2} \int \prod_{k=1}^{N-1} dq_k \exp\left\{i \frac{m}{2\epsilon} \sum_{k=1}^N (q_k - q_{k-1})^2\right\}. \quad (1.34)$$

One can successively integrate over q_1, q_2 , etc. The integral over q_1 gives

$$\begin{aligned} U(q_f, q_i; t) &= \frac{1}{\sqrt{2}} \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i t}\right)^{(N-1)/2} \\ &\times \int \prod_{k=2}^{N-1} dq_k \exp\left\{i \frac{m}{4\epsilon} (q_2 - q_i)^2 + i \frac{m}{2\epsilon} \sum_{k=3}^N (q_k - q_{k-1})^2\right\}. \end{aligned} \quad (1.35)$$

Integrating then over q_2 yields

$$\begin{aligned} U(q_f, q_i; t) &= \frac{1}{\sqrt{3}} \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i t}\right)^{(N-2)/2} \\ &\times \int \prod_{k=3}^{N-1} dq_k \exp\left\{i \frac{m}{6\epsilon} (q_3 - q_i)^2 + i \frac{m}{2\epsilon} \sum_{k=4}^N (q_k - q_{k-1})^2\right\}, \end{aligned} \quad (1.36)$$

and we easily deduce the final result

$$U(q_f, q_i; t) = \left(\frac{m}{2\pi i t}\right)^{1/2} \exp\left(i \frac{m(q_f - q_i)^2}{2t}\right). \quad (1.37)$$

We recognize in the exponential i times the classical action: the classical path gives the exact propagator for a free particle. The result (1.37) can also be directly obtained from the definition (1.11) of the propagator using the eigenstates $\varphi_p(q) = L^{-1/2} e^{ipq}$ with $\epsilon_p = p^2/2m$.

Let us now consider the harmonic oscillator action

$$S[q] = \frac{m}{2} \int_{t_i}^{t_f} dt (\dot{q}^2 - \omega^2 q^2). \quad (1.38)$$

Although it is possible to do the calculation in discrete time (see e.g. Ref. [5]), we take the continuum time limit. (The discrete time calculation is carried out below for the partition function.) To compute the propagator, we write $q(t) = q_c(t) + r(t)$. The classical trajectory q_c satisfies the equation of motion $\ddot{q} + \omega^2 q^2 = 0$ and reads

$$q_c(t) = A \cos(\omega t) + B \sin(\omega t) \quad (1.39)$$

with the boundary conditions

$$q_i = A \cos(\omega t_i) + B \sin(\omega t_i) \quad \text{and} \quad q_f = A \cos(\omega t_f) + B \sin(\omega t_f), \quad (1.40)$$

while the classical action is given by

$$S[q_c] = \frac{m\omega}{2 \sin(\omega(t_f - t_i))} [(q_f^2 + q_i^2) \cos(\omega(t_f - t_i)) - 2q_i q_f]. \quad (1.41)$$

Writing

$$\begin{aligned} q(t) &= q_c + r(t), \\ S[q] &= S[q_c] + \frac{m}{2} \int_{t_i}^{t_f} dt (\dot{r}^2 - \omega^2 r^2) \end{aligned} \quad (1.42)$$

(with $r(t_i) = r(t_f) = 0$), one obtains

$$U(q_f, q_i; t_f - t_i) = e^{iS[q_c]} \int \mathcal{D}[r] \exp \left\{ i \frac{m}{2} \int_{t_i}^{t_f} dt (\dot{r}^2 - r^2) \right\}. \quad (1.43)$$

Taking advantage of the boundary conditions $r(t_i) = r(t_f) = 0$, one can expand $r(t)$ in a Fourier series.

$$r(t) = \sum_{l=1}^{\infty} a_l \sin \left(\frac{l\pi(t - t_i)}{T} \right). \quad (1.44)$$

with $T = t_f - t_i$. The action then reads

$$S[r] = \frac{mT}{4} \sum_{l=1}^{\infty} a_l^2 \left(\frac{l^2 \pi^2}{T^2} - \omega^2 \right) \quad (1.45)$$

and the integration over $r(t)$ becomes an integration over the coefficients a_l ,

$$\mathcal{D}[r] \rightarrow J(T) \prod_{l=1}^{\infty} \int_{-\infty}^{\infty} da_l, \quad (1.46)$$

with a Jacobian $J(T)$ that depends on T but not on ω . We then find

$$\begin{aligned} \int \mathcal{D}[r] \exp\{iS[r]\} &\propto \prod_{l=1}^{\infty} \int_{-\infty}^{\infty} da_l \exp \left[i \frac{mT}{4} \left(\frac{l^2 \pi^2}{T^2} - \omega^2 \right) a_l^2 \right] \\ &\propto \prod_{l=1}^{\infty} \left(\frac{l^2 \pi^2}{T^2} - \omega^2 \right)^{-1/2} \\ &\propto \left(\frac{\omega T}{\sin(\omega T)} \right)^{1/2}, \end{aligned} \quad (1.47)$$

where at each step the proportionality constant is independent of ω . We have used the identity

$$\prod_{l=1}^{\infty} \left(1 - \frac{z^2}{l^2 \pi^2}\right) = \frac{\sin z}{z}. \quad (1.48)$$

We then have

$$U(q_f, q_i; T) = \mathcal{N}(T) \left(\frac{\omega T}{\sin(\omega T)} \right)^{1/2} e^{iS[q_c]}. \quad (1.49)$$

For $\omega \rightarrow 0$, we must reproduce the free particle result (1.37), which fixes the constant $\mathcal{N}(T)$, so that

$$U(q_f, q_i; t_f - t_i) = \left(\frac{m\omega}{2\pi i \sin(\omega(t_f - t_i))} \right)^{1/2} \times \exp \left\{ i \frac{m\omega}{2 \sin(\omega(t_f - t_i))} [(q_f^2 + q_i^2) \cos(\omega(t_f - t_i)) - 2q_i q_f] \right\}. \quad (1.50)$$

By setting $t_f - t_i \rightarrow -i\beta$, one obtains the imaginary time propagator

$$U(q_f, q_i, -i\beta) = \left(\frac{m\omega}{2\pi \sinh(\beta\omega)} \right)^{1/2} \times \exp \left\{ -\frac{m\omega}{2 \sinh(\beta\omega)} [(q_f^2 + q_i^2) \cosh(\beta\omega) - 2q_i q_f] \right\}. \quad (1.51)$$

and the partition function

$$Z = \int_{-\infty}^{\infty} dq U(q, q, -i\beta) = \frac{e^{-\beta\omega/2}}{1 - e^{-\beta\omega}} \quad (1.52)$$

of the harmonic oscillator.

Alternatively, one can calculate the partition function directly in the Euclidean formalism by writing

$$q_k = \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} a_l e^{-i\omega_l \tau_k}, \quad (1.53)$$

where $\tau_k = k\epsilon = k\beta/N$, $\omega_l = l2\pi/\beta$, $a_l^* = a_{N-l}$ and $a_0 = a_0^*$ (q_k is real). The action reads

$$S_E[a] = \frac{m}{\epsilon} \sum_{l=0}^{N-1} \left\{ [1 - \cos(\omega_l \epsilon)] + \frac{1}{2} \epsilon^2 \omega^2 \right\} a_l^* a_l, \quad (1.54)$$

and the partition function is given by a product of Gaussian integrals (Appendix 1.E),

$$\begin{aligned} Z &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi\epsilon} \right)^{N/2} \int \prod_{l=0}^{N-1} da_l^* da_l e^{-S_E[a]} \\ &= \lim_{N \rightarrow \infty} \left(\frac{1}{2\epsilon} \right)^{N/2} \prod_{l=0}^{N-1} \left\{ \frac{1}{\epsilon} [1 - \cos(\omega_l \epsilon)] + \frac{1}{2} \epsilon \omega^2 \right\}^{-1/2} \end{aligned} \quad (1.55)$$

(the exponent 1/2 is due to the constraints $a_l^* = a_{N-l}$ and $a_0^* = a_0$). Writing $\cosh \theta = 1 + \epsilon^2 \omega^2 / 2$ and using the identity

$$\prod_{l=0}^{N-1} [\cosh \theta - \cos(\omega_l \epsilon)] = 2^{1-N} [\cosh(N\theta) - 1], \quad (1.56)$$

one reproduces the result (1.52).

Let us finally try to calculate the partition function directly in the continuum time limit. With

$$q(\tau) = \frac{1}{\sqrt{\beta}} \sum_{l=-\infty}^{\infty} a_l e^{-i\omega_l \tau} \quad (1.57)$$

and $a_l^* = a_{-l}$ ($q(\tau)$ is real), the Euclidean action becomes

$$S_E[a] = \frac{m}{2} \sum_{l=-\infty}^{\infty} (\omega_l^2 + \omega^2) |a_l|^2, \quad (1.58)$$

which leads to the partition function

$$Z = \int \mathcal{D}[q] e^{-S_E[q]} \propto \prod_{l=-\infty}^{\infty} \frac{1}{\sqrt{\omega_l^2 + \omega^2}}, \quad (1.59)$$

making use of the result for Gaussian integration (Appendix 1.E). The product in the rhs vanishes. To get a finite result for the partition function, one should take into account the infinite factor included in the integration measure $\mathcal{D}[q]$ (that was dropped in (1.59)). This infinite factor being ω independent, the derivative of $\ln Z$ wrt ω is however well defined,

$$\frac{\partial \ln Z}{\partial \omega} = - \sum_{l=-\infty}^{\infty} \frac{\omega}{\omega_l^2 + \omega^2} = - \frac{\beta}{2 \tanh(\beta\omega/2)} \quad (1.60)$$

(the method to compute the sum over ω_l in (1.60) is explained in Appendix 1.F), so that

$$Z = \frac{\mathcal{N}}{\sinh(\beta\omega/2)}, \quad (1.61)$$

where the constant \mathcal{N} is independent of ω . Since \mathcal{N} is dimensionless, it cannot be a function of β alone and is therefore a pure number. It can be determined by noting that $\lim_{\beta \rightarrow \infty} Z = e^{-\beta\epsilon_0}$ with $\epsilon_0 = \omega/2$ the energy of the ground state. This yields $\mathcal{N} = 2$ and in turn the result (1.52).

Path integral with vector potential⁷

To quantize a classical Hamiltonian $H(p, q)$, it is not always sufficient to replace the classical variables p and q by the corresponding quantum operators. When this correspondence rule yields products of the non-commuting operators \hat{p} and \hat{q} , the order of the operators should be determined by additional conditions such as the hermiticity of the Hamiltonian. These difficulties also show up in the path integral formulation: the path integral should be carefully defined in order to respect the proper ordering of the operators.

As an example, we consider a free particle moving in a three-dimensional space in the presence of a magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$. Its dynamics is governed by the Lagrangian

$$L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2} m \dot{\mathbf{q}}^2 + e \dot{\mathbf{q}} \cdot \mathbf{A}(\mathbf{q}) \quad (1.62)$$

⁷This section closely follows chapter 5 and Sec. I.A of the Supplements in Ref. [3]. See also Ref. [4].

(e is the charge of the particle). The conjugated momentum is defined by $\mathbf{p} = \partial L / \partial \dot{\mathbf{q}} = m\dot{\mathbf{q}} + e\mathbf{A}(\mathbf{q})$ and the classical Hamiltonian reads

$$H(\mathbf{p}, \mathbf{q}) = \frac{[\mathbf{p} - e\mathbf{A}(\mathbf{q})]^2}{2m}. \quad (1.63)$$

In order to determine the quantum Hamiltonian, one has to choose the order of the operators in the product $\hat{\mathbf{p}} \cdot \mathbf{A}(\hat{\mathbf{q}})$. By requiring the Hamiltonian to be hermitian, one obtains

$$\hat{H} = \frac{1}{2m} [\hat{\mathbf{p}}^2 - e\hat{\mathbf{p}} \cdot \mathbf{A}(\hat{\mathbf{q}}) - e\mathbf{A}(\hat{\mathbf{q}}) \cdot \hat{\mathbf{p}} + e^2 \mathbf{A}(\hat{\mathbf{q}})^2] = \frac{[\hat{\mathbf{p}} - e\mathbf{A}(\hat{\mathbf{q}})]^2}{2m}. \quad (1.64)$$

This expression can also be deduced from gauge invariance, which implies that the Hamiltonian can only be a function of the gauge invariant combination $\hat{\mathbf{p}} - e\mathbf{A}(\hat{\mathbf{q}})$. Any other quantification choice would add to the Hamiltonian a term proportional to the commutator $e[\hat{\mathbf{p}}, \mathbf{A}(\hat{\mathbf{q}})] = -ie\nabla \cdot \mathbf{A}(\hat{\mathbf{q}})$ which would violate both hermiticity and gauge invariance.

Because of the additional term $e\dot{\mathbf{q}} \cdot \mathbf{A}(\mathbf{q})$ in the Lagrangian (1.62), we expect the action $S(\mathbf{q}_k, \mathbf{q}_{k-1}; \epsilon)$ along the infinitesimal trajectory $(\mathbf{q}_k, \mathbf{q}_{k-1})$ to write

$$S(\mathbf{q}_k, \mathbf{q}_{k-1}; \epsilon) = \frac{m(\mathbf{q}_k - \mathbf{q}_{k-1})^2}{2\epsilon} + e(\mathbf{q}_k - \mathbf{q}_{k-1}) \cdot \mathbf{A}(\mathbf{q}), \quad (1.65)$$

but it is not clear whether $\mathbf{A}(\mathbf{q})$ should be evaluated at \mathbf{q}_k , \mathbf{q}_{k-1} , or somewhere in between. Since typical paths satisfy $|\mathbf{q}_k - \mathbf{q}_{k-1}| \sim \sqrt{\epsilon}$, different discretizations of $\dot{\mathbf{q}} \cdot \mathbf{A}(\mathbf{q})$ lead to changes in the action of order ϵ which cannot be ignored. The proper choice can be obtained by noting that the hermiticity of the Hamiltonian implies $U(\mathbf{q}_k, \mathbf{q}_{k-1}; \epsilon)^* = U(\mathbf{q}_{k-1}, \mathbf{q}_k; -\epsilon)$ and therefore $S(\mathbf{q}_k, \mathbf{q}_{k-1}; \epsilon) = -S(\mathbf{q}_{k-1}, \mathbf{q}_k; -\epsilon)$. The only possibility is then to evaluate the vector potential at the midpoint $(\mathbf{q}_k + \mathbf{q}_{k-1})/2$. The choice $[\mathbf{A}(\mathbf{q}_k) + \mathbf{A}(\mathbf{q}_{k-1})]/2$ (or any other combination symmetric in $\mathbf{q}_k, \mathbf{q}_{k-1}$) is also possible, since two symmetric combinations differ by a term $\mathcal{O}[(\mathbf{q}_k - \mathbf{q}_{k-1})^2] = \mathcal{O}(\epsilon)$ and the corresponding actions by a negligible term $\mathcal{O}(\epsilon^{3/2})$.

The “midpoint” rule that follows from the hermiticity of the Hamiltonian is the only choice compatible with gauge invariance. In the gauge transformation $\mathbf{A} \rightarrow \mathbf{A} + \nabla\Lambda$, the action along the path $(\mathbf{q}_i, t_i) \rightarrow (\mathbf{q}_f, t_f)$ changes by a term

$$e \int_{t_i}^{t_f} dt \dot{\mathbf{q}} \cdot \nabla\Lambda(\mathbf{q}) = e \int_{\mathbf{q}_i}^{\mathbf{q}_f} d\mathbf{q} \cdot \nabla\Lambda(\mathbf{q}) = e[\Lambda(\mathbf{q}_f) - \Lambda(\mathbf{q}_i)]. \quad (1.66)$$

The corresponding change in the propagator,

$$U(\mathbf{q}_f, \mathbf{q}_i; t_f - t_i) \rightarrow e^{ie\Lambda(\mathbf{q}_f)} U(\mathbf{q}_f, \mathbf{q}_i; t_f - t_i) e^{-ie\Lambda(\mathbf{q}_i)}, \quad (1.67)$$

reflects the change in the phase of the wavefunctions

$$\varphi(\mathbf{q}) \rightarrow e^{ie\Lambda(\mathbf{q})} \varphi(\mathbf{q}) \quad (1.68)$$

(see Eq. (1.11)). Up to a trivial phase factor, the propagator is independent of the function Λ (gauge invariance). In the path integration formulation, the change in the action is given by

$$e \sum_{k=1}^N (\mathbf{q}_k - \mathbf{q}_{k-1}) \cdot \nabla\Lambda(\mathbf{u}_k), \quad (1.69)$$

if we choose to evaluate the vector potential in (1.65) at the point \mathbf{u}_k . To see whether (1.66) and (1.69) agree, we assume Λ to be a well-behaved function and rewrite (1.66) as

$$\begin{aligned}\Lambda(\mathbf{q}_f) - \Lambda(\mathbf{q}_i) &= \sum_{k=1}^N [\Lambda(\mathbf{q}_k) - \Lambda(\mathbf{q}_{k-1})] \\ &= \sum_{k=1}^N \left\{ (\mathbf{q}_k - \mathbf{q}_{k-1}) \cdot \nabla \Lambda(\mathbf{u}_k) \right. \\ &\quad \left. + \frac{1}{2}(1-2\theta)[(\mathbf{q}_k - \mathbf{q}_{k-1}) \cdot \nabla]^2 \Lambda(\mathbf{u}_k) + \mathcal{O}[(\mathbf{q}_k - \mathbf{q}_{k-1})^3] \right\},\end{aligned}\quad (1.70)$$

where $\mathbf{u}_k = \mathbf{q}_{k-1} + \theta(\mathbf{q}_k - \mathbf{q}_{k-1})$ (with $0 \leq \theta \leq 1$). Since $|\mathbf{q}_k - \mathbf{q}_{k-1}|^2$ is of order ϵ for typical paths, the second term in the rhs of the last equation does not vanish in the limit $\epsilon \rightarrow 0$ unless $\theta = 1/2$, i.e. $\mathbf{u}_k = (\mathbf{q}_k + \mathbf{q}_{k-1})/2$ (midpoint rule). With this choice, equations (1.66) and (1.69) agree.

We conclude this section by showing that the midpoint rule can also be obtained from an explicit calculation of the propagator $U(\mathbf{q}_k, \mathbf{q}_{k-1}; \epsilon)$. We rewrite the latter as

$$U(\mathbf{q}_k, \mathbf{q}_{k-1}; \epsilon) = \frac{1}{(2i\pi)^{3/2}} \int d^3u e^{\frac{i}{2}\mathbf{u}^2} \langle \mathbf{q}_k | e^{-i\bar{\epsilon}\mathbf{u} \cdot [\hat{\mathbf{p}} - eA(\hat{\mathbf{q}})]} | \mathbf{q}_{k-1} \rangle, \quad (1.71)$$

where $\bar{\epsilon} = \sqrt{\epsilon/m}$. Contrary to what was done previously, it is not possible to factorize the exponential. This would introduce an error of order $\bar{\epsilon}^2 = \epsilon/m$, whereas we need the error to be smaller than ϵ to construct the path integral over a finite time interval $t_f - t_i$. This difficulty can be circumvented by using the relation

$$e^{\bar{\epsilon}(\hat{A} + \hat{B})} = e^{\frac{\bar{\epsilon}}{2}\hat{B}} e^{\bar{\epsilon}\hat{A}} e^{\frac{\bar{\epsilon}}{2}\hat{B}} + \mathcal{O}(\bar{\epsilon}^3), \quad (1.72)$$

which can be checked by a direct expansion of the exponentials. We then deduce

$$\langle \mathbf{q}_k | e^{-i\bar{\epsilon}\mathbf{u} \cdot [\hat{\mathbf{p}} - eA(\hat{\mathbf{q}})]} | \mathbf{q}_{k-1} \rangle = e^{\frac{i}{2}e\bar{\epsilon}\mathbf{u} \cdot \mathbf{A}(\mathbf{q}_k)} \langle \mathbf{q}_k | e^{-i\bar{\epsilon}\mathbf{u} \cdot \hat{\mathbf{p}} + \mathcal{O}(\epsilon^{3/2})} | \mathbf{q}_{k-1} \rangle e^{\frac{i}{2}e\bar{\epsilon}\mathbf{u} \cdot \mathbf{A}(\mathbf{q}_{k-1})}, \quad (1.73)$$

where the $\mathcal{O}(\epsilon^{3/2})$ error can now be ignored. The matrix element in (1.73) is calculated by inserting the closure relation $\sum_{\mathbf{p}} |\mathbf{p}\rangle \langle \mathbf{p}| = 1$,

$$\begin{aligned}\langle \mathbf{q}_k | e^{-i\bar{\epsilon}\mathbf{u} \cdot \hat{\mathbf{p}}} | \mathbf{q}_{k-1} \rangle &= \sum_{\mathbf{p}, \mathbf{p}'} \langle \mathbf{q}_k | \mathbf{p} \rangle \langle \mathbf{p} | e^{-i\bar{\epsilon}\mathbf{u} \cdot \hat{\mathbf{p}}} | \mathbf{p}' \rangle \langle \mathbf{p}' | \mathbf{q}_{k-1} \rangle \\ &= \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p} \cdot (\mathbf{q}_k - \mathbf{q}_{k-1} - \bar{\epsilon}\mathbf{u})} = \frac{1}{\bar{\epsilon}^3} \delta\left(\frac{\mathbf{q}_k - \mathbf{q}_{k-1}}{\bar{\epsilon}} - \mathbf{u}\right),\end{aligned}\quad (1.74)$$

which gives

$$\begin{aligned}U(\mathbf{q}_k, \mathbf{q}_{k-1}; \epsilon) &= \left(\frac{m}{2i\pi\epsilon}\right)^{3/2} \exp\left\{i\bar{\epsilon}\left[\frac{m}{2}\frac{(\mathbf{q}_k - \mathbf{q}_{k-1})^2}{\epsilon^2}\right.\right. \\ &\quad \left.\left.+ \frac{e}{2}\frac{\mathbf{q}_k - \mathbf{q}_{k-1}}{\epsilon} \cdot (\mathbf{A}(\mathbf{q}_k) + \mathbf{A}(\mathbf{q}_{k-1}))\right]\right\}.\end{aligned}\quad (1.75)$$

We recognize in the exponential i times the action (1.65) with the vector potential $\mathbf{A}(\mathbf{q})$ approximated by $[\mathbf{A}(\mathbf{q}_k) + \mathbf{A}(\mathbf{q}_{k-1})]/2$ which, as discussed above, is equivalent to the midpoint rule.⁸

Many-particle systems

With little more effort, we can now write a path integral for the partition function – or the propagator – of a system with N particles interacting via a two-body potential $v(q_i - q_j)$ (we consider a one-dimensional system for simplicity). The Hilbert space is defined as the subspace of the tensor product $\mathcal{H} \otimes \cdots \otimes \mathcal{H}$ (\mathcal{H} denotes the one-particle Hilbert space) containing all N -particle states properly symmetrized or antisymmetrized according to the quantum statistics of the particles. The partition function can be written as (see Sec. 1.2)

$$Z = \frac{1}{N!} \sum_{p \in S_N} \epsilon_p \int dq_1 \cdots dq_N (q_1 \cdots q_N | e^{-\beta \hat{H}} | q_{p(1)} \cdots q_{p(N)}), \quad (1.76)$$

where $|q_1 \cdots q_N\rangle = |q_1\rangle \otimes \cdots \otimes |q_N\rangle$. The sum in (1.76) is over all permutations p of $\{1, \dots, N\}$. ϵ^p equals one for bosons and the signature of the permutation p for fermions. Proceeding as in the one-particle case and inserting the closure relation

$$\int dq_1 \cdots dq_N |q_1 \cdots q_N\rangle \langle q_1 \cdots q_N| = 1 \quad (1.77)$$

at each time step, we obtain the path integral

$$Z = \frac{1}{N!} \sum_{p \in S_N} \epsilon_p \int_{q_i(\beta) = q_{p(i)}(0)} \mathcal{D}[q] \exp \{-S_E[q]\} \quad (1.78)$$

with the Euclidean action

$$S_E[q] = \int_0^\beta d\tau \left[\frac{m}{2} \sum_{i=1}^N \dot{q}_i^2 + \sum_{\substack{i,j=1 \\ (i < j)}}^N v(q_i - q_j) \right]. \quad (1.79)$$

This expression bears an obvious similarity with that obtained for a single particle. It is however not well suited for the study of a many-particle system. In Sec. 1.4 we shall introduce a path integral or, more precisely, a functional integral representation of the partition function that turns out to be much more convenient. This functional integral is based on the coherent states introduced in Sec. 1.3 and involves an integration over all configurations of a field weighted by an appropriate action. This turns out to be an essential aspect of (quantum) statistical physics and field theory: systems with an infinite number of degrees of freedom are naturally described by fields, rather than the set of coordinates of all particles. Before embarking on the study of field theories of quantum systems, we consider in the next section an elementary example of field theory.

⁸One can also directly verify that $U(\mathbf{q}_k, \mathbf{q}_{k-1}; \epsilon)$ yields the time evolution of the wavefunction as obtained from the Hamiltonian (1.64) [3]. This provides a definitive proof of the validity of the path integral.

1.1.2 Functional integral in statistical physics

In this section, we consider the functional integral approach to the quantum harmonic string. This simple example already exhibits many essential aspects of the field theory of (more complicated, i.e. anharmonic) quantum systems.⁹

The classical harmonic string

We consider a one-dimension harmonic string of length L and mass per unit length ρ . We denote by $\phi(x, t)$ the displacement of the infinitesimal mass ρdx located between x and $x + dx$ at equilibrium. The dynamics of the chain is governed by the Lagrangian

$$L[\phi] = \int_0^L dx \mathcal{L}(\partial_x \phi, \dot{\phi}), \quad (1.80)$$

$$\mathcal{L}(\partial_x \phi, \dot{\phi}) = \frac{1}{2} \rho \dot{\phi}^2 - \frac{1}{2} \kappa (\partial_x \phi)^2,$$

where \mathcal{L} is referred to as the Lagrangian density. The first term in the rhs of (1.80) corresponds to the kinetic energy while the second one gives the energy cost associated to the deformation of the string. The harmonic string can be seen as the low-energy or long-wavelength limit of a one-dimensional “crystal” consisting of masses $m = \rho a$ separated by a distance a (at equilibrium) and connected by springs with stiffness κ/a .¹⁰

The Euler-Lagrange equation

$$\frac{d}{dt} \frac{\partial \mathcal{L}(\partial_x \phi, \dot{\phi})}{\partial \dot{\phi}} + \frac{d}{dx} \frac{\partial \mathcal{L}(\partial_x \phi, \dot{\phi})}{\partial (\partial_x \phi)} = 0 \quad (1.81)$$

gives the wave equation

$$\rho \ddot{\phi} - \kappa \partial_x^2 \phi = 0. \quad (1.82)$$

The solutions are plane waves $\phi(x, t) \propto e^{i(kx - c|k|t)} + \text{c.c.}$ propagating with the velocity $c = \sqrt{\kappa/\rho}$, where $k = p \frac{2\pi}{L}$ (p integer) for periodic boundary conditions $\phi(x + L, t) = \phi(x, t)$.

The quantum harmonic string

The momentum conjugated to $\phi(x, t)$ is

$$\Pi(x, t) = \frac{\partial \mathcal{L}(\partial_x \phi, \dot{\phi})}{\partial \dot{\phi}(x, t)} = \rho \dot{\phi}(x, t) \quad (1.83)$$

⁹In a particle language, an “harmonic” system (i.e. a system whose Lagrangian is quadratic in its variables) corresponds to non-interacting particles, whereas an “anharmonic” system includes interactions between particles. These particles do not necessary correspond to the bare particles but can refer to elementary excitations (a concept that will be explained in the forthcoming chapters).

¹⁰The Lagrangian of the one-dimensional crystal reads $L(q_i, \dot{q}_i) = \frac{1}{2} \sum_{i=1}^n [m \dot{q}_i^2 - k_s (q_{i+1} - q_i)^2]$, where q_i denotes the displacement of the i th atom with respect to its equilibrium position. We leave it as an exercise to show that the normal modes (phonons) of this system propagate with frequencies $\omega_k = \sqrt{2k_s/m(1 - \cos ka)}^{1/2}$. In the long wavelength limit $|k|a \ll 1$, one recovers the spectrum $\omega = c|k|$ of the harmonic continuous string.

and the Hamiltonian is defined by

$$H = \int_0^L dx \left[\Pi \dot{\phi} - \mathcal{L}(\partial_x \phi, \dot{\phi}) \right] = \int_0^L dx \left[\frac{\Pi^2}{2\rho} + \frac{1}{2} \kappa (\partial_x \phi)^2 \right]. \quad (1.84)$$

To quantize the string, we promote ϕ and Π to operators satisfying the commutation relations

$$[\hat{\phi}(x), \hat{\Pi}(x')] = i\delta(x - x'). \quad (1.85)$$

It is convenient to introduce the Fourier transformed operators

$$\begin{aligned} \hat{\phi}(k) &= \frac{1}{\sqrt{L}} \int_0^L dx e^{-ikx} \hat{\phi}(x) = \hat{\phi}^\dagger(-k), \\ \hat{\Pi}(k) &= \frac{1}{\sqrt{L}} \int_0^L dx e^{-ikx} \hat{\Pi}(x) = \hat{\Pi}^\dagger(-k) \end{aligned} \quad (1.86)$$

satisfying the commutation relations

$$[\hat{\phi}(k), \hat{\phi}(k')] = [\hat{\Pi}(k), \hat{\Pi}(k')] = 0 \quad \text{and} \quad [\hat{\phi}(k), \hat{\Pi}^\dagger(k')] = i\delta_{k,k'}. \quad (1.87)$$

This allows us to write the Hamiltonian as a sum of harmonic oscillators,

$$\hat{H} = \sum_k \left[\frac{1}{2\rho} \hat{\Pi}^\dagger(k) \hat{\Pi}(k) + \frac{1}{2} \rho \omega_k^2 \hat{\phi}^\dagger(k) \hat{\phi}(k) \right], \quad (1.88)$$

where $\omega_k = c|k|$ and the sum is over all vectors $k = p2\pi/L$ (p integer) satisfying the boundary conditions $e^{ikL} = 1$. \hat{H} is diagonalized by introducing the ladder operators

$$\begin{aligned} \hat{a}(k) &= \sqrt{\frac{\rho\omega_k}{2}} \left[\hat{\phi}(k) + \frac{i}{\rho\omega_k} \hat{\Pi}(k) \right], \\ \hat{a}^\dagger(k) &= \sqrt{\frac{\rho\omega_k}{2}} \left[\hat{\phi}^\dagger(k) - \frac{i}{\rho\omega_k} \hat{\Pi}^\dagger(k) \right]. \end{aligned} \quad (1.89)$$

Using the commutation relations

$$[\hat{a}(k), \hat{a}(k')] = [\hat{a}^\dagger(k), \hat{a}^\dagger(k')] = 0, \quad [\hat{a}(k), \hat{a}^\dagger(k')] = \delta_{k,k'}, \quad (1.90)$$

one easily finds

$$\hat{H} = \sum_k \omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right). \quad (1.91)$$

The eigenstates of the harmonic oscillator indexed by k are defined by

$$\begin{aligned} |n_k\rangle &= \frac{1}{\sqrt{n_k!}} (\hat{a}_k^\dagger)^{n_k} |0\rangle, \\ \omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) |n_k\rangle &= \omega_k \left(n_k + \frac{1}{2} \right) |n_k\rangle, \end{aligned} \quad (1.92)$$

where $|0\rangle = |n_k = 0\rangle$ is the normalized vacuum state: $\hat{a}_k |0\rangle = 0$. The ladder operators \hat{a}_k and \hat{a}_k^\dagger satisfy

$$\begin{aligned} \hat{a}_k |n_k\rangle &= \sqrt{n_k} |n_k - 1\rangle, \\ \hat{a}_k^\dagger |n_k\rangle &= \sqrt{n_k + 1} |n_k + 1\rangle, \end{aligned} \quad (1.93)$$

and can be seen as annihilation and creation operators of an elementary excitation (phonon) with momentum k . $n_k = \langle n_k | \hat{a}_k^\dagger \hat{a}_k | n_k \rangle$ denotes the number of phonons in the state $|n_k\rangle$. The eigenstates of the Hamiltonian (1.91) are obtained from the tensor product of the states $|n_k\rangle$,

$$\begin{aligned} |n_{k_1} \cdots n_{k_i} \cdots\rangle &= |n_{k_1}\rangle \otimes \cdots \otimes |n_{k_i}\rangle \otimes \cdots = \prod_i \frac{(\hat{a}_{k_i}^\dagger)^{n_{k_i}}}{\sqrt{n_{k_i}!}} |\text{vac}\rangle, \\ \hat{H} |n_{k_1} \cdots n_{k_i} \cdots\rangle &= \sum_j \left(n_{k_j} + \frac{1}{2} \right) \omega_{k_j} |n_{k_1} \cdots n_{k_i} \cdots\rangle, \end{aligned} \quad (1.94)$$

where $|\text{vac}\rangle$ is the vacuum, i.e. the normalized state defined by $\hat{a}_k |\text{vac}\rangle = 0$ (for any k). The eigenstate $|n_{k_1} \cdots n_{k_i} \cdots\rangle$ has a total number of phonons $n = \sum_i n_{k_i}$. The Hilbert space can be written as the direct sum $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_n \oplus \cdots$ where \mathcal{H}_n is the Hilbert space with n phonons. This type of Hilbert space, generically referred to as a Fock space, is at the basis of the second-quantization formalism described in Sec. 1.2.

Functional integral formulation

A functional integral formulation can be obtained following the same procedure as in the single particle case. $\hat{\phi}(x)$ and $\hat{\Pi}(x)$ play the role of the position and momentum operator \hat{q} and \hat{p} of the single particle (the only difference being that they are labeled by x). One can introduce states $|\phi\rangle$ and $|\Pi\rangle$ satisfying $\hat{\phi}(x)|\phi\rangle = \phi(x)|\phi\rangle$ and $\hat{\Pi}(x)|\Pi\rangle = \Pi(x)|\Pi\rangle$. Since both sets of states $\{|\phi\rangle\}$ and $\{|\Pi\rangle\}$ form a complete basis of the Hilbert space, we have the closure relations

$$\begin{aligned} \mathcal{N} \lim_{a \rightarrow 0} \int \prod_{l=0}^{L/a} d\phi(la) |\phi\rangle \langle \phi| &= 1, \\ \mathcal{N}' \lim_{a \rightarrow 0} \int \prod_{l=0}^{L/a} d\Pi(la) |\Pi\rangle \langle \Pi| &= 1. \end{aligned} \quad (1.95)$$

Here we have discretized the chain; the continuous variable x becomes a discrete variable $x = la$. The harmonic chain is recovered in the limit $a \rightarrow 0$. This step is necessary to properly define the closure relations (1.95) as well as the functional integration measures below [Eq. (1.99)]. \mathcal{N} and \mathcal{N}' are unimportant normalization constants that contribute a factor to the partition function but do not affect the average values. They will be dropped in the following.

Proceeding as in section 1.1.1, one finds that the partition function

$$Z = \int_{\phi(x,\beta)=\phi(x,0)} \mathcal{D}[\Pi, \phi] \exp \left\{ - \int_0^\beta d\tau \int_0^L dx \left[\frac{\Pi^2}{2\rho} + \frac{\kappa}{2} (\partial_x \phi)^2 - i\Pi \dot{\phi} \right] \right\} \quad (1.96)$$

can be written as a functional integral in imaginary time over the real fields $\phi(x, \tau)$

and $\Pi(x, \tau)$.¹¹ Performing the Gaussian functional integral over Π ,¹² one obtains

$$Z = \int_{\phi(x, \beta) = \phi(x, 0)} \mathcal{D}[\phi] e^{-S_E[\phi]} \quad (1.97)$$

with the Euclidean action

$$S_E[\phi] = \frac{1}{2} \int_0^\beta d\tau \int_0^L dx \left[\rho \dot{\phi}^2 + \kappa (\partial_x \phi)^2 \right]. \quad (1.98)$$

The integration measure in (1.97) is defined as

$$\mathcal{D}[\phi] = \lim_{N \rightarrow \infty} \lim_{a \rightarrow 0} \prod_{k=1}^N \prod_{l=0}^{L/a} d\phi(la, k\beta/N) \quad (1.99)$$

(up to a multiplicative factor). Performing a Wick rotation ($\tau = it$), we see that the real-time action is given by the classical action $S[\phi] = \int dt \int_0^L dx \mathcal{L}(\partial_x \phi, \dot{\phi})$.

Since the field $\phi(x, \tau)$ is periodic in time, it can be expanded as a Fourier series,

$$\begin{aligned} \phi(x, \tau) &= \frac{1}{\sqrt{\beta}} \sum_{\omega_n} e^{-i\omega_n \tau} \phi(x, i\omega_n), \\ \phi(x, i\omega_n) &= \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau e^{i\omega_n \tau} \phi(x, \tau), \end{aligned} \quad (1.100)$$

where the discrete frequency

$$\omega_n = \frac{2\pi}{\beta} n \quad (n \text{ integer}) \quad (1.101)$$

is called a Matsubara (imaginary) frequency. The Fourier transformed field $\phi(k, i\omega_n)$ diagonalizes the action,

$$S_E[\phi] = \frac{\rho}{2} \sum_{k, \omega_n} \phi(-k, -i\omega_n) (\omega_n^2 + \omega_k^2) \phi(k, i\omega_n), \quad (1.102)$$

so that the partition function (1.97) is given by a product of Gaussian integrals. Note that $\phi(-k, -i\omega_n) = \phi^*(k, i\omega_n)$ since $\phi(x, \tau)$ is real.

The functional integral approach to the quantum harmonic string already exhibits many essential aspects of the field theory of (more complicated) quantum systems:

- Equation (1.97) is an exact representation of the partition function. Since the action is quadratic in the field, the integral can be done exactly:¹³

$$Z = \prod_k \frac{e^{-\frac{\beta}{2} \omega_k}}{1 - e^{-\beta \omega_k}}, \quad (1.103)$$

¹¹Equation (1.96) is analog to (1.25).

¹²Gaussian functional integration is discussed in Sec. 1.E.

¹³See the calculation of the partition function of the harmonic oscillator in section 1.1.1 (in particular Eqs. (1.58, 1.59)).

which is the standard result for a set of decoupled harmonic oscillators. More generally, all results that can be obtained from the Hamiltonian (1.91) can also be derived from the functional integral (1.97). When the action is not quadratic, for example when it contains a term

$$S_{\text{int}}[\phi] = \int_0^\beta d\tau \int_0^L dx V(\phi) \quad (1.104)$$

with $V(\phi)$ a potential of order 4 or higher, the functional integral cannot be done exactly and one has to resort to approximate strategies such as perturbative expansion (Sec. 1.5) or saddle-point approximation (Sec. 1.7).

- Requiring the action to be stationary, $\delta S_E / \delta \phi(x, \tau) = 0$, one obtains the classical equation of motion $\rho \partial_\tau^2 \phi + \kappa \partial_x^2 \phi = 0$ in imaginary time [see Eq. (1.82)].
- The continuous string model cannot be valid at arbitrary small length scales. For example, if it corresponds to the low-energy description of a one-dimensional crystal (as discussed at the beginning of this section), it is valid only for momenta k much smaller than $1/a$ where a is the lattice spacing. In general the dispersion ω_k is bounded by a maximum value ω_0 . At high temperature, when $\omega_0 \ll T$, the partition function is dominated by the zero Matsubara frequency $\omega_{n=0} = 0$. The action

$$S_E[\phi] \simeq \frac{\rho}{2} \sum_k \phi(-k, -i\omega_{n=0}) \omega_k^2 \phi(k, i\omega_{n=0}) = \frac{\kappa}{2T} \int_0^L dx (\partial_x \phi)^2 \quad (1.105)$$

then yields the classical partition function

$$Z_{\text{cl}} = \int \mathcal{D}[\phi] \exp \left\{ -\frac{\kappa}{2T} \int_0^L dx (\partial_x \phi)^2 \right\}. \quad (1.106)$$

A quantum system at sufficiently high temperature behaves classically. When $T \sim \omega_0$, the system enters the quantum regime and non-zero Matsubara frequencies cannot be ignored. Thus the quantum-mechanical behavior of the system shows up in the imaginary time dependence of the field.

- In the limit $T \rightarrow 0$ ($\beta \rightarrow \infty$), the imaginary time τ varies in the interval $[0, \infty[$ and the discrete Matsubara frequency ω_n becomes a continuous variable ω . By rescaling the time variable, we can rewrite the action as

$$S_E[\phi] = \frac{\kappa}{2c} \int d^2 r [\nabla \phi(\mathbf{r})]^2 \quad (1.107)$$

(we assume both $\beta \rightarrow \infty$ and $L \rightarrow \infty$), where $\mathbf{r} = (x, c\tau)$. The action of the quantum one-dimensional string reduces to the action of a classical two-dimensional string. More generally, zero-temperature d -dimensional quantum systems behave as $(d+1)$ -dimensional classical systems or, when time and space do not enter the action symmetrically, $(d+z)$ -dimensional systems.

- The fact that the excitation energies ω_k can be directly read off from the partition function (1.97,1.102) illustrates the connection between thermodynamics and dynamics in a quantum system. The relevant tool to study the dynamics of the system is the (imaginary-time) propagator of the ϕ field – also called the (imaginary-time) Green function – defined as the correlation function

$$\begin{aligned} G(k, i\omega_n) &\equiv \langle \phi(k, i\omega_n) \phi(-k, -i\omega_n) \rangle \\ &= \frac{1}{Z} \int \mathcal{D}[\phi] \phi(k, i\omega_n) \phi(-k, -i\omega_n) e^{-S_E[\phi]}. \end{aligned} \quad (1.108)$$

The action (1.102) being quadratic, it can be calculated exactly,¹²

$$G(k, i\omega_n) = \frac{1}{\rho} \frac{1}{\omega_n^2 + \omega_k^2}. \quad (1.109)$$

To obtain the dynamics in real time, one performs an analytical continuation $i\omega_n \rightarrow \omega + i\eta$ to real frequencies ω . The infinitesimal $\eta \rightarrow 0^+$ is crucial for the analytical continuation to be well defined in the general case (chapter 3). The resulting correlation function

$$G^R(k, \omega) = G(k, \omega + i\eta) = -\frac{1}{\rho} \frac{1}{(\omega + i\eta)^2 - \omega_k^2} \quad (1.110)$$

is called the retarded Green function (Sec. 1.2.3). Its poles $\omega = \pm\omega_k$ directly give the excitation energies of the quantum string. The excitation spectrum also shows up in the spectral function

$$A(k, \omega) = \Im[G^R(k, \omega)] = \frac{\pi}{2\rho\omega_k} [\delta(\omega - \omega_k) - \delta(\omega + \omega_k)]. \quad (1.111)$$

This is a very general result: Green functions – or correlation functions – contain information about the excitation spectrum of the system and are therefore the main quantities of interest besides the thermodynamic potential $\Omega = -\frac{1}{\beta} \ln Z$. We shall see in chapter 3 that correlation functions also determine the linear response of the system to an external field.

1.2 Second quantization and Green functions

In quantum statistical physics we are interested in systems with a large number of particles. The state vectors describing the possible physical states should be symmetric or antisymmetric under the exchange of two particles, depending on the statistics of the particles (bosons or fermions). Furthermore, the number of particles fluctuates when the system can exchange particles with a reservoir – as for instance in the grand canonical ensemble. Second quantization provides a natural formalism to describe many-particle systems (the main results are summarized in Table 1.1). It yields the concept of quantum field and in turn the possibility to express the partition function as a functional integral over suitably defined coherent states (Secs. 1.3.1, 1.3.3 and 1.4).

1.2.1 Fock space

The Fock space is defined as the direct sum

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \cdots = \oplus_{n=0}^{\infty} \mathcal{H}_n, \quad (1.112)$$

where \mathcal{H}_n is the Hilbert space corresponding to a system of n particles. \mathcal{H}_0 contains only the vacuum state $|\text{vac}\rangle$ and \mathcal{H}_1 is the Hilbert used when studying the quantum mechanics of a single particle.

Let us first focus on the Hilbert space \mathcal{H}_n . \mathcal{H}_n contains all n -particle states properly symmetrized (bosons) or antisymmetrized (fermions). It is a subspace of the direct product $\bar{\mathcal{H}}_n = \mathcal{H}_0 \otimes \mathcal{H}_0 \otimes \cdots \mathcal{H}_0$. If we know an orthonormal basis $\{|\alpha\rangle\}$ of \mathcal{H}_1 , then we can obtain an orthonormal basis of $\bar{\mathcal{H}}_n$ from the tensor product

$$|\alpha_1 \cdots \alpha_n\rangle = |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_n\rangle. \quad (1.113)$$

Note that we use the notation $|\cdots\rangle$ (with a curly bracket) to denote this n -particle state. The overlap of two vectors is simply

$$\langle \alpha'_1 \cdots \alpha'_n | \alpha_1 \cdots \alpha_n \rangle = \langle \alpha'_1 | \alpha_1 \rangle \cdots \langle \alpha'_n | \alpha_n \rangle = \delta_{\alpha'_1, \alpha_1} \cdots \delta_{\alpha'_n, \alpha_n} \quad (1.114)$$

and the completeness of the basis gives the closure relation

$$\sum_{\alpha_1 \cdots \alpha_n} |\alpha_1 \cdots \alpha_n\rangle \langle \alpha_1 \cdots \alpha_n| = 1, \quad (1.115)$$

where “1” in the rhs means the unit operator in $\bar{\mathcal{H}}_n$. A wave function in coordinate space is obtained by multiplying the ket $|\alpha_1 \cdots \alpha_n\rangle$ by the bra $\langle \mathbf{r}_1 \cdots \mathbf{r}_n | = \langle \mathbf{r}_1 | \otimes \cdots \otimes \langle \mathbf{r}_n |$,

$$\langle \mathbf{r}_1 \cdots \mathbf{r}_n | \alpha_1 \cdots \alpha_n \rangle = \varphi_{\alpha_1}(\mathbf{r}_1) \cdots \varphi_{\alpha_n}(\mathbf{r}_n), \quad (1.116)$$

where $\varphi_{\alpha}(\mathbf{r}) = \langle \mathbf{r} | \alpha \rangle$ is the coordinate-representation wave function of a particle in the quantum state $|\alpha\rangle$.

To obtain a basis of \mathcal{H}_n , we should (anti)symmetrize the tensor product (1.113),

$$\begin{aligned} |\alpha_1 \cdots \alpha_n\rangle &= \sqrt{n!} \mathcal{P}_{\zeta} |\alpha_1 \cdots \alpha_n\rangle \\ &= \frac{1}{\sqrt{n!}} \sum_{p \in S_n} \zeta^p |\alpha_{p(1)} \cdots \alpha_{p(n)}\rangle. \end{aligned} \quad (1.117)$$

\mathcal{P}_+ (\mathcal{P}_-) is a symmetrization (antisymmetrization) operator and $\zeta = +1$ for bosons and -1 for fermions. The sum in (1.117) is over all permutations p of S_n . ζ^p equals one for bosons and the signature of the permutation p for fermions. One can easily verify that \mathcal{P}_{ζ} is a projector, i.e. $\mathcal{P}_{\zeta}^2 = \mathcal{P}_{\zeta}$. Note that for fermions the state $|\alpha_1 \cdots \alpha_n\rangle$ vanishes if two of the α_i 's are identical (Pauli principle). The states $|\alpha_1 \cdots \alpha_n\rangle$ form a basis of \mathcal{H}_n . The closure relation (1.115) in $\bar{\mathcal{H}}_n$ becomes a closure relation in \mathcal{H}_n ,

$$\begin{aligned} 1 &= \sum_{\alpha_1 \cdots \alpha_n} \mathcal{P}_{\zeta} |\alpha_1 \cdots \alpha_n\rangle \langle \alpha_1 \cdots \alpha_n| \mathcal{P}_{\zeta} \\ &= \frac{1}{n!} \sum_{\alpha_1 \cdots \alpha_n} |\alpha_1 \cdots \alpha_n\rangle \langle \alpha_1 \cdots \alpha_n|, \end{aligned} \quad (1.118)$$

and the overlap between two states is given by

$$\begin{aligned} \{\alpha'_1 \cdots \alpha'_n | \alpha_1 \cdots \alpha_n\} &= n! (\alpha'_1 \cdots \alpha'_n | \mathcal{P}_\zeta^2 | \alpha_1 \cdots \alpha_n) \\ &= \sum_p \zeta^p (\alpha'_1 \cdots \alpha'_n | \alpha_{p(1)} \cdots \alpha_{p(n)}). \end{aligned} \quad (1.119)$$

The permutations p contributing to the sum must satisfy $\alpha'_1 = \alpha_{p(1)}, \dots, \alpha'_n = \alpha_{p(n)}$. Since for fermions all α_i 's should be different, there is only one such permutation and the overlap reduces to

$$\{\alpha'_1 \cdots \alpha'_n | \alpha_1 \cdots \alpha_n\} = (-1)^p \quad (\text{fermions}). \quad (1.120)$$

In the case of bosons, several particles can occupy the same one-body state, and any permutation which interchanges particles in the same state contributes to the sum in (1.119). The number of these permutations is $n_{\alpha_1}! \cdots n_{\alpha_p}!$ if we denote by n_{α_i} the number of bosons in the one-body state $|\alpha_i\rangle$ (with $\alpha_1, \dots, \alpha_p$ all different). We therefore find

$$\{\alpha'_1 \cdots \alpha'_n | \alpha_1 \cdots \alpha_n\} = n_{\alpha_1}! \cdots n_{\alpha_p}! \quad (\text{bosons}). \quad (1.121)$$

A normalized basis of \mathcal{H}_n is obtained by normalizing the states $|\alpha_1 \cdots \alpha_n\rangle$,

$$\begin{aligned} |\alpha_1 \cdots \alpha_n\rangle &= \frac{1}{(\prod_{i=1}^p n_{\alpha_i}!)^{1/2}} |\alpha_1 \cdots \alpha_n\rangle \\ &= \frac{1}{(n! \prod_{i=1}^p n_{\alpha_i}!)^{1/2}} \sum_p \zeta^p |\alpha_{p(1)} \cdots \alpha_{p(n)}\rangle. \end{aligned} \quad (1.122)$$

The coordinate-representation wave function is given by

$$\begin{aligned} (\mathbf{r}_1 \cdots \mathbf{r}_n | \alpha_1 \cdots \alpha_n) &= \frac{1}{(n! \prod_{i=1}^p n_{\alpha_i}!)^{1/2}} \sum_p \zeta^p \varphi_{\alpha_{p(1)}}(\mathbf{r}_1) \cdots \varphi_{\alpha_{p(n)}}(\mathbf{r}_n) \\ &= \begin{cases} \frac{1}{\sqrt{n!}} \det(\varphi_{\alpha_i}(\mathbf{r}_j)) & (\text{fermions}), \\ \frac{1}{(n! \prod_{i=1}^p n_{\alpha_i}!)^{1/2}} \text{per}(\varphi_{\alpha_i}(\mathbf{r}_j)) & (\text{bosons}). \end{cases} \end{aligned} \quad (1.123)$$

We thus obtain a basis of permanents for bosons and determinants for fermions. The latter are known as Slater determinants.

It is also possible to define an (anti)symmetrized many-body state in the coordinate representation,

$$\begin{aligned} |\mathbf{r}_1 \sigma_1, \dots, \mathbf{r}_n \sigma_n\rangle &= \frac{1}{\sqrt{n!}} \sum_{p \in S_n} \zeta^p |\mathbf{r}_{p(1)} \sigma_{p(1)}, \dots, \mathbf{r}_{p(n)} \sigma_{p(n)}\rangle \\ &= \frac{1}{V^{n/2}} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_n} e^{i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_n \cdot \mathbf{r}_n)} |\mathbf{k}_1 \sigma_1, \dots, \mathbf{k}_n \sigma_n\rangle, \end{aligned} \quad (1.124)$$

although the states $|\mathbf{r}\sigma\rangle$ are not normalized. σ denotes the spin index (as well as other discrete indices if necessary) and \mathbf{k} the momentum.

Creation and annihilation operators

To complete the description of many-particle systems, we need to introduce operators which couple \mathcal{H}_n to $\mathcal{H}_{n\pm 1}$, i.e. which add or remove a particle from the system. The creation operator $\hat{\psi}_\alpha^\dagger$ is defined by

$$\begin{aligned}\hat{\psi}_\alpha^\dagger|\alpha_1 \cdots \alpha_n\rangle &= |\alpha\alpha_1 \cdots \alpha_n\rangle, \\ \hat{\psi}_\alpha^\dagger|\alpha_1 \cdots \alpha_n\rangle &= \sqrt{n_\alpha + 1}|\alpha\alpha_1 \cdots \alpha_n\rangle.\end{aligned}\tag{1.125}$$

$\hat{\psi}_\alpha^\dagger$ adds a particle in the one-body state α and (anti)symmetrizes the resulting many-body state. When acting on the vacuum state, it gives the one-body state $|\alpha\rangle$: $\hat{\psi}_\alpha^\dagger|\text{vac}\rangle = |\alpha\rangle$. More generally,

$$\begin{aligned}|\alpha_1 \cdots \alpha_n\rangle &= \hat{\psi}_{\alpha_1}^\dagger \cdots \hat{\psi}_{\alpha_n}^\dagger|\text{vac}\rangle, \\ |\alpha_1 \cdots \alpha_n\rangle &= \frac{1}{(\prod_{i=1}^n n_{\alpha_i}!)^{1/2}} \hat{\psi}_{\alpha_1}^\dagger \cdots \hat{\psi}_{\alpha_n}^\dagger|\text{vac}\rangle.\end{aligned}\tag{1.126}$$

The annihilation operator $\hat{\psi}_\alpha$ is defined as the adjoint of the creation operator $\hat{\psi}_\alpha^\dagger$. From (1.125), we find

$$\begin{aligned}\{\alpha_1 \cdots \alpha_n|\hat{\psi}_\alpha|\alpha'_1 \cdots \alpha'_m\rangle &= \{\alpha'_1 \cdots \alpha'_m|\hat{\psi}_\alpha^\dagger|\alpha_1 \cdots \alpha_n\rangle^* \\ &= \{\alpha\alpha_1 \cdots \alpha_n|\alpha'_1 \cdots \alpha'_m\rangle.\end{aligned}\tag{1.127}$$

The result is finite only if $n = m - 1$ so that $\hat{\psi}_\alpha$ removes a particle from the system. This means in particular that $\hat{\psi}_\alpha|\text{vac}\rangle = 0$. Using the closure relation in the Fock space \mathcal{H} ,

$$\sum_{n=0}^{\infty} \sum_{\alpha_1 \cdots \alpha_n} \frac{1}{n!} |\alpha_1 \cdots \alpha_n\rangle \langle \alpha_1 \cdots \alpha_n| = 1,\tag{1.128}$$

we obtain

$$\begin{aligned}\hat{\psi}_\alpha|\alpha'_1 \cdots \alpha'_m\rangle &= \sum_{n=0}^{\infty} \sum_{\alpha_1 \cdots \alpha_n} \frac{1}{n!} \{\alpha_1 \cdots \alpha_n|\hat{\psi}_\alpha|\alpha'_1 \cdots \alpha'_m\rangle|\alpha_1 \cdots \alpha_n\rangle \\ &= \frac{1}{(m-1)!} \sum_{\alpha_1 \cdots \alpha_{m-1}} \{\alpha\alpha_1 \cdots \alpha_{m-1}|\alpha'_1 \cdots \alpha'_m\rangle|\alpha_1 \cdots \alpha_{m-1}\rangle \\ &= \frac{1}{(m-1)!} \sum_{p \in S_m} \zeta^p \langle \alpha|\alpha'_{p(1)}\rangle |\alpha'_{p(2)} \cdots \alpha'_{p(m)}\rangle,\end{aligned}\tag{1.129}$$

where we have used (1.114) and (1.119). The permutation $(p(2), \dots, p(m)) \rightarrow (1, \dots, p(1)-1, p(1)+1, \dots, m)$ has a signature $\zeta^{p+p(1)-1}$,¹⁴ so that we finally obtain¹⁵

$$\begin{aligned}\hat{\psi}_\alpha|\alpha'_1 \cdots \alpha'_m\rangle &= \frac{1}{(m-1)!} \sum_{p \in S_m} \zeta^{p(1)-1} \delta_{\alpha, \alpha'_{p(1)}} |\alpha'_1 \cdots \alpha'_{p(1)-1}, \alpha'_{p(1)+1} \cdots \alpha'_m\rangle \\ &= \sum_{i=1}^m \zeta^{i-1} \delta_{\alpha, \alpha'_i} |\alpha'_1 \cdots \hat{\alpha}'_i \cdots \alpha'_m\rangle,\end{aligned}\tag{1.130}$$

¹⁴The permutation $(p(1), p(2), \dots, p(m)) \rightarrow (p(1), 2, \dots, p(1)-1, p(1)+1, \dots, m)$ can be written as the permutation $p^{-1} [(p(1), p(2), \dots, p(m)) \rightarrow (1, 2, \dots, m), \text{signature } \zeta^p]$ followed by $p(1)-1$ transpositions $[(1, 2, \dots, m) \rightarrow (p(1), 2, \dots, p(1)-1, p(1)+1, \dots, m), \text{signature } \zeta^{p(1)-1}]$.

¹⁵One can easily verify that (1.130) reproduces (1.127).

where $\hat{\alpha}'_i$ indicates that α'_i is omitted. The analogous result for the normalized states reads

$$\hat{\psi}_\alpha |\alpha'_1 \cdots \alpha'_m\rangle = \frac{1}{\sqrt{n_\alpha}} \sum_{i=1}^m \zeta^{i-1} \delta_{\alpha, \alpha'_i} |\alpha'_1 \cdots \hat{\alpha}'_i \cdots \alpha'_m\rangle. \quad (1.131)$$

For bosons, it is sometimes convenient to introduce the states

$$|n_{\alpha_1} \cdots n_{\alpha_p}\rangle = \frac{1}{(\prod_{i=1}^p n_{\alpha_i}!)^{1/2}} (\hat{\psi}_{\alpha_1}^\dagger)^{n_{\alpha_1}} \cdots (\hat{\psi}_{\alpha_p}^\dagger)^{n_{\alpha_p}} |\text{vac}\rangle, \quad (1.132)$$

where n_{α_i} denotes the occupation number of the one-body state α_i (with $\alpha_1 \cdots \alpha_p$ all different). These states form an orthonormal basis of the Fock space \mathcal{H} and satisfy the closure relation

$$\sum_{\{\alpha_i\}} |n_{\alpha_1} \cdots n_{\alpha_i} \cdots\rangle \langle n_{\alpha_1} \cdots n_{\alpha_i} \cdots| = 1 \quad (1.133)$$

as well as

$$\begin{aligned} \hat{\psi}_\alpha^\dagger |n_{\alpha_1} \cdots n_{\alpha_p}\rangle &= \sqrt{n_\alpha + 1} |n_{\alpha_1} \cdots (n_\alpha + 1) \cdots n_{\alpha_p}\rangle, \\ \hat{\psi}_\alpha |n_{\alpha_1} \cdots n_{\alpha_p}\rangle &= \sum_{i=1}^p \delta_{\alpha, \alpha_i} \sqrt{n_\alpha} |n_{\alpha_1} \cdots (n_\alpha - 1) \cdots n_{\alpha_p}\rangle, \end{aligned} \quad (\text{bosons}). \quad (1.134)$$

They are therefore eigenstates of the operator $\hat{n}_\alpha = \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha$ which measures the number of particles in the one-body state $|\alpha\rangle$,

$$\hat{n}_\alpha |n_{\alpha_1} \cdots n_{\alpha_p}\rangle = \sum_{i=1}^p \delta_{\alpha, \alpha_i} n_{\alpha_i} |n_{\alpha_1} \cdots n_{\alpha_p}\rangle. \quad (1.135)$$

(Anti)commutation relations

The symmetry properties of the states $|\alpha_1 \cdots \alpha_n\rangle$ under the exchange of two particles have important consequences for the operators $\hat{\psi}_\alpha, \hat{\psi}_\alpha^\dagger$. We have

$$\begin{aligned} \hat{\psi}_\alpha^\dagger \hat{\psi}_{\alpha'}^\dagger |\alpha_1 \cdots \alpha_n\rangle &= |\alpha \alpha' \alpha_1 \cdots \alpha_n\rangle \\ &= \zeta |\alpha' \alpha \alpha_1 \cdots \alpha_n\rangle \\ &= \zeta \hat{\psi}_{\alpha'}^\dagger \hat{\psi}_\alpha^\dagger |\alpha_1 \cdots \alpha_n\rangle. \end{aligned} \quad (1.136)$$

Since (1.136) holds for any state $|\alpha_1 \cdots \alpha_n\rangle$, we deduce

$$[\hat{\psi}_\alpha^\dagger, \hat{\psi}_{\alpha'}^\dagger]_{-\zeta} = [\hat{\psi}_\alpha, \hat{\psi}_{\alpha'}]_{-\zeta} = 0 \quad (1.137)$$

(the second equation is deduced from the first by taking the adjoint). $[\cdot, \cdot]_-$ and $[\cdot, \cdot]_+$ denote the commutator and the anticommutator, respectively. By comparing

$$\begin{aligned} \hat{\psi}_\alpha \hat{\psi}_{\alpha'}^\dagger |\alpha_1 \cdots \alpha_n\rangle &= \hat{\psi}_\alpha |\alpha' \alpha_1 \cdots \alpha_n\rangle \\ &= \delta_{\alpha, \alpha'} |\alpha_1 \cdots \alpha_n\rangle + \sum_{i=1}^n \zeta^i \delta_{\alpha, \alpha_i} |\alpha' \alpha_1 \cdots \hat{\alpha}_i \cdots \alpha_n\rangle \end{aligned} \quad (1.138)$$

and

$$\begin{aligned}\hat{\psi}_{\alpha'}^\dagger \hat{\psi}_\alpha |\alpha_1 \cdots \alpha_n\rangle &= \hat{\psi}_{\alpha'}^\dagger \sum_{i=1}^n \zeta^{i-1} \delta_{\alpha, \alpha_i} |\alpha_1 \cdots \hat{\alpha}_i \cdots \alpha_n\rangle \\ &= \sum_{i=1}^n \zeta^{i-1} \delta_{\alpha, \alpha_i} |\alpha' \alpha_1 \cdots \hat{\alpha}_i \cdots \alpha_n\rangle,\end{aligned}\quad (1.139)$$

we also obtain

$$[\hat{\psi}_\alpha, \hat{\psi}_{\alpha'}^\dagger]_{-\zeta} = \delta_{\alpha, \alpha'}.\quad (1.140)$$

Equations (1.137) and (1.140) are fundamental relations satisfied by the creation and annihilation operators $\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha$. Recall the crucial assumption that $\{|\alpha\rangle\}$ forms an orthonormal basis of the single-particle Hilbert space \mathcal{H}_1 .

Change of basis

Creation and annihilation operators in another basis $\{|\tilde{\alpha}\rangle\}$ can be straightforwardly obtained from the operators $\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha$. Making use of $|\tilde{\alpha}\rangle = \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle|\alpha\rangle$, we deduce

$$\begin{aligned}\hat{\psi}_{\tilde{\alpha}}^\dagger |\alpha_1 \cdots \alpha_n\rangle &= |\tilde{\alpha} \alpha_1 \cdots \alpha_n\rangle \\ &= \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle |\alpha \alpha_1 \cdots \alpha_n\rangle \\ &= \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle \hat{\psi}_\alpha^\dagger |\alpha_1 \cdots \alpha_n\rangle,\end{aligned}\quad (1.141)$$

and therefore

$$\begin{aligned}\hat{\psi}_{\tilde{\alpha}}^\dagger &= \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle \hat{\psi}_\alpha^\dagger, \\ \hat{\psi}_{\tilde{\alpha}} &= \sum_\alpha \langle\tilde{\alpha}|\alpha\rangle \hat{\psi}_\alpha.\end{aligned}\quad (1.142)$$

The transformed operators satisfy the (anti)commutation relations

$$\begin{aligned}[\hat{\psi}_{\tilde{\alpha}}^\dagger, \hat{\psi}_{\tilde{\alpha}'}^\dagger]_{-\zeta} &= [\hat{\psi}_{\tilde{\alpha}}, \hat{\psi}_{\tilde{\alpha}'}]_{-\zeta} = 0, \\ [\hat{\psi}_{\tilde{\alpha}}, \hat{\psi}_{\tilde{\alpha}'}^\dagger]_{-\zeta} &= \langle\tilde{\alpha}|\tilde{\alpha}'\rangle.\end{aligned}\quad (1.143)$$

If the new basis is orthonormal, the (anti)commutation relations are preserved; the transformation $\{\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha\} \rightarrow \{\hat{\psi}_{\tilde{\alpha}}^\dagger, \hat{\psi}_{\tilde{\alpha}}\}$ is unitary.

Field operators

The “field operators” are defined by

$$\begin{aligned}\hat{\psi}_\sigma(\mathbf{r}) &= \sum_\alpha \langle\mathbf{r}, \sigma|\alpha\rangle \hat{\psi}_\alpha = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\psi}_\sigma(\mathbf{k}), \\ \hat{\psi}_\sigma^\dagger(\mathbf{r}) &= \sum_\alpha \langle\alpha|\mathbf{r}, \sigma\rangle \hat{\psi}_\alpha^\dagger = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \hat{\psi}_\sigma^\dagger(\mathbf{k}),\end{aligned}\quad (1.144)$$

where the sum extends over all states α of the orthonormal basis. The last relations are obtained by choosing the momentum-representation basis $\{|\mathbf{k}, \sigma\rangle\}$. The field operators satisfy the (anti)commutation relations

$$\begin{aligned} [\hat{\psi}_\sigma^\dagger(\mathbf{r}), \hat{\psi}_{\sigma'}^\dagger(\mathbf{r}')]_{-\zeta} &= [\hat{\psi}_\sigma(\mathbf{r}), \hat{\psi}_{\sigma'}(\mathbf{r}')]_{-\zeta} = 0, \\ [\hat{\psi}_\sigma(\mathbf{r}), \hat{\psi}_{\sigma'}^\dagger(\mathbf{r}')]_{-\zeta} &= \delta_{\sigma, \sigma'} \delta(\mathbf{r} - \mathbf{r}'). \end{aligned} \quad (1.145)$$

From equations (1.125) and (1.130), we deduce that

$$\begin{aligned} \hat{\psi}_\sigma^\dagger(\mathbf{r})|\mathbf{r}_1\sigma_1, \dots, \mathbf{r}_n\sigma_n\rangle &= |\mathbf{r}\sigma, \mathbf{r}_1\sigma_1, \dots, \mathbf{r}_n\sigma_n\rangle, \\ \hat{\psi}_\sigma(\mathbf{r})|\mathbf{r}_1\sigma_1, \dots, \mathbf{r}_n\sigma_n\rangle &= \sum_{i=1}^n \zeta^{i-1} \delta(\mathbf{r} - \mathbf{r}_i) |\mathbf{r}_1\sigma_1, \dots, \widehat{\mathbf{r}_i\sigma_i}, \dots, \mathbf{r}_n\sigma_n\rangle, \end{aligned} \quad (1.146)$$

where $\widehat{\mathbf{r}_i\sigma_i}$ means that $\mathbf{r}_i\sigma_i$ is omitted. Thus the field operator $\hat{\psi}_\sigma^\dagger(\mathbf{r})$ adds a spin- σ particle at point \mathbf{r} and (anti)symmetrizes the resulting many-body state.

1.2.2 Operators in second-quantized form

Any operator acting within the Fock space can be written in terms of the creation and annihilation operators. In the following, we discuss in detail one- and two-body operators before generalizing to n -body operators.

An operator $\hat{V}^{(1)}$ is a one-body operator if it acts on each particle separately,¹⁶

$$\begin{aligned} \hat{V}^{(1)}|\alpha_1 \dots \alpha_n\rangle &= \sum_{i=1}^n \hat{V}_i|\alpha_1 \dots \alpha_n\rangle, \\ \hat{V}^{(1)}|\alpha_1 \dots \alpha_n\rangle &= \frac{1}{\sqrt{n!}} \sum_p \zeta^p \sum_{i=1}^n \hat{V}_i|\alpha_{p(1)} \dots \alpha_{p(n)}\rangle, \end{aligned} \quad (1.147)$$

where \hat{V}_i operates only on the i th particle. $\hat{V}_1|\alpha_1 \dots \alpha_n\rangle = (\hat{V}|\alpha_1\rangle) \otimes |\alpha_2\rangle \otimes \dots \otimes |\alpha_n\rangle$, etc. Let us first choose a basis where the operator \hat{V} is diagonal,

$$\hat{V}|\alpha\rangle = \langle\alpha|\hat{V}|\alpha\rangle|\alpha\rangle \equiv V_\alpha|\alpha\rangle. \quad (1.148)$$

We then have

$$\begin{aligned} \hat{V}^{(1)}|\alpha_1 \dots \alpha_n\rangle &= \frac{1}{\sqrt{n!}} \sum_p \zeta^p \sum_{i=1}^n V_{\alpha_{p(i)}} |\alpha_{p(1)} \dots \alpha_{p(n)}\rangle \\ &= \sum_{i=1}^n V_{\alpha_i} |\alpha_1 \dots \alpha_n\rangle \\ &= \sum_{\alpha} V_{\alpha} \hat{n}_{\alpha} |\alpha_1 \dots \alpha_n\rangle, \end{aligned} \quad (1.149)$$

¹⁶Recall that in first-quantization, one would write $\hat{V}^{(1)} = \sum_{i=1}^n V(\hat{\mathbf{r}}_i, \hat{\mathbf{p}}_i, \hat{\sigma}_i)$ where the sum extends over the n particles present in the system.

where the sum extends over the complete set of one-body states α and $\hat{n}_\alpha = \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha$. We deduce

$$\hat{V}^{(1)} = \sum_{\alpha} \langle \alpha | \hat{V} | \alpha \rangle \hat{n}_\alpha. \quad (1.150)$$

Using (1.142), we obtain the general expression for one-body operators,

$$\hat{V}^{(1)} = \sum_{\alpha, \alpha'} \langle \alpha | \hat{V} | \alpha' \rangle \hat{\psi}_\alpha^\dagger \hat{\psi}_{\alpha'}, \quad (1.151)$$

valid in any complete basis. In particular

$$\hat{V}^{(1)} = \int d^d r d^d r' \sum_{\sigma, \sigma'} \langle \mathbf{r}, \sigma | \hat{V} | \mathbf{r}', \sigma' \rangle \hat{\psi}_\sigma^\dagger(\mathbf{r}) \hat{\psi}_{\sigma'}(\mathbf{r}') \quad (1.152)$$

in terms of the field operators. Note that the expressions (1.151, 1.152) make no reference to the total number of particles actually present in the system (to be compared with the first-quantized form of a one-body operator acting on a n -particle state¹⁶).

Examples. The density $\hat{n}(\mathbf{r})$ of particles at point \mathbf{r} reads $\sum_{i=1}^n \delta(\mathbf{r} - \hat{\mathbf{r}}_i)$ in first quantization and

$$\begin{aligned} \hat{n}(\mathbf{r}) &= \int d^d r_1 d^d r_2 \sum_{\sigma, \sigma'} \langle \mathbf{r}_1, \sigma | \delta(\mathbf{r} - \hat{\mathbf{r}}) | \mathbf{r}_2, \sigma' \rangle \hat{\psi}_\sigma^\dagger(\mathbf{r}_1) \hat{\psi}_{\sigma'}(\mathbf{r}_2) \\ &= \sum_{\sigma} \hat{\psi}_\sigma^\dagger(\mathbf{r}) \hat{\psi}_\sigma(\mathbf{r}) \end{aligned} \quad (1.153)$$

in second-quantized form. The number of particles operator is given by

$$\hat{N} = \int d^d r \hat{n}(\mathbf{r}) = \sum_{\alpha} \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha \quad (1.154)$$

for any complete basis of one-body states $|\alpha\rangle$. For a one-body potential $V^{(1)} = \sum_{i=1}^n V(\hat{\mathbf{r}}_i)$, one finds

$$\begin{aligned} V^{(1)} &= \int d^d r_1 d^d r_2 \sum_{\sigma, \sigma'} \langle \mathbf{r}_1, \sigma | V(\hat{\mathbf{r}}) | \mathbf{r}_2, \sigma' \rangle \hat{\psi}_\sigma^\dagger(\mathbf{r}_1) \hat{\psi}_{\sigma'}(\mathbf{r}_2) \\ &= \int d^d r V(\mathbf{r}) \sum_{\sigma} \hat{\psi}_\sigma^\dagger(\mathbf{r}) \hat{\psi}_\sigma(\mathbf{r}) = \int d^d r V(\mathbf{r}) \hat{n}(\mathbf{r}). \end{aligned} \quad (1.155)$$

The kinetic energy operator $\hat{T} = \sum_{i=1}^n \hat{\mathbf{p}}_i^2 / 2m$ is most easily calculated in the plane-wave basis,

$$\hat{T} = \sum_{\substack{\mathbf{k}, \mathbf{k}' \\ \sigma, \sigma'}} \langle \mathbf{k}, \sigma | \frac{\hat{\mathbf{p}}^2}{2m} | \mathbf{k}', \sigma' \rangle \hat{\psi}_\sigma^\dagger(\mathbf{k}) \hat{\psi}_{\sigma'}(\mathbf{k}') = \sum_{\mathbf{k}, \sigma} \frac{\mathbf{k}^2}{2m} \hat{\psi}_\sigma^\dagger(\mathbf{k}) \hat{\psi}_\sigma(\mathbf{k}). \quad (1.156)$$

In direct space, this gives

$$\hat{T} = - \int d^d r \sum_{\sigma} \hat{\psi}_\sigma^\dagger(\mathbf{r}) \frac{\nabla^2}{2m} \hat{\psi}_\sigma(\mathbf{r}) = \frac{1}{2m} \sum_{\sigma} \int d^d r \nabla \hat{\psi}_\sigma^\dagger(\mathbf{r}) \cdot \nabla \hat{\psi}_\sigma(\mathbf{r}). \quad (1.157)$$

The last line is obtained from an integration by part assuming that the fields vanish at infinity (or satisfy periodic boundary conditions). For the current operator $\hat{\mathbf{j}}(\mathbf{r}) = \frac{1}{2m} \sum_i [\hat{\mathbf{p}}_i \delta(\mathbf{r} - \hat{\mathbf{r}}_i) + \delta(\mathbf{r} - \hat{\mathbf{r}}_i) \hat{\mathbf{p}}_i]$, one obtains

$$\begin{aligned} \hat{\mathbf{j}}(\mathbf{r}) &= \frac{1}{2m} \int d^d r_1 d^d r_2 \sum_{\sigma} \langle \mathbf{r}_1 | \hat{\mathbf{p}} \delta(\mathbf{r} - \hat{\mathbf{r}}) + \delta(\mathbf{r} - \hat{\mathbf{r}}) \hat{\mathbf{p}} | \mathbf{r}_2 \rangle \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}_1) \hat{\psi}_{\sigma}(\mathbf{r}_2) \\ &= -\frac{i}{2m} \sum_{\sigma} \left[\hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \nabla \hat{\psi}_{\sigma}(\mathbf{r}) - \text{h.c.} \right]. \end{aligned} \quad (1.158)$$

The most general form of the grand-canonical Hamiltonian of non-interacting particles is $\hat{H}_0 = \sum_{\alpha} \xi_{\alpha} \hat{\psi}_{\alpha}^{\dagger} \hat{\psi}_{\alpha}$ in the diagonal basis $\{|\alpha\rangle\}$, where $\xi_{\alpha} = \epsilon_{\alpha} - \mu$ denotes the energy of the one-body state $|\alpha\rangle$ wrt the chemical potential μ .

An operator $\hat{V}^{(2)}$ is a two-body operator if it acts only on pairs of particles,

$$\begin{aligned} \hat{V}^{(2)} |\alpha_1 \cdots \alpha_n\rangle &= \sum_{\substack{i,j=1 \\ (i < j)}}^n \hat{V}_{ij} |\alpha_1 \cdots \alpha_n\rangle, \\ \hat{V}^{(2)} |\alpha_1 \cdots \alpha_n\rangle &= \frac{1}{\sqrt{n!}} \sum_p \zeta^p \sum_{\substack{i,j=1 \\ (i < j)}}^n \hat{V}_{ij} |\alpha_{p(1)} \cdots \alpha_{p(n)}\rangle, \end{aligned} \quad (1.159)$$

where \hat{V}_{ij} acts only on particles i and j . In the basis $\{|\alpha\rangle\}$ where \hat{V} is diagonal,

$$\hat{V} |\alpha\beta\rangle = (\alpha\beta | \hat{V} | \alpha\beta) |\alpha\beta\rangle \equiv V_{\alpha\beta} |\alpha\beta\rangle, \quad (1.160)$$

one has

$$\begin{aligned} \hat{V}^{(2)} |\alpha_1 \cdots \alpha_n\rangle &= \frac{1}{\sqrt{n!}} \sum_p \zeta^p \sum_{\substack{i,j=1 \\ (i < j)}}^n V_{\alpha_{p(i)} \alpha_{p(j)}} |\alpha_{p(1)} \cdots \alpha_{p(n)}\rangle \\ &= \sum_{\substack{i,j=1 \\ (i < j)}}^n V_{\alpha_i \alpha_j} |\alpha_1 \cdots \alpha_n\rangle \\ &= \frac{1}{2} \sum_{i,j=1}^n (V_{\alpha_i \alpha_j} - \delta_{i,j} V_{\alpha_i \alpha_i}) |\alpha_1 \cdots \alpha_n\rangle \\ &= \frac{1}{2} \sum_{\alpha, \beta} V_{\alpha\beta} (\hat{n}_{\alpha} \hat{n}_{\beta} - \delta_{\alpha, \beta} \hat{n}_{\alpha}) |\alpha_1 \cdots \alpha_n\rangle, \end{aligned} \quad (1.161)$$

where the sum extends over all states α, β of the complete basis of the one-body states. Using the (anti)commutation relations (1.137, 1.140), one finds $\hat{n}_{\alpha} \hat{n}_{\beta} - \delta_{\alpha, \beta} \hat{n}_{\alpha} = \hat{\psi}_{\alpha}^{\dagger} \hat{\psi}_{\beta}^{\dagger} \hat{\psi}_{\beta} \hat{\psi}_{\alpha}$, which leads to

$$\hat{V}^{(2)} = \frac{1}{2} \sum_{\alpha, \beta} (\alpha\beta | \hat{V} | \alpha\beta) \hat{\psi}_{\alpha}^{\dagger} \hat{\psi}_{\beta}^{\dagger} \hat{\psi}_{\beta} \hat{\psi}_{\alpha}. \quad (1.162)$$

Transforming to an arbitrary basis, we finally find the general expression of a two-body operator,

$$\begin{aligned}\hat{V}^{(2)} &= \frac{1}{2} \sum_{\alpha_1 \dots \alpha'_2} (\alpha_1 \alpha_2 | \hat{V} | \alpha'_1 \alpha'_2) \hat{\psi}_{\alpha_1}^\dagger \hat{\psi}_{\alpha_2}^\dagger \hat{\psi}_{\alpha'_2} \hat{\psi}_{\alpha'_1} \\ &= \frac{1}{2} \int d\mathbf{r}_1 \dots d^d r'_2 \sum_{\sigma_1 \dots \sigma'_2} (\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2 | \hat{V} | \mathbf{r}'_1 \sigma'_1, \mathbf{r}'_2 \sigma'_2) \hat{\psi}_{\sigma_1}^\dagger(\mathbf{r}_1) \hat{\psi}_{\sigma_2}^\dagger(\mathbf{r}_2) \hat{\psi}_{\sigma'_2}(\mathbf{r}'_2) \hat{\psi}_{\sigma'_1}(\mathbf{r}'_1).\end{aligned}\quad (1.163)$$

Notice the respecting order of α'_1 and α'_2 in the matrix element and in the product of annihilation operators. It is sometimes convenient to use a variant of (1.163) where the matrix element is (anti)symmetrized,

$$\hat{V}^{(2)} = \frac{1}{4} \sum_{\alpha_1, \dots, \alpha'_2} \{ \alpha_1 \alpha_2 | \hat{V} | \alpha'_1 \alpha'_2 \} \hat{\psi}_{\alpha_1}^\dagger \hat{\psi}_{\alpha_2}^\dagger \hat{\psi}_{\alpha'_2} \hat{\psi}_{\alpha'_1}, \quad (1.164)$$

with

$$\{ \alpha_1 \alpha_2 | \hat{V} | \alpha'_1 \alpha'_2 \} = (\alpha_1 \alpha_2 | \hat{V} | \alpha'_1 \alpha'_2) + \zeta (\alpha_1 \alpha_2 | \hat{V} | \alpha'_2 \alpha'_1). \quad (1.165)$$

Example. For a two-body potential $\hat{V}^{(2)} = \sum_{i < j} v(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j)$ (in first-quantized form), one finds

$$\begin{aligned}\hat{V}^{(2)} &= \frac{1}{2} \int d\mathbf{r}_1 \dots d^d r'_2 \sum_{\sigma_1 \dots \sigma'_2} (\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2 | v(\hat{\mathbf{r}} - \hat{\mathbf{r}}') | \mathbf{r}'_1 \sigma'_1, \mathbf{r}'_2 \sigma'_2) \\ &\quad \times \hat{\psi}_{\sigma_1}^\dagger(\mathbf{r}_1) \hat{\psi}_{\sigma_2}^\dagger(\mathbf{r}_2) \hat{\psi}_{\sigma'_2}(\mathbf{r}'_2) \hat{\psi}_{\sigma'_1}(\mathbf{r}'_1) \\ &= \frac{1}{2} \int d^d r_1 d^d r_2 \sum_{\sigma_1, \sigma_2} v(\mathbf{r}_1 - \mathbf{r}_2) \hat{\psi}_{\sigma_1}^\dagger(\mathbf{r}_1) \hat{\psi}_{\sigma_2}^\dagger(\mathbf{r}_2) \hat{\psi}_{\sigma_2}(\mathbf{r}_2) \hat{\psi}_{\sigma_1}(\mathbf{r}_1).\end{aligned}\quad (1.166)$$

Here we have used the fact that $v(\hat{\mathbf{r}} - \hat{\mathbf{r}}')$ is diagonal in the coordinate representation: $v(\hat{\mathbf{r}} - \hat{\mathbf{r}}') | \mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2 \rangle = v(\mathbf{r}_1 - \mathbf{r}_2) | \mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2 \rangle$. In Fourier space, equation (1.166) becomes

$$\hat{V}^{(2)} = \frac{1}{2V} \sum_{\substack{\mathbf{k}, \mathbf{k}', \mathbf{q} \\ \sigma, \sigma'}} v(\mathbf{q}) \hat{\psi}_\sigma^\dagger(\mathbf{k} + \mathbf{q}) \hat{\psi}_{\sigma'}^\dagger(\mathbf{k}' - \mathbf{q}) \hat{\psi}_{\sigma'}(\mathbf{k}') \hat{\psi}_\sigma(\mathbf{k}), \quad (1.167)$$

where $v(\mathbf{q})$ is the Fourier transformed of $v(\mathbf{r})$.

To conclude this section, we give without proof the expression of a n -body operator in second-quantized form,

$$\begin{aligned}\hat{V}^{(n)} &= \frac{1}{n!} \sum_{\{\alpha_i, \alpha'_i\}} (\alpha_1 \dots \alpha_n | \hat{V} | \alpha'_1 \dots \alpha'_n) \hat{\psi}_{\alpha_1}^\dagger \dots \hat{\psi}_{\alpha_n}^\dagger \hat{\psi}_{\alpha'_n} \dots \hat{\psi}_{\alpha'_1} \\ &= \frac{1}{(n!)^2} \sum_{\{\alpha_i, \alpha'_i\}} \{ \alpha_1 \dots \alpha_n | \hat{V} | \alpha'_1 \dots \alpha'_n \} \hat{\psi}_{\alpha_1}^\dagger \dots \hat{\psi}_{\alpha_n}^\dagger \hat{\psi}_{\alpha'_n} \dots \hat{\psi}_{\alpha'_1}.\end{aligned}\quad (1.168)$$

| | |
|-------------------------------------|---|
| Many-body states | $ \alpha_1 \cdots \alpha_n\rangle = \alpha_1\rangle \otimes \cdots \otimes \alpha_n\rangle$ $ \alpha_1 \cdots \alpha_n\rangle = \frac{1}{\sqrt{n!}} \sum_p \zeta^p \alpha_{p(1)} \cdots \alpha_{p(n)}\rangle$ $ \alpha_1 \cdots \alpha_n\rangle = \frac{1}{(\prod_{i=1}^n n_{\alpha_i}!)^{1/2}} \alpha_1 \cdots \alpha_n\rangle$ |
| Closure relation | $\sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\alpha_1 \cdots \alpha_n} \alpha_1 \cdots \alpha_n\rangle \langle \alpha_1 \cdots \alpha_n = 1$ |
| Creation and annihilation operators | $\hat{\psi}_{\alpha}^{\dagger} \alpha_1 \cdots \alpha_n\rangle = \alpha \alpha_1 \cdots \alpha_n\rangle$ $\hat{\psi}_{\alpha} \alpha_1 \cdots \alpha_n\rangle = \sum_{i=1}^n \zeta^{i-1} \delta_{\alpha, \alpha_i} \alpha_1 \cdots \hat{\alpha}_i \cdots \alpha_n\rangle$ $\hat{\psi}_{\alpha}^{\dagger} \alpha_1 \cdots \alpha_n\rangle = \sqrt{n_{\alpha} + 1} \alpha \alpha_1 \cdots \alpha_n\rangle$ $\hat{\psi}_{\alpha} \alpha_1 \cdots \alpha_n\rangle = \frac{1}{\sqrt{n_{\alpha}}} \sum_{i=1}^n \zeta^{i-1} \delta_{\alpha, \alpha_i} \alpha_1 \cdots \hat{\alpha}_i \cdots \alpha_n\rangle$ |
| Commutation relations | $[\hat{\psi}_{\alpha}, \hat{\psi}_{\alpha'}]_{-\zeta} = [\hat{\psi}_{\alpha}^{\dagger}, \hat{\psi}_{\alpha'}^{\dagger}]_{-\zeta} = 0$ $[\hat{\psi}_{\alpha}, \hat{\psi}_{\alpha'}^{\dagger}]_{-\zeta} = \delta_{\alpha, \alpha'}$ |
| Field operators | $\hat{\psi}_{\sigma}(\mathbf{r}) = \sum_{\alpha} \langle \mathbf{r}, \sigma \alpha \rangle \hat{\psi}_{\alpha}$ $\hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) = \sum_{\alpha} \langle \alpha \mathbf{r}, \sigma \rangle \hat{\psi}_{\alpha}^{\dagger}$ $[\hat{\psi}_{\sigma}(\mathbf{r}), \hat{\psi}_{\sigma'}(\mathbf{r}')]_{-\zeta} = [\hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}), \hat{\psi}_{\sigma'}^{\dagger}(\mathbf{r}')]_{-\zeta} = 0$ $[\hat{\psi}_{\sigma}(\mathbf{r}), \hat{\psi}_{\sigma'}^{\dagger}(\mathbf{r}')]_{-\zeta} = \delta_{\sigma, \sigma'} \delta(\mathbf{r} - \mathbf{r}')$ |
| One-body operator | $\hat{V}^{(1)} = \sum_{\alpha, \alpha'} \langle \alpha \hat{V} \alpha' \rangle \hat{\psi}_{\alpha}^{\dagger} \hat{\psi}_{\alpha'}$ $= \int d^d r d^d r' \sum_{\sigma, \sigma'} \langle \mathbf{r}, \sigma \hat{V} \mathbf{r}', \sigma' \rangle \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma'}(\mathbf{r}')$ |
| Two-body operator | $\hat{V}^{(2)} = \frac{1}{2} \sum_{\alpha_1 \cdots \alpha'_2} (\alpha_1 \alpha_2 \hat{V} \alpha'_1 \alpha'_2) \hat{\psi}_{\alpha_1}^{\dagger} \hat{\psi}_{\alpha_2}^{\dagger} \hat{\psi}_{\alpha'_2} \hat{\psi}_{\alpha'_1}$ |

Table 1.1: Main results from second quantification.

1.2.3 Green functions

Retarded Green function

When studying the quantum mechanics of a single particle in Sec. 1.1.1, we introduced the propagator

$$G^R(\mathbf{r}, \mathbf{r}'; t) = -i\Theta(t)\langle \mathbf{r} | e^{-i\hat{H}t} | \mathbf{r}' \rangle = -i\Theta(t) \sum_n e^{-i\epsilon_n t} \varphi_n(\mathbf{r}) \varphi_n^*(\mathbf{r}') \quad (1.169)$$

describing the propagation of a particle from $(\mathbf{r}', 0)$ to (\mathbf{r}, t) . We ignore for the time being the spin of the particle. To make causality explicit, we have added the factor $\Theta(t)$: the particle can propagate only forward in time. The sum in (1.169) extends over a complete set $\{\varphi_n(\mathbf{r}), \epsilon_n\}$ of one-body eigenstates. G^R is called the retarded propagator or retarded Green function. Its Fourier transform is defined by

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \int_{-\infty}^{\infty} dt e^{i(\omega+i\eta)t} G^R(\mathbf{r}, \mathbf{r}'; t) = \sum_n \frac{\varphi_n(\mathbf{r}) \varphi_n^*(\mathbf{r}')}{\omega + i\eta - \epsilon_n}, \quad (1.170)$$

where the infinitesimal $\eta \rightarrow 0^+$ is introduced to ensure the convergence of the integral.¹⁷ Thus the energies ϵ_n of the eigenstates $|n\rangle$ show up as poles of the retarded Green function while the residues give information about the wavefunctions $\varphi_n(\mathbf{r}) = \langle \mathbf{r} | n \rangle$. Since $|\mathbf{r}\rangle = \hat{\psi}^\dagger(\mathbf{r})|\text{vac}\rangle$, G^R can be rewritten as

$$G^R(\mathbf{r}, \mathbf{r}'; t) = -i\Theta(t)\langle \text{vac} | \hat{\psi}(\mathbf{r}) e^{-i\hat{H}t} \hat{\psi}^\dagger(\mathbf{r}') | \text{vac} \rangle. \quad (1.171)$$

In a many-body system, it is tempting to generalize (1.171) as

$$\begin{aligned} G^R(\mathbf{r}, \mathbf{r}'; t) &= -i\Theta(t)\langle 0 | \hat{\psi}(\mathbf{r}) e^{-i\hat{H}t} \hat{\psi}^\dagger(\mathbf{r}') | 0 \rangle \\ &= -i\Theta(t)\langle 0 | \hat{\psi}(\mathbf{r}, t) \hat{\psi}^\dagger(\mathbf{r}', 0) | 0 \rangle, \end{aligned} \quad (1.172)$$

where we take $\epsilon_0 = 0$ for the energy of the many-body ground state $|0\rangle$.

$$\begin{aligned} \hat{\psi}(\mathbf{r}, t) &= e^{i\hat{H}t} \hat{\psi}(\mathbf{r}) e^{-i\hat{H}t}, \\ \hat{\psi}^\dagger(\mathbf{r}, t) &= e^{i\hat{H}t} \hat{\psi}^\dagger(\mathbf{r}) e^{-i\hat{H}t} \end{aligned} \quad (1.173)$$

are the field operators in the Heisenberg picture. In the grand canonical formalism, the term $-\mu\hat{N}$ is included in the Hamiltonian. Contrary to (1.169), the definition (1.172) does not satisfy $G^R(\mathbf{r}, t^+; \mathbf{r}', t) = -i\delta(\mathbf{r} - \mathbf{r}')$ – an expected result for a “propagator” since within an infinitesimal time the particle has no time to propagate. The latter relation is however satisfied if we choose

$$G^R(\mathbf{r}, \mathbf{r}'; t) = -i\Theta(t)\langle 0 | [\hat{\psi}(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', 0)]_{-\zeta} | 0 \rangle. \quad (1.174)$$

This expression reflects the fact that in a many-body system we can not only add but also remove a particle. At finite temperature the ground state expectation value

¹⁷The physical meaning of η is further discussed in chapter 3.

should be replaced by a statistical average and we can define the retarded Green function as

$$\begin{aligned} G^R(\alpha, \alpha'; t) &= -i\Theta(t) \langle [\hat{\psi}_\alpha(t), \hat{\psi}_{\alpha'}^\dagger]_{-\zeta} \rangle \\ &= -i\Theta(t) \frac{1}{Z} \text{Tr} \left\{ e^{-\beta \hat{H}} [\hat{\psi}_\alpha(t), \hat{\psi}_{\alpha'}^\dagger]_{-\zeta} \right\} \end{aligned} \quad (1.175)$$

for any complete set $\{|\alpha\rangle\}$ of one-body states. α includes a spin index as well as other internal indices if necessary.

For a non-interacting system with Hamiltonian $\hat{H}_0 = \sum_\alpha \xi_\alpha \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha$ ($\xi_\alpha = \epsilon_\alpha - \mu$) in the diagonal basis, the field operators satisfy the equations of motion

$$\begin{aligned} \partial_t \hat{\psi}_\alpha(t) &= i[\hat{H}_0, \hat{\psi}_\alpha(t)] = -i\xi_\alpha \hat{\psi}_\alpha(t), \\ \partial_t \hat{\psi}_\alpha^\dagger(t) &= i[\hat{H}_0, \hat{\psi}_\alpha^\dagger(t)] = i\xi_\alpha \hat{\psi}_\alpha^\dagger(t), \end{aligned} \quad (1.176)$$

and are therefore given by

$$\begin{aligned} \hat{\psi}_\alpha(t) &= e^{-i\xi_\alpha t} \hat{\psi}_\alpha, \\ \hat{\psi}_\alpha^\dagger(t) &= e^{i\xi_\alpha t} \hat{\psi}_\alpha^\dagger. \end{aligned} \quad (1.177)$$

From (1.175), we then deduce

$$G_0^R(\alpha, t) = -i\Theta(t) e^{-i\xi_\alpha t} \langle [\hat{\psi}_\alpha, \hat{\psi}_\alpha^\dagger]_{-\zeta} \rangle = -i\Theta(t) e^{-i\xi_\alpha t}, \quad (1.178)$$

and

$$G_0^R(\alpha, \omega) = \int_{-\infty}^{\infty} dt e^{i(\omega + i\eta)t} G_0^R(\alpha, t) = \frac{1}{\omega + i\eta - \xi_\alpha}. \quad (1.179)$$

As in the single-particle case [Eq. (1.170)], the poles of the retarded Green function give the single-particle excitation energies, i.e. the energy of the many-body states obtained by adding (or removing) a particle to the equilibrium state. In chapter 3, we shall study in detail the properties of the retarded Green function in interacting systems and show that its poles are indeed related to the single-particle excitation energies.

Matsubara Green function

The retarded Green function is not the one that is calculated in the first place. Instead, one generally focuses on the Matsubara Green function

$$\begin{aligned} G(\alpha, \alpha'; \tau) &= -\langle T_\tau \hat{\psi}_\alpha(\tau) \hat{\psi}_{\alpha'}^\dagger \rangle \\ &= -\Theta(\tau) \langle \hat{\psi}_\alpha(\tau) \hat{\psi}_{\alpha'}^\dagger \rangle - \zeta \Theta(-\tau) \langle \hat{\psi}_{\alpha'}^\dagger \hat{\psi}_\alpha(\tau) \rangle, \end{aligned} \quad (1.180)$$

where the time ordering operator T_τ is defined by the second line. For fermions, the interchange of the two operators when $\tau < 0$ implies a sign change. The imaginary time operators in (1.180) are defined by

$$\begin{aligned} \hat{\psi}_\alpha(\tau) &= e^{\tau \hat{H}} \hat{\psi}_\alpha e^{-\tau \hat{H}}, \\ \hat{\psi}_\alpha^\dagger(\tau) &= e^{\tau \hat{H}} \hat{\psi}_\alpha^\dagger e^{-\tau \hat{H}}. \end{aligned} \quad (1.181)$$

For $\tau = it$, they reduce to the real-time Heisenberg operators (1.173). Note that $\hat{\psi}_\alpha^\dagger(\tau)$ is not the adjoint $[\hat{\psi}_\alpha(\tau)]^\dagger$ of $\hat{\psi}_\alpha(\tau)$. For $\tau > 0$, $G(\alpha, \alpha'; \tau)$ describes the creation of a particle and its propagation in the system, while for $\tau < 0$ it describes the annihilation of a particle and the propagation of the corresponding “hole”. There is no need to specify here how the equal-time ($\tau = 0$) Green function is defined. As we shall see, $G(\alpha, \alpha'; 0)$ will always be interpreted as either as $G(\alpha, \alpha'; 0^+)$ or $G(\alpha, \alpha'; 0^-)$.

We shall see later that we need to know $G(\alpha, \alpha'; \tau)$ only for $\tau \in [-\beta, \beta]$. For $-\beta < \tau < 0$, one obtains

$$\begin{aligned} G(\alpha, \alpha'; \tau) &= -\zeta \langle \hat{\psi}_{\alpha'}^\dagger \hat{\psi}_\alpha(\tau) \rangle \\ &= -\zeta e^{\beta\Omega} \text{Tr} [e^{-\beta\hat{H}} \hat{\psi}_{\alpha'}^\dagger e^{\tau\hat{H}} \hat{\psi}_\alpha e^{-\tau\hat{H}}] \\ &= -\zeta e^{\beta\Omega} \text{Tr} [e^{\tau\hat{H}} \hat{\psi}_\alpha e^{-(\tau+\beta)\hat{H}} \hat{\psi}_{\alpha'}^\dagger] \\ &= -\zeta e^{\beta\Omega} \text{Tr} [e^{-\beta\hat{H}} \hat{\psi}_\alpha(\tau + \beta) \hat{\psi}_{\alpha'}^\dagger] \\ &= \zeta G(\alpha, \alpha'; \tau + \beta) \end{aligned} \quad (1.182)$$

(with $\Omega = -\frac{1}{\beta} \ln Z$ the thermodynamic potential) making use of the cyclic invariance of the trace. A similar reasoning gives

$$G(\alpha, \alpha'; \tau) = \zeta G(\alpha, \alpha'; \tau - \beta) \quad (1.183)$$

for $0 < \tau < \beta$. Since $G(\alpha, \alpha'; \tau)$ is (anti)periodic for $\tau \in [-\beta, \beta]$ with period β , it can be expanded in a Fourier series,

$$\begin{aligned} G(\alpha, \alpha'; \tau) &= \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n \tau} G(\alpha, \alpha'; i\omega_n), \\ G(\alpha, \alpha'; i\omega_n) &= \int_0^\beta d\tau e^{i\omega_n \tau} G(\alpha, \alpha'; \tau), \end{aligned} \quad (1.184)$$

where $\sum_{\omega_n} = \sum_{n=-\infty}^\infty$ and the discrete frequencies

$$\omega_n = \begin{cases} \frac{2\pi}{\beta} n & (\text{bosons}), \\ \frac{2\pi}{\beta} (n + \frac{1}{2}) & (\text{fermions}), \end{cases} \quad (1.185)$$

are called Matsubara frequencies.

The Matsubara Green function can be easily calculated for a non-interacting system with Hamiltonian $\hat{H}_0 = \sum_\alpha \xi_\alpha \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha$. Inserting $\hat{\psi}_\alpha(\tau) = e^{-\xi_\alpha \tau} \hat{\psi}_\alpha$ and $\hat{\psi}_\alpha^\dagger(\tau) = e^{-\xi_\alpha \tau} \hat{\psi}_\alpha^\dagger$ in (1.180), we obtain

$$G_0(\alpha, \tau) = -e^{-\xi_\alpha \tau} [\Theta(\tau)(1 + \zeta n_\alpha) + \Theta(-\tau)\zeta n_\alpha], \quad (1.186)$$

where the occupation number $n_\alpha = \langle \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha \rangle$ is given by the Fermi-Dirac function $n_F(\xi_\alpha)$ for fermions and the Bose-Einstein function $n_B(\xi_\alpha)$ for bosons. In frequency space

$$G_0(\alpha, i\omega_n) = \frac{1}{i\omega_n - \xi_\alpha}. \quad (1.187)$$

Comparing (1.179) and (1.187), we see that the retarded Green function can be obtained from the Matsubara one by an analytical continuation

$$G_0^R(\alpha, \omega) = G_0(\alpha, i\omega_n \rightarrow \omega + i\eta). \quad (1.188)$$

This result turns out to be valid also in interacting systems. The retarded Green function, which contains physical information about the system, can be deduced from the Matsubara Green function which is the natural quantity to consider in (finite temperature) interacting systems. We postpone a detailed study of the properties of Green functions to chapter 3 and in the following sections of this chapter discuss how we can define and compute Green functions in the functional integral formalism.

Many-particle Green function

The Green function we have discussed so far is called the one-particle Green function since it describes the propagation of a single particle. One can also define higher-order Green functions

$$\begin{aligned} G^{(2n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n; \alpha'_1 \tau'_1, \dots, \alpha'_n \tau'_n) \\ = (-1)^n \langle T_\tau \hat{\psi}_{\alpha_1}(\tau_1) \cdots \hat{\psi}_{\alpha_n}(\tau_n) \hat{\psi}_{\alpha'_1}^\dagger(\tau'_1) \cdots \hat{\psi}_{\alpha'_n}^\dagger(\tau'_n) \rangle. \end{aligned} \quad (1.189)$$

Note that the superscript $(2n)$ corresponds to the number of operators rather than the number n of particles propagating in the system. We shall often denote the single-particle Green function $G^{(2)}$ merely by G . As in (1.180), the operator T_τ chronologically orders the operators from left to right with the latest time to the left,

$$T_\tau \hat{A}_{\alpha_1}(\tau_1) \cdots \hat{A}_{\alpha_n}(\tau_n) = \zeta^p \hat{A}_{\alpha_{p(1)}}(\tau_{p(1)}) \cdots \hat{A}_{\alpha_{p(n)}}(\tau_{p(n)}) \quad (1.190)$$

($\tau_{p(1)} > \tau_{p(2)} > \cdots > \tau_{p(n)}$), where ζ^p equals one for bosons and the signature of the permutation p for fermions.

Real-time Green function

Finally, we can define Green functions in real time,

$$\begin{aligned} G^{(2n)}(\alpha_1 t_1, \dots, \alpha_n t_n; \alpha'_1 t'_1, \dots, \alpha'_n t'_n) \\ = (-i)^n \langle T \hat{\psi}_{\alpha_1}(t_1) \cdots \hat{\psi}_{\alpha_n}(t_n) \hat{\psi}_{\alpha'_1}^\dagger(t'_1) \cdots \hat{\psi}_{\alpha'_n}^\dagger(t'_n) \rangle, \end{aligned} \quad (1.191)$$

where T is the time-ordering operator (not to be confused with the temperature) defined as its imaginary-time counterpart T_τ , and $\hat{\psi}_\alpha(t), \hat{\psi}_\alpha^\dagger(t)$ the Heisenberg picture operators (1.173). The relation between the various Green functions introduced in this section will be studied in sections 3.2.7 and 3.5.

1.3 Coherent states

The quantum mechanical behavior of a single particle is usually described in terms of the position and momentum operators $\hat{\mathbf{q}}$ and $\hat{\mathbf{p}}$. When constructing a path integral representation of the propagator or the partition function, it therefore appears natural

to introduce the closure relations $\int d^d q |\mathbf{q}\rangle\langle\mathbf{q}| = 1$ and/or $\sum_{\mathbf{p}} |\mathbf{p}\rangle\langle\mathbf{p}| = 1$ at each time step (Sec. 1.1.1). Since second quantization is the natural formalism for studying many-particle systems, we should try to construct the path integral using a closure relation based on the eigenstates of the creation or annihilation operators.

Now it is clear that an arbitrary state

$$|\psi\rangle = \sum_{\alpha_1 \dots \alpha_n} C_{\alpha_1 \dots \alpha_n} |\alpha_1 \dots \alpha_n\rangle \quad (1.192)$$

cannot be an eigenstate of the creation operator $\hat{\psi}_\alpha^\dagger$. $|\psi\rangle$ has necessarily a component with a minimum number n_0 of particles. Applying $\hat{\psi}_\alpha^\dagger$ to this component will either increase n_0 by 1 or yields zero if the single-particle state α is already occupied and the particles are fermions. In all cases, the minimum numbers of particles in $|\psi\rangle$ and $\hat{\psi}_\alpha^\dagger |\psi\rangle$ differ. On the other hand there is *a priori* nothing that prevents $|\psi\rangle$ to be an eigenstate of $\hat{\psi}_\alpha$. Suppose that $|\psi\rangle$ is an eigenstate of the annihilation operators,

$$\hat{\psi}_\alpha |\psi\rangle = \psi_\alpha |\psi\rangle \quad \forall \alpha. \quad (1.193)$$

Then the (anti)commutation relations

$$[\hat{\psi}_\alpha, \hat{\psi}_\beta]_{-\zeta} = 0 \quad (1.194)$$

imply

$$\begin{aligned} \hat{\psi}_\alpha \hat{\psi}_\beta |\psi\rangle &= \hat{\psi}_\alpha \psi_\beta |\psi\rangle = \psi_\alpha \psi_\beta |\psi\rangle \\ &= \zeta \hat{\psi}_\beta \hat{\psi}_\alpha |\psi\rangle = \zeta \hat{\psi}_\beta \psi_\alpha |\psi\rangle = \zeta \psi_\beta \psi_\alpha |\psi\rangle, \end{aligned} \quad (1.195)$$

i.e.

$$[\psi_\alpha, \psi_\beta]_{-\zeta} = 0. \quad (1.196)$$

Thus, for fermions, the eigenvalues cannot be ordinary numbers. We shall need to introduce anticommuting variables called Grassmann numbers.¹⁸ Postponing the case of fermions to sections 1.3.2 and 1.3.3, we now restrict our discussion to the case of bosons.

1.3.1 Boson coherent states

It is straightforward to verify that the so-called boson coherent states

$$\begin{aligned} |\psi\rangle &= \exp\left\{\sum_{\alpha} \psi_{\alpha} \hat{\psi}_{\alpha}^{\dagger}\right\} |\text{vac}\rangle \\ &= \sum_{n_{\alpha_1}, n_{\alpha_2}, \dots=0}^{\infty} \frac{(\psi_{\alpha_1}^{n_{\alpha_1}} \dots \psi_{\alpha_p}^{n_{\alpha_p}} \dots)}{(n_{\alpha_1}! \dots n_{\alpha_p}! \dots)^{1/2}} |n_{\alpha_1} \dots n_{\alpha_p} \dots\rangle \end{aligned} \quad (1.197)$$

(ψ_{α} is a *c*-number) are eigenstates of the annihilation operators,¹⁹

$$\hat{\psi}_{\alpha} |\psi\rangle = \psi_{\alpha} |\psi\rangle. \quad (1.198)$$

¹⁸Note that when ψ_{α} is an anticommuting variable, (1.195) holds regardless of whether ψ_{α} commutes or anticommutes with the operator $\hat{\psi}_{\beta}$.

¹⁹Expand the exponential in (1.197) and use $[\hat{\psi}_{\alpha}, (\hat{\psi}_{\beta}^{\dagger})^n]_{-} = \delta_{\alpha, \beta} n (\hat{\psi}_{\alpha}^{\dagger})^{n-1}$.

The action of the creation operator $\hat{\psi}_\alpha^\dagger$ on the coherent states is given by

$$\hat{\psi}_\alpha^\dagger|\psi\rangle = \frac{\partial}{\partial\psi_\alpha}|\psi\rangle. \quad (1.199)$$

By taking the Hermitian conjugate in (1.198) and (1.199), we deduce

$$\begin{aligned} \langle\psi|\hat{\psi}_\alpha^\dagger &= \langle\psi|\psi_\alpha^*, \\ \langle\psi|\hat{\psi}_\alpha &= \frac{\partial}{\partial\psi_\alpha^*}\langle\psi|, \end{aligned} \quad (1.200)$$

where

$$\langle\psi| = \langle\text{vac}|\exp\left\{\sum_\alpha\psi_\alpha^*\hat{\psi}_\alpha\right\} \quad (1.201)$$

is the bra corresponding to the ket $|\psi\rangle$ and ψ_α^* the complex conjugate of ψ_α .

The overlap between two states is given by

$$\langle\psi|\psi'\rangle = \exp\left\{\sum_\alpha\psi_\alpha^*\psi'_\alpha\right\}. \quad (1.202)$$

Another crucial property of the coherent states is their overcompleteness in the Fock space,²⁰ which results in the closure relation

$$\int \prod_\alpha \frac{d\psi_\alpha^* d\psi_\alpha}{2i\pi} e^{-\sum_\alpha |\psi_\alpha|^2} |\psi\rangle\langle\psi| = 1, \quad (1.203)$$

where

$$\frac{d\psi_\alpha^* d\psi_\alpha}{2i\pi} = \frac{1}{\pi} d\Re(\psi_\alpha) d\Im(\psi_\alpha). \quad (1.204)$$

For a single degree of freedom, writing $\psi = \rho e^{i\theta}$, one finds

$$\begin{aligned} \int \frac{d\psi^* d\psi}{2i\pi} e^{-|\psi|^2} |\psi\rangle\langle\psi| &= \frac{1}{\pi} \int_0^\infty \rho d\rho \int_0^{2\pi} d\theta e^{-\rho^2} \sum_{n,m=0}^\infty \frac{\rho^{n+m} e^{i(n-m)\theta}}{(n!m!)^{1/2}} |n\rangle\langle m| \\ &= 2 \int_0^\infty \rho d\rho e^{-\rho^2} \sum_{n=0}^\infty \frac{\rho^{2n}}{n!} |n\rangle\langle n| \\ &= \sum_{n=0}^\infty |n\rangle\langle n| = 1. \end{aligned} \quad (1.205)$$

This result is generalized to many degrees of freedom by writing the coherent state $|\psi\rangle$ in terms of the states $|n_{\alpha_1} \cdots\rangle$ [Eq. (1.197)] and using the closure relation (1.133) in Fock space.

Let us now consider an operator $\hat{A} \equiv A(\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha)$ where all creation operators stand to the left of the annihilation operators. Such an operator is said to be normal ordered. Its matrix element between coherent states takes the simple form

$$\langle\psi|A(\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha)|\psi'\rangle = e^{\sum_\alpha \psi_\alpha^* \psi'_\alpha} A(\psi_\alpha^*, \psi'_\alpha). \quad (1.206)$$

²⁰The basis is said to be overcomplete because the coherent states are not pairwise orthogonal.

To conclude this section, we note that the occupation numbers n_α in the coherent state $|\psi\rangle$ are Poisson distributed with mean values $|\psi_\alpha|^2$,

$$|\langle n_{\alpha_1} \cdots n_{\alpha_p} \cdots | \psi \rangle|^2 = \prod_{\alpha} \frac{|\psi_\alpha|^{2n_\alpha}}{n_\alpha!}. \quad (1.207)$$

The total number of particle has the average value

$$N = \langle \hat{N} \rangle = \frac{\langle \psi | \hat{N} | \psi \rangle}{\langle \psi | \psi \rangle} = \sum_{\alpha} |\psi_\alpha|^2 \quad (1.208)$$

(recall that $\hat{N} = \sum_{\alpha} \hat{\psi}_{\alpha}^{\dagger} \hat{\psi}_{\alpha}$) and variance

$$\sigma^2 = \langle (\hat{N} - \langle \hat{N} \rangle)^2 \rangle = \langle \hat{N} \rangle. \quad (1.209)$$

In the thermodynamic limit where $N \rightarrow \infty$, $\sigma/N = 1/\sqrt{N} \rightarrow 0$ and the particle number distribution becomes sharply peaked around N , reflecting the fact that a product of Poisson distributions approaches a normal distribution.

The physical meaning of the boson coherent states can be understood from the study of a one-dimensional harmonic oscillator,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2, \quad (1.210)$$

with $[\hat{x}, \hat{p}] = i$. The ladder operators

$$\hat{a} = \sqrt{\frac{m\omega}{2}} \left(\hat{x} + i \frac{\hat{p}}{m\omega} \right), \quad \hat{a}^{\dagger} = \sqrt{\frac{m\omega}{2}} \left(\hat{x} - i \frac{\hat{p}}{m\omega} \right) \quad (1.211)$$

satisfy canonical bosonic commutation relations, $[\hat{a}, \hat{a}^{\dagger}] = 1$, and enable to rewrite the Hamiltonian as

$$\hat{H} = \omega \left(\hat{a}^{\dagger} \hat{a} + \frac{1}{2} \right). \quad (1.212)$$

The states $|n\rangle = \frac{(\hat{a}^{\dagger})^n}{\sqrt{n!}} |\text{vac}\rangle$ are eigenstates with eigenvalues $(n + \frac{1}{2})\omega$.

Let us now consider the normalized coherent state

$$|z\rangle = \exp\left(-\frac{|z|^2}{2} + z\hat{a}^{\dagger}\right) |\text{vac}\rangle. \quad (1.213)$$

A simple calculation yields

$$\begin{aligned} \langle z | \hat{x} | z \rangle &= \sqrt{\frac{2}{m\omega}} \Re(z), & \langle z | \hat{x}^2 | z \rangle &= \frac{1}{2m\omega} [4\Re(z)^2 + 1], \\ \langle z | \hat{p} | z \rangle &= \sqrt{2m\omega} \Im(z), & \langle z | \hat{p}^2 | z \rangle &= \frac{m\omega}{2} [4\Im(z)^2 + 1], \end{aligned} \quad (1.214)$$

and therefore

$$\Delta x^2 = \frac{1}{2m\omega}, \quad \Delta p^2 = \frac{m\omega}{2}. \quad (1.215)$$

Thus the coherent state $|z\rangle$ yields the minimum position and momentum fluctuations compatible with the uncertainty relation $\Delta x \Delta p \geq \hbar/2$ (we have restored Planck constant).

In order to further study the relation between coherent states and the classical limit of the harmonic oscillator, we consider the dynamics of the eigenstates $|n\rangle$ in the Schrödinger picture,

$$e^{-i\hat{H}t}|n\rangle = e^{-i(n+\frac{1}{2})\omega t}|n\rangle. \quad (1.216)$$

From (1.216) we deduce the time evolution of the coherent states,

$$e^{-i\hat{H}t}|z\rangle = e^{-\frac{|z|^2}{2}} \sum_{n=0}^{\infty} \frac{(z\hat{a}^\dagger)^n}{\sqrt{n!}} e^{-i\hat{H}t}|n\rangle = e^{-\frac{i}{2}\omega t} |e^{-i\omega t}z\rangle. \quad (1.217)$$

Apart from the unimportant phase factor $e^{-\frac{i}{2}\omega t}$, the dynamics of the coherent state $|z\rangle$ is simply obtained by replacing z by $z(t) = ze^{-i\omega t}$. One then finds that the quantum averages

$$\begin{aligned} \langle \hat{x} \rangle(t) &= \langle z(t) | \hat{x} | z(t) \rangle = \sqrt{\frac{2}{m\omega}} z(0) \cos(\omega t), \\ \langle \hat{p} \rangle(t) &= \langle z(t) | \hat{p} | z(t) \rangle = \sqrt{2m\omega} z(0) \sin(\omega t) \end{aligned} \quad (1.218)$$

(we assume $z(0) = z$ to be real) satisfy the classical equations of motion $\dot{x} = \partial H / \partial p = p/m$ and $\dot{p} = -\partial H / \partial x = -m\omega^2 x$. The amplitude $|z(0)|$ of the oscillations is related to the mean value of $\hat{N} = \hat{a}^\dagger \hat{a}$,

$$\langle \hat{N} \rangle = \langle z(t) | \hat{a}^\dagger \hat{a} | z(t) \rangle = |z(t)|^2 = |z(0)|^2. \quad (1.219)$$

The time independence of $\langle \hat{N} \rangle$ follows from $[\hat{H}, \hat{N}] = 0$ (see Appendix 1.B and chapter 2). When $\langle \hat{N} \rangle = |z(0)|^2 \gg 1$, $|\langle \hat{x} \rangle(t)| \gg \Delta x$ and $|\langle \hat{p} \rangle(t)| \gg \Delta p$ for most times t (with Δx and Δp given by (1.215)). A coherent state with large occupation number $\langle \hat{N} \rangle = |z(0)|^2$ therefore corresponds to a quasi-classical behavior of the harmonic oscillator. Boson coherent states are sometimes referred to as quasi-classical states.

1.3.2 Grassmann variables

A Grassmann algebra is an algebra of anticommuting variables (or Grassmann variables).²¹ It is defined by a set $\{\psi_1, \dots, \psi_n\}$ of n generators whose product is anticommutative,

$$[\psi_i, \psi_j]_+ = \psi_i \psi_j + \psi_j \psi_i = 0. \quad (1.220)$$

This implies that the square ψ_i^2 of any generator vanishes. An element of the Grassmann algebra is a polynomial of first order in the generators,

$$f(\psi_1, \dots, \psi_n) = c_0 + \sum_{k=1}^n \sum_{i_1 \dots i_k=1}^n c_{i_1 \dots i_k} \psi_{i_1} \dots \psi_{i_k}, \quad (1.221)$$

where the coefficients c_0 and $c_{i_1 \dots i_k}$ are complex and we assume that the indices $i_1 < i_2 < \dots < i_k$ are ordered. For example, the elements of a Grassmann algebra with only one or two generators are

$$\begin{aligned} f(\psi) &= c_0 + c_1 \psi, \\ f(\psi_1, \psi_2) &= c_0 + c_1 \psi_1 + c_2 \psi_2 + c_{12} \psi_1 \psi_2. \end{aligned} \quad (1.222)$$

²¹Recall that an algebra is a vector space endowed with a multiplication rule.

Differentiation with respect to Grassmann numbers is defined by

$$\frac{\partial}{\partial \psi_i} \psi_j = \delta_{i,j}. \quad (1.223)$$

As with ordinary numbers, this is a linear operation. The anticommutation relations (1.220) imply

$$[\partial_{\psi_i}, \partial_{\psi_j}]_+ = 0. \quad (1.224)$$

The operator ∂_{ψ_i} is therefore nilpotent, $\partial_{\psi_i}^2 = 0$, reflecting the fact that the function $f(\psi_1, \dots, \psi_n)$ is at most of order 1 in each variable. Equation (1.223) defines a left differentiation,

$$\partial_{\psi_i} \psi_j \psi_i = -\partial_{\psi_i} \psi_i \psi_j = -\psi_j \quad (i \neq j). \quad (1.225)$$

For ∂_{ψ_i} to act on ψ_i , one should first shift ψ_i to the left of the monomial. The chain rule for differentiation then reads

$$\frac{\partial}{\partial \psi_i} f(g) = \frac{\partial g}{\partial \psi_i} \frac{\partial f}{\partial g}. \quad (1.226)$$

Contrary to ordinary variables, the order of the terms in the rhs matters.

For Grassmann numbers, integration and differentiation are identical,

$$\int d\psi_i f(\psi_1, \dots, \psi_n) = \frac{\partial}{\partial \psi_i} f(\psi_1, \dots, \psi_n). \quad (1.227)$$

This property ensures that two fundamental properties of ordinary integrals over functions vanishing at infinity are satisfied. The integral of an exact differential form is zero,

$$\int d\psi_i \frac{\partial}{\partial \psi_i} f(\psi_1, \dots, \psi_n) = 0, \quad (1.228)$$

and the integral over ψ_i of $f(\psi_1, \dots, \psi_n)$ does not depend on ψ_i so that its derivative vanishes,

$$\frac{\partial}{\partial \psi_i} \int d\psi_i f(\psi_1, \dots, \psi_n) = 0. \quad (1.229)$$

Both properties (1.228) and (1.229) follow from the definition (1.227) and the nilpotence of the differential operator ∂_{ψ_i} . For a Grassmann algebra with a single generator, one has

$$\begin{aligned} f(\psi) &= c_0 + c_1 \psi, \\ \frac{\partial f}{\partial \psi} &= \int d\psi f = c_1. \end{aligned} \quad (1.230)$$

Other properties of Grassmann integration are discussed in Appendix 1.E.

It will often be convenient to consider Grassmann algebras with $2n$ generators $\{\psi_1, \dots, \psi_n, \psi_1^*, \dots, \psi_n^*\}$. One can then define a (complex) conjugation for Grassmann variables,

$$\begin{aligned} (\psi_i)^* &= \psi_i^*, \\ (\psi_i^*)^* &= \psi_i, \\ (c\psi_i)^* &= c^* \psi_i^* \quad (c \in \mathbb{C}), \\ (\psi_i \psi_j)^* &= \psi_j^* \psi_i^*. \end{aligned} \quad (1.231)$$

The general element of a Grassmann algebra with two generators $\{\psi, \psi^*\}$ reads

$$f(\psi, \psi^*) = c_0 + c_1 \psi^* + c_2 \psi + c_{12} \psi^* \psi. \quad (1.232)$$

Using the differentiation and integration rules, one easily finds

$$\begin{aligned} \frac{\partial f}{\partial \psi} &= \int d\psi f = c_2 - c_{12} \psi^*, \\ \frac{\partial f}{\partial \psi^*} &= \int d\psi^* f = c_1 + c_{12} \psi, \\ \frac{\partial^2 f}{\partial \psi^* \partial \psi} &= \int d\psi^* d\psi f = -c_{12}. \end{aligned} \quad (1.233)$$

1.3.3 Fermion coherent states

Grassmann variables enable to define coherent states analog to the ones introduced for bosons. Given a set $\{\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha\}$ of annihilation operators, we define a Grassmann algebra by associating a generator ψ_α to $\hat{\psi}_\alpha$ and a generator ψ_α^* to $\hat{\psi}_\alpha^\dagger$ for any α . We also require

$$\begin{aligned} [\psi_\alpha^{(*)}, \hat{\psi}_\beta^{(\dagger)}]_+ &= 0, \\ (\psi_\alpha \hat{\psi}_\beta)^\dagger &= \hat{\psi}_\beta^\dagger \psi_\alpha^*, \quad (\psi_\alpha \hat{\psi}_\beta^\dagger)^\dagger = \hat{\psi}_\beta \psi_\alpha^*, \quad \text{etc.} \end{aligned} \quad (1.234)$$

A fermion coherent state is defined by the ket

$$|\psi\rangle = \exp\left\{-\sum_\alpha \psi_\alpha \hat{\psi}_\alpha^\dagger\right\} |\text{vac}\rangle = \prod_\alpha (1 - \psi_\alpha \hat{\psi}_\alpha^\dagger) |\text{vac}\rangle \quad (1.235)$$

and the corresponding bra

$$\langle\psi| = \langle\text{vac}| \exp\left\{\sum_\alpha \psi_\alpha^* \hat{\psi}_\alpha\right\} = \langle\text{vac}| \prod_\alpha (1 + \psi_\alpha^* \hat{\psi}_\alpha). \quad (1.236)$$

It is straightforward to show that the properties (1.198-1.200) obtained previously for the boson coherent states carry over to the fermionic case,²²

$$\begin{aligned} \hat{\psi}_\alpha |\psi\rangle &= \psi_\alpha |\psi\rangle, \\ \hat{\psi}_\alpha^\dagger |\psi\rangle &= -\frac{\partial}{\partial \psi_\alpha} |\psi\rangle, \\ \langle\psi| \hat{\psi}_\alpha^\dagger &= \langle\psi| \psi_\alpha^*, \\ \langle\psi| \hat{\psi}_\alpha &= \frac{\partial}{\partial \psi_\alpha^*} \langle\psi|. \end{aligned} \quad (1.237)$$

²²For instance, the first equation in (1.237) is obtained from $\hat{\psi}_\alpha |\psi\rangle = \hat{\psi}_\alpha \prod_\beta (1 - \psi_\beta \hat{\psi}_\beta^\dagger) |\text{vac}\rangle = \prod_{\beta \neq \alpha} (1 - \psi_\beta \hat{\psi}_\beta^\dagger) \hat{\psi}_\alpha (1 - \psi_\alpha \hat{\psi}_\alpha^\dagger) |\text{vac}\rangle = \prod_{\beta \neq \alpha} (1 - \psi_\beta \hat{\psi}_\beta^\dagger) \psi_\alpha |\text{vac}\rangle = \prod_{\beta \neq \alpha} (1 - \psi_\beta \hat{\psi}_\beta^\dagger) \psi_\alpha (1 - \psi_\alpha \hat{\psi}_\alpha^\dagger) |\text{vac}\rangle = \psi_\alpha |\psi\rangle$.

The overlap between two states is given by

$$\langle \psi | \psi' \rangle = \exp \left\{ \sum_{\alpha} \psi_{\alpha}^* \psi'_{\alpha} \right\}, \quad (1.238)$$

and for a normal ordered operator $\hat{A} = A(\hat{\psi}_{\alpha}^{\dagger}, \hat{\psi}_{\alpha})$,

$$\langle \psi | A(\hat{\psi}_{\alpha}^{\dagger}, \hat{\psi}_{\alpha}) | \psi' \rangle = e^{\sum_{\alpha} \psi_{\alpha}^* \psi'_{\alpha}} A(\psi_{\alpha}^*, \psi'_{\alpha}). \quad (1.239)$$

The overcompleteness of the coherent state basis reflects into the closure relation

$$\int \prod_{\alpha} d\psi_{\alpha}^* d\psi_{\alpha} e^{-\sum_{\alpha} \psi_{\alpha}^* \psi_{\alpha}} |\psi\rangle \langle \psi| = 1. \quad (1.240)$$

This relation can be proven by considering the matrix element of the lhs of (1.240) between two arbitrary states of the Fock space. From

$$\begin{aligned} \langle \alpha_1 \cdots \alpha_n | \psi \rangle &= \langle \text{vac} | \hat{\psi}_{\alpha_n} \cdots \hat{\psi}_{\alpha_1} | \psi \rangle = \psi_{\alpha_n} \cdots \psi_{\alpha_1}, \\ \langle \psi | \beta_1 \cdots \beta_m \rangle &= \langle \psi | \hat{\psi}_{\beta_1}^{\dagger} \cdots \hat{\psi}_{\beta_m}^{\dagger} | \text{vac} \rangle = \psi_{\beta_1}^* \cdots \psi_{\beta_m}^* \end{aligned} \quad (1.241)$$

($\langle \text{vac} | \psi \rangle = 1$), we deduce

$$\begin{aligned} &\int \prod_{\alpha} d\psi_{\alpha}^* d\psi_{\alpha} e^{-\sum_{\alpha} \psi_{\alpha}^* \psi_{\alpha}} \langle \alpha_1 \cdots \alpha_n | \psi \rangle \langle \psi | \beta_1 \cdots \beta_m \rangle \\ &= \int \prod_{\alpha} d\psi_{\alpha}^* d\psi_{\alpha} \prod_{\alpha} (1 - \psi_{\alpha}^* \psi_{\alpha}) \psi_{\alpha_n} \cdots \psi_{\alpha_1} \psi_{\beta_1}^* \cdots \psi_{\beta_m}^*. \end{aligned} \quad (1.242)$$

Four types of integrals appear in (1.242),

$$\int d\psi_{\alpha}^* d\psi_{\alpha} (1 - \psi_{\alpha}^* \psi_{\alpha}) \begin{pmatrix} \psi_{\alpha} \psi_{\alpha}^* \\ \psi_{\alpha} \\ \psi_{\alpha}^* \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \quad (1.243)$$

Thus each α should belong to both $\{\alpha_i\}$ and $\{\beta_i\}$ or be absent from both sets for (1.242) to be nonzero. In this case $n = m$ and $\beta_i = \alpha_{p(i)}$ with $p \in S_n$ a permutation, and equation (1.242) reduces to

$$\begin{aligned} &\int \prod_{\alpha} d\psi_{\alpha}^* d\psi_{\alpha} \prod_{\alpha} (1 - \psi_{\alpha}^* \psi_{\alpha}) \psi_{\alpha_n} \cdots \psi_{\alpha_1} \psi_{\alpha_{p(1)}}^* \cdots \psi_{\alpha_{p(m)}}^* \\ &= \int \prod_{\alpha} d\psi_{\alpha}^* d\psi_{\alpha} \prod_{\alpha} (1 - \psi_{\alpha}^* \psi_{\alpha}) (-1)^p \psi_{\alpha_n} \cdots \psi_{\alpha_1} \psi_{\alpha_1}^* \cdots \psi_{\alpha_m}^* = (-1)^p. \end{aligned} \quad (1.244)$$

This result should be compared with

$$\langle \alpha_1 \cdots \alpha_n | \beta_1 \cdots \beta_m \rangle = \delta_{n,m} \sum_{p \in S_n} (-1)^p \delta_{\alpha_i, \beta_{p(i)}}, \quad (1.245)$$

| | |
|-------------------------|---|
| Definition | $ \psi\rangle = \exp\left\{\zeta \sum_{\alpha} \psi_{\alpha} \hat{\psi}_{\alpha}^{\dagger}\right\} \text{vac}\rangle$ $\langle\psi = \langle\text{vac} \exp\left\{\sum_{\alpha} \psi_{\alpha}^* \hat{\psi}_{\alpha}\right\}$ |
| | $\hat{\psi}_{\alpha} \psi\rangle = \psi_{\alpha} \psi\rangle, \quad \langle\psi \hat{\psi}_{\alpha}^{\dagger} = \langle\psi \psi_{\alpha}^*$ |
| Overlap | $\langle\psi \psi'\rangle = \exp\left\{\sum_{\alpha} \psi_{\alpha}^* \psi'_{\alpha}\right\}$ |
| Closure relation | $\int \prod_{\alpha} \frac{d\psi_{\alpha}^* d\psi_{\alpha}}{\mathcal{N}} e^{-\sum_{\alpha} \psi_{\alpha} ^2} \psi\rangle \langle\psi = 1$ |
| Normal ordered operator | $\langle\psi A(\hat{\psi}_{\alpha}^{\dagger}, \hat{\psi}_{\alpha}) \psi'\rangle = e^{\sum_{\alpha} \psi_{\alpha}^* \psi'_{\alpha}} A(\psi_{\alpha}^*, \psi'_{\alpha})$ |

Table 1.2: Main properties of coherent states. ψ_{α} denotes a complex variable for bosons ($\zeta = 1$) and a Grassmann number for fermions ($\zeta = -1$). $\mathcal{N} = 2i\pi$ for bosons and $\mathcal{N} = 1$ for fermions.

which proves the closure relation (1.240).

To conclude this section, we note that fermion coherent states are not physical states of the system; they do not belong to the Fock space. For instance, the expectation value of the particle number operator $\hat{N} = \sum_{\alpha} \hat{\psi}_{\alpha}^{\dagger} \hat{\psi}_{\alpha}$ in the coherent state $|\psi\rangle$,

$$\frac{\langle\psi|\hat{N}|\psi\rangle}{\langle\psi|\psi\rangle} = \sum_{\alpha} \psi_{\alpha}^* \psi_{\alpha}, \quad (1.246)$$

is not a real number.

1.4 Functional integral in many-particle systems

We are now in a position to derive a functional integral representation of the partition function of a many-particle system following the general procedure outlined in Sec. 1.1.

1.4.1 Coherent-state functional integral

Partition function

Making use of the closure relation (1.203) or (1.240), we can write the partition function as

$$Z = \sum_n \langle n | e^{-\beta \hat{H}} | n \rangle = \sum_n \int d(\psi^*, \psi) e^{-\sum_{\alpha} \psi_{\alpha}^* \psi_{\alpha}} \langle n | \psi \rangle \langle \psi | e^{-\beta \hat{H}} | n \rangle, \quad (1.247)$$

where \hat{H} is the grand canonical Hamiltonian of the system (including the term $-\mu \hat{N}$), and $\{|n\rangle\}$ a basis in the Fock space. $|\psi\rangle$ is a coherent state, and ψ_{α} a c-number for

bosons and a Grassmann variable for fermions. We use the notation

$$d(\psi^*, \psi) = \begin{cases} \prod_{\alpha} \frac{d\psi_{\alpha}^* d\psi_{\alpha}}{2i\pi} & (\text{bosons}), \\ \prod_{\alpha} d\psi_{\alpha}^* d\psi_{\alpha} & (\text{fermions}). \end{cases} \quad (1.248)$$

For bosons, we can interchange the two terms $\langle n|\psi\rangle$ and $\langle\psi|e^{-\beta\hat{H}}|n\rangle$ in (1.247) and then use $\sum_n |n\rangle\langle n| = 1$. For fermions, this interchange should be realized with care. Let us write $e^{-\beta\hat{H}}|n\rangle = \sum_m a_m|m\rangle$. Since \hat{H} conserves the particle number, the kets $|n\rangle$ and $|m\rangle$ must have the same number of particles. Writing

$$\begin{aligned} |n\rangle &= \hat{\psi}_{\alpha_1}^{\dagger} \cdots \hat{\psi}_{\alpha_p}^{\dagger} |\text{vac}\rangle, \\ |m\rangle &= \hat{\psi}_{\gamma_1}^{\dagger} \cdots \hat{\psi}_{\gamma_p}^{\dagger} |\text{vac}\rangle, \end{aligned} \quad (1.249)$$

we obtain

$$\begin{aligned} \langle n|\psi\rangle\langle\psi|m\rangle &= \psi_{\alpha_p} \cdots \psi_{\alpha_1} \psi_{\gamma_1}^* \cdots \psi_{\gamma_p}^* \\ &= \zeta^{p^2} \psi_{\gamma_1}^* \cdots \psi_{\gamma_p}^* \psi_{\alpha_p} \cdots \psi_{\alpha_1} \\ &= \langle\zeta\psi|m\rangle\langle n|\psi\rangle \end{aligned} \quad (1.250)$$

(note that $\zeta^{p^2} = \zeta^p$). We therefore deduce

$$\langle n|\psi\rangle\langle\psi|e^{-\beta\hat{H}}|n\rangle = \sum_m a_m \langle\zeta\psi|m\rangle\langle n|\psi\rangle = \langle\zeta\psi|e^{-\beta\hat{H}}|n\rangle\langle n|\psi\rangle \quad (1.251)$$

and the partition function can be written as

$$Z = \int d(\psi^*, \psi) e^{-\sum_{\alpha} \psi_{\alpha}^* \psi_{\alpha}} \langle\zeta\psi|e^{-\beta\hat{H}}|\psi\rangle. \quad (1.252)$$

Dividing the imaginary time β into $N = \beta/\epsilon$ steps and inserting $N - 1$ times the closure relation (1.203) or (1.240), we obtain

$$Z = \int \prod_{k=1}^N d(\psi_k^*, \psi_k) e^{-\sum_{k=1}^N \sum_{\alpha} \psi_{k,\alpha}^* \psi_{k,\alpha}} \prod_{k=1}^N \langle\psi_k|e^{-\epsilon\hat{H}}|\psi_{k-1}\rangle, \quad (1.253)$$

with the boundary conditions $\psi_{N,\alpha} = \zeta\psi_{0,\alpha}$ and $\psi_{N,\alpha}^* = \zeta\psi_{0,\alpha}^*$. If the Hamiltonian $\hat{H} = H(\hat{\psi}_{\alpha}^{\dagger}, \hat{\psi}_{\alpha})$ is normal ordered,

$$\langle\psi_k|e^{-\epsilon\hat{H}}|\psi_{k-1}\rangle = \langle\psi_k|\psi_{k-1}\rangle e^{-\epsilon H(\psi_k^*, \psi_{k-1})} + \mathcal{O}(\epsilon^2), \quad (1.254)$$

one finds

$$Z = \int \prod_{k=1}^N d(\psi_k^*, \psi_k) \exp \left\{ -\epsilon \sum_{k=1}^N \left[\sum_{\alpha} \psi_{k,\alpha}^* \frac{(\psi_{k,\alpha} - \psi_{k-1,\alpha})}{\epsilon} + H(\psi_{k,\alpha}^*, \psi_{k-1,\alpha}) \right] \right\} \quad (1.255)$$

for $\epsilon \rightarrow 0$. As for the Feynman path integral (Sec. 1.1), in the limit $N \rightarrow \infty$ it is convenient to represent the set $\{\psi_{0,\alpha}, \dots, \psi_{N,\alpha}\}$ by a continuous trajectory $\psi_\alpha(\tau)$ with τ an imaginary time varying between 0 and β and the boundary conditions

$$\psi_\alpha(\beta) = \zeta \psi_\alpha(0), \quad \psi_\alpha^*(\beta) = \zeta \psi_\alpha^*(0). \quad (1.256)$$

We can then (symbolically) write

$$\begin{aligned} \epsilon \sum_{k=1}^N &\rightarrow \int_0^\beta d\tau, \\ \psi_{k,\alpha}^* \frac{(\psi_{k,\alpha} - \psi_{k-1,\alpha})}{\epsilon} &\rightarrow \psi_\alpha^*(\tau) \partial_\tau \psi_\alpha(\tau), \\ H(\psi_{k,\alpha}^*, \psi_{k-1,\alpha}) &\rightarrow H(\psi_\alpha^*(\tau^+), \psi_\alpha(\tau)), \end{aligned} \quad (1.257)$$

so that the partition takes the final form

$$Z = \int_{\substack{\psi(\beta) = \zeta \psi(0) \\ \psi^*(\beta) = \zeta \psi^*(0)}} \mathcal{D}[\psi^*, \psi] \exp\{-S[\psi^*, \psi]\} \quad (1.258)$$

with the Euclidean action²³

$$S[\psi^*, \psi] = \int_0^\beta d\tau \left[\sum_\alpha \psi_\alpha^*(\tau) \partial_\tau \psi_\alpha(\tau) + H(\psi_\alpha^*(\tau^+), \psi_\alpha(\tau)) \right]. \quad (1.259)$$

The notation τ^+ reminds us that the creation field is always evaluated infinitesimally later than the annihilation field (see (1.257)). Note that for fermions the notation $\partial_\tau \psi_\alpha(\tau)$ is purely symbolic since there is no sense in which $\psi_{k,\alpha} - \psi_{k-1,\alpha}$ is small. The symbol $\partial_\tau \psi_\alpha(\tau)$ should be understood as $\lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} (\psi_{k,\alpha} - \psi_{k-1,\alpha})$. The measure in the functional integral (1.258) is defined as

$$\mathcal{D}[\psi^*, \psi] = \lim_{N \rightarrow \infty} \prod_{k=1}^N d(\psi_k^*, \psi_k). \quad (1.260)$$

For a system with a non-interacting one-body Hamiltonian \hat{h}_0 and a two-body interaction \hat{v} , the action reads

$$\begin{aligned} S[\psi^*, \psi] &= \int_0^\beta d\tau \left\{ \sum_{\alpha, \alpha'} \psi_\alpha^*(\tau) \left[\delta_{\alpha, \alpha'} \partial_\tau + \langle \alpha | \hat{h}_0 | \alpha' \rangle \right] \psi_{\alpha'}(\tau) \right. \\ &\quad \left. + \frac{1}{2} \sum_{\alpha_1, \alpha_2, \alpha'_1, \alpha'_2} (\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2) \psi_{\alpha_1}^*(\tau^+) \psi_{\alpha_2}^*(\tau^+) \psi_{\alpha'_2}(\tau) \psi_{\alpha'_1}(\tau) \right\}. \end{aligned} \quad (1.261)$$

Green functions

Let us now consider the Green function $G(\alpha\tau, \alpha'\tau') = -\langle T_\tau \hat{\psi}_\alpha(\tau) \hat{\psi}_{\alpha'}^\dagger(\tau') \rangle$ introduced in section 1.2.3. For $\tau > \tau'$ it reads

$$G(\alpha\tau, \alpha'\tau') = -\frac{1}{Z} \text{Tr} \left[e^{-(\beta-\tau)\hat{H}} \hat{\psi}_\alpha e^{-(\tau-\tau')\hat{H}} \hat{\psi}_{\alpha'}^\dagger e^{-\tau'\hat{H}} \right]. \quad (1.262)$$

²³For simplicity we denote the Euclidean action merely by S (and not S_E).

We now split the times $\beta - \tau$, $\tau - \tau'$ and τ' in infinitesimal steps $\epsilon = \beta/N$. If we assume that τ corresponds to the discrete time $\tau_{k_1} = k_1\epsilon$ and τ' to $\tau_{k_2} = k_2\epsilon$, we obtain

$$G(\alpha\tau, \alpha'\tau') = -\frac{1}{Z} \int \prod_{k=1}^N d(\psi_k^*, \psi_k) e^{-\sum_{k=1}^N \sum_{\alpha} \psi_{k,\alpha}^* \psi_{k,\alpha}} \langle \psi_N | e^{-\epsilon \hat{H}} | \psi_{N-1} \rangle \cdots \langle \psi_{k_1+1} | e^{-\epsilon \hat{H}} \hat{\psi}_{\alpha} | \psi_{k_1} \rangle \cdots \langle \psi_{k_2} | \hat{\psi}_{\alpha'}^{\dagger} e^{-\epsilon \hat{H}} | \psi_{k_2-1} \rangle \cdots \langle \psi_1 | e^{-\epsilon \hat{H}} | \psi_0 \rangle, \quad (1.263)$$

with the boundary conditions $\psi_N = \zeta \psi_0$ and $\psi_N^* = \zeta \psi_0^*$. We deduce

$$\begin{aligned} G(\alpha\tau, \alpha'\tau') &= -\frac{1}{Z} \int \prod_{k=1}^N d(\psi_k^*, \psi_k) \psi_{k_1,\alpha} \psi_{k_2,\alpha'}^* \exp\{-S(\psi_k^*, \psi_k)\} \\ &\equiv -\frac{1}{Z} \int \mathcal{D}[\psi^*, \psi] \psi_{\alpha}(\tau) \psi_{\alpha'}^*(\tau') \exp\{-S[\psi^*, \psi]\}, \end{aligned} \quad (1.264)$$

where $S(\psi_k^*, \psi_k)$ is the action defined in (1.255) and $S[\psi^*, \psi]$ its continuum time limit (1.259). For $\tau < \tau'$, we can follow a similar reasoning. Starting from

$$G(\alpha\tau, \alpha'\tau') = -\frac{\zeta}{Z} \text{Tr} \left[e^{-(\beta-\tau')\hat{H}} \hat{\psi}_{\alpha'}^{\dagger} e^{-(\tau'-\tau)\hat{H}} \hat{\psi}_{\alpha} e^{-\tau\hat{H}} \right], \quad (1.265)$$

one obtains

$$\begin{aligned} G(\alpha\tau, \alpha'\tau') &= -\frac{\zeta}{Z} \int \mathcal{D}[\psi^*, \psi] \psi_{\alpha'}^*(\tau') \psi_{\alpha}(\tau) \exp\{-S[\psi^*, \psi]\} \\ &= -\frac{1}{Z} \int \mathcal{D}[\psi^*, \psi] \psi_{\alpha}(\tau) \psi_{\alpha'}^*(\tau') \exp\{-S[\psi^*, \psi]\}. \end{aligned} \quad (1.266)$$

Thus the Green function can be written as a functional integral. This result generalizes to the n -particle Green function (1.189) and any statistical average of a time ordered product of operators,

$$\begin{aligned} &\langle T_{\tau} A_1(\hat{\psi}_{\alpha}^{\dagger}(\tau_1), \hat{\psi}_{\alpha}(\tau_1)) \cdots A_n(\hat{\psi}_{\alpha}^{\dagger}(\tau_n), \hat{\psi}_{\alpha}(\tau_n)) \rangle \\ &= \frac{1}{Z} \text{Tr} \left[e^{-\beta \hat{H}} T_{\tau} A_1(\hat{\psi}_{\alpha}^{\dagger}(\tau_1), \hat{\psi}_{\alpha}(\tau_1)) \cdots A_n(\hat{\psi}_{\alpha}^{\dagger}(\tau_n), \hat{\psi}_{\alpha}(\tau_n)) \right] \\ &= \frac{1}{Z} \int \mathcal{D}[\psi^*, \psi] A_1(\psi_{\alpha}^*(\tau_1), \psi_{\alpha}(\tau_1)) \cdots A_n(\psi_{\alpha}^*(\tau_n), \psi_{\alpha}(\tau_n)) e^{-S[\psi^*, \psi]}. \end{aligned} \quad (1.267)$$

1.4.2 Non-interacting particles

For non-interacting particles with grand canonical Hamiltonian $\hat{H}_0 = \sum_{\alpha} \xi_{\alpha} \hat{\psi}_{\alpha}^{\dagger} \hat{\psi}_{\alpha}$, the action reads

$$S_0 = \sum_{\alpha} \sum_{k=1}^N [\psi_{\alpha,k}^* (\psi_{\alpha,k}^* - \psi_{\alpha,k-1}) + \epsilon \xi_{\alpha} \psi_{\alpha,k}^* \psi_{\alpha,k-1}]. \quad (1.268)$$

In order to diagonalize the action, we expand the fields in Fourier series,

$$\psi_{\alpha,k} = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} a_{\alpha,n} e^{-i\omega_n \tau_k}, \quad \psi_{\alpha,k}^* = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} a_{\alpha,n}^* e^{i\omega_n \tau_k}, \quad (1.269)$$

where $\tau_k = k\epsilon$ and the Matsubara frequencies ω_n are defined in (1.185). The a_n 's are complex variables for bosons and Grassmann numbers for fermions. Since the transformation $\psi^{(*)} \rightarrow a^{(*)}$ has unit Jacobian,²⁴ one obtains

$$\begin{aligned} Z_0 &= \lim_{N \rightarrow \infty} \int \prod_{n=0}^{N-1} d(a_n^*, a_n) \exp \left\{ - \sum_{\alpha} \sum_{n=0}^{N-1} |a_{\alpha,n}|^2 [1 + (\epsilon \xi_{\alpha} - 1) e^{i\omega_n \epsilon}] \right\} \\ &= \lim_{N \rightarrow \infty} \prod_{\alpha} \prod_{n=0}^{N-1} [1 + (\epsilon \xi_{\alpha} - 1) e^{i\omega_n \epsilon}]^{-\zeta} \end{aligned} \quad (1.270)$$

using the results of Appendix 1.E. Writing $1 - \epsilon \xi_{\alpha} = e^{-\theta_{\alpha}}$ and using the identity

$$\prod_{n=0}^{N-1} (1 - e^{i\omega_n \epsilon - \theta}) = 1 - \zeta e^{-N\theta}, \quad (1.271)$$

we finally deduce

$$Z_0 = \lim_{N \rightarrow \infty} \prod_{\alpha} (1 - \zeta e^{-N\theta_{\alpha}})^{-\zeta} = \prod_{\alpha} (1 - \zeta e^{-\beta \xi_{\alpha}})^{-\zeta}, \quad (1.272)$$

which is the familiar result for non-interacting particles.

The Fourier transform of the one-particle Green function is obtained from

$$\begin{aligned} -\langle a_{\alpha,n} a_{\alpha,n}^* \rangle &= - \lim_{N \rightarrow \infty} \frac{1}{Z} \int \prod_{n=0}^{N-1} d(a_n^*, a_n) a_{\alpha,n} a_{\alpha,n}^* e^{-S_0} \\ &= \lim_{N \rightarrow \infty} [(1 - \epsilon \xi_{\alpha}) e^{i\omega_n \epsilon} - 1]^{-1} \\ &= \frac{1}{\epsilon i\omega_n - \xi_{\alpha}}. \end{aligned} \quad (1.273)$$

Up to a factor $1/\epsilon$ we recover the Green function $G_0(\alpha, i\omega_n) = (i\omega_n - \xi_{\alpha})^{-1}$ of the non-interacting system [Eq. (1.187)]. Equation (1.273) yields the Green function²⁵

$$\begin{aligned} G_0(\alpha, \tau_{k_1} - \tau_{k_2}) &= - \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} \langle a_{\alpha,n} a_{\alpha,n}^* \rangle e^{-i\omega_n(\tau_{k_1} - \tau_{k_2})} \\ &= \begin{cases} - \lim_{N \rightarrow \infty} \frac{\zeta a^{N+k_1-k_2}}{1 - \zeta a^N} = -\zeta n_{\alpha} e^{\xi_{\alpha}(\tau_{k_1} - \tau_{k_2})} & \text{if } \tau_{k_1} < \tau_{k_2}, \\ - \lim_{N \rightarrow \infty} \frac{a^{k_1-k_2}}{1 - \zeta a^N} = -(1 + \zeta n_{\alpha}) e^{\xi_{\alpha}(\tau_{k_1} - \tau_{k_2})} & \text{if } \tau_{k_1} \geq \tau_{k_2}, \end{cases} \end{aligned} \quad (1.275)$$

where $a = 1 - \epsilon \xi_{\alpha}$ and

$$n_{\alpha} = \frac{1}{e^{\beta \xi_{\alpha}} - \zeta} \quad (1.276)$$

²⁴See Appendix 1.E.3 for change of variables in a Grassmannian integral.

²⁵To convince oneself that (1.275) is correct, one can verify it for small values of N . See also the direct calculation of $G_0(\alpha, \tau)$ below.

if the occupation number $n_B(\xi_\alpha)$ for bosons and $n_F(\xi_\alpha)$ for fermions. One may rewrite (1.275) as

$$G_0(\alpha, \tau) = -e^{\xi_\alpha \tau} [\Theta(\tau)(1 + \zeta n_\alpha) + \Theta(-\tau)\zeta n_\alpha], \quad (1.277)$$

where $\tau = \tau_{k_1} - \tau_{k_2} \in [-\beta, \beta]$, in agreement with (1.186).

It is also possible to calculate the partition function Z_0 directly from (1.268) without introducing the Fourier transformed variables $a_{\alpha, n}^{(*)}$. To this end, we write the action as

$$S_0 = \sum_{\alpha} \sum_{k, k'=1}^N \psi_{k, \alpha}^* S_{k, k'}^{(\alpha)} \psi_{k', \alpha}, \quad (1.278)$$

where $S^{(\alpha)}$ is the $N \times N$ matrix

$$S^{(\alpha)} = \begin{pmatrix} 1 & 0 & \cdots & \cdots & 0 & -\zeta a \\ -a & 1 & 0 & & & 0 \\ 0 & -a & 1 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & 1 & \ddots & \vdots \\ \vdots & & \ddots & -a & 1 & 0 \\ 0 & \cdots & \cdots & 0 & -a & 1 \end{pmatrix} \quad (1.279)$$

with $a = 1 - \frac{\beta}{N}\xi_\alpha$. Expanding with respect to the first line, we obtain

$$\lim_{N \rightarrow \infty} \det S^{(\alpha)} = \lim_{N \rightarrow \infty} [1 + (-\zeta a)(-1)^{N-1}(-a)^{N-1}] = 1 - \zeta e^{-\beta \xi_\alpha},$$

and finally

$$Z_0 = \lim_{N \rightarrow 0} \prod_{\alpha} [\det S^{(\alpha)}]^{-\zeta} = \prod_{\alpha} (1 - \zeta e^{-\beta \xi_\alpha})^{-\zeta}. \quad (1.280)$$

Similarly we can calculate the one-particle Green function

$$\begin{aligned} G_0(\alpha, \tau_{k_1} - \tau_{k_2}) &= - \lim_{N \rightarrow \infty} \frac{1}{Z_0} \int \prod_{k=1}^N d(\psi_k^*, \psi_k) \psi_{k_1, \alpha} \psi_{k_2, \alpha}^* \exp \left\{ - \sum_{k, k'=1}^N \sum_{\alpha} \psi_{k, \alpha}^* S_{k, k'}^{(\alpha)} \psi_{k', \alpha} \right\} \\ &= - \lim_{N \rightarrow \infty} (S^{(\alpha)-1})_{k_1, k_2}, \end{aligned} \quad (1.281)$$

where $\tau_k = k\beta/N$. The inverse matrix $S^{(\alpha)-1}$ being given by

$$S^{(\alpha)-1} = \frac{1}{1 - \zeta a^N} \begin{pmatrix} 1 & \zeta a^{N-1} & \zeta a^{N-2} & \cdots & \cdots & \zeta a \\ a & 1 & \zeta a^{N-1} & \ddots & & \vdots \\ a^2 & a & 1 & \zeta a^{N-1} & \ddots & \vdots \\ \vdots & \ddots & a & 1 & \zeta a^{N-1} & \zeta a^{N-2} \\ \vdots & & \ddots & a & 1 & \zeta a^{N-1} \\ a^{N-1} & \cdots & \cdots & a^2 & a & 1 \end{pmatrix}, \quad (1.282)$$

we obtain

$$G_0(\alpha, \tau_{k_1} - \tau_{k_2}) = - \lim_{N \rightarrow \infty} \begin{cases} \frac{\zeta a^{N+k_1-k_2}}{1 - \zeta a^N} & \text{if } \tau_{k_1} < \tau_{k_2}, \\ \frac{\zeta a^{k_1-k_2}}{1 - \zeta a^N} & \text{if } \tau_{k_1} \geq \tau_{k_2}, \end{cases} \quad (1.283)$$

i.e.

$$G_0(\alpha, \tau_{k_1} - \tau_{k_2}) = \begin{cases} -\zeta n_\alpha e^{\xi_\alpha(\tau_{k_1} - \tau_{k_2})} & \text{if } \tau_{k_1} < \tau_{k_2}, \\ -(1 + \zeta n_\alpha) e^{\xi_\alpha(\tau_{k_1} - \tau_{k_2})} & \text{if } \tau_{k_1} \geq \tau_{k_2}. \end{cases} \quad (1.284)$$

Continuum time limit

In the continuum time limit, the variables $a_n^{(*)}$ become Fourier transformed fields $\psi_\alpha^{(*)}(i\omega_n)$ defined by

$$\begin{aligned} \psi_\alpha(\tau) &= \frac{1}{\sqrt{\beta}} \sum_{\omega_n} e^{-i\omega_n \tau} \psi_\alpha(i\omega_n), & \psi_\alpha(i\omega_n) &= \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau e^{i\omega_n \tau} \psi_\alpha(\tau), \\ \psi_\alpha^*(\tau) &= \frac{1}{\sqrt{\beta}} \sum_{\omega_n} e^{i\omega_n \tau} \psi_\alpha^*(i\omega_n), & \psi_\alpha^*(i\omega_n) &= \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau e^{-i\omega_n \tau} \psi_\alpha^*(\tau), \end{aligned} \quad (1.285)$$

and the action reads

$$\begin{aligned} S_0[\psi^*, \psi] &= \int_0^\beta d\tau \sum_\alpha \psi_\alpha^*(\tau) (\partial_\tau + \xi_\alpha) \psi_\alpha(\tau), \\ &= \sum_{\alpha, \omega_n} \psi_\alpha^*(i\omega_n) (-i\omega_n + \xi_\alpha) \psi_\alpha(i\omega_n), \end{aligned} \quad (1.286)$$

while the functional integral measure is given by

$$\mathcal{D}[\psi^*, \psi] = \prod_{\alpha, \omega_n} d(\psi_\alpha^*(i\omega_n), \psi_\alpha(i\omega_n)). \quad (1.287)$$

If we try to compute directly the partition function from the continuum time limit, we obtain

$$\begin{aligned} Z_0 &= \prod_{\alpha, \omega_n} (-i\omega_n + \xi_\alpha)^{-\zeta}, \\ \Omega_0 &= -\frac{1}{\beta} \ln Z_0 = \frac{\zeta}{\beta} \sum_{\alpha, \omega_n} \ln(-i\omega_n + \xi_\alpha). \end{aligned} \quad (1.288)$$

The Matsubara sum in (1.288) is divergent; the continuum time limit of the partition function is therefore ill-defined. To understand the origin of this difficulty, consider the mean particle number derived from the preceding equation,

$$N = -\frac{\partial \Omega_0}{\partial \mu} = -\frac{\zeta}{\beta} \sum_{\alpha, \omega_n} \frac{1}{i\omega_n - \xi_\alpha}. \quad (1.289)$$

This expression should be compared with the result directly obtained from the action (1.268),

$$N = \frac{\epsilon}{\beta} \sum_{\alpha} \sum_{k=1}^N \langle \psi_{\alpha,k}^* \psi_{\alpha,k-1} \rangle = \sum_{\alpha} \langle \psi_{\alpha}^*(\tau_k) \psi_{\alpha}(\tau_{k-1}) \rangle, \quad (1.290)$$

where the last result holds for any τ_k and follows from time translation invariance. Thus, in the continuum time limit, the correct definition of the average particle number should be $N = \sum_{\alpha} \langle \psi_{\alpha}^*(\tau^+) \psi_{\alpha}(\tau) \rangle$ with $\tau^+ = \tau + \eta$ ($\eta \rightarrow 0^+$). This gives

$$N = -\zeta \sum_{\alpha} G_0(\alpha, -\eta) = -\frac{\zeta}{\beta} \sum_{\alpha, \omega_n} G_0(\alpha, i\omega_n) e^{i\omega_n \eta}, \quad (1.291)$$

where the Green function

$$\begin{aligned} G_0(\alpha, i\omega_n) &= -\langle \psi_{\alpha}(i\omega_n) \psi_{\alpha}^*(i\omega_n) \rangle \\ &= -\frac{1}{Z_0} \int \mathcal{D}[\psi^*, \psi] \psi_{\alpha}(i\omega_n) \psi_{\alpha}^*(i\omega_n) e^{-S_0[\psi^*, \psi]} \\ &= \frac{1}{i\omega_n - \xi_{\alpha}} \end{aligned} \quad (1.292)$$

is obtained using standard results of Gaussian integration (Appendix 1.E). Performing the Matsubara sum in (1.291),²⁶ we obtain $N = \sum_{\alpha} n_{\alpha}$ with n_{α} defined in (1.276). In order for this result to be consistent with $N = -\partial\Omega_0/\partial\mu$, we should reexpress the thermodynamic potential as

$$\Omega_0 = \frac{\zeta}{\beta} \sum_{\alpha, \omega_n} \ln(-i\omega_n + \xi_{\alpha}) e^{i\omega_n \eta}. \quad (1.293)$$

The Matsubara sum is now converging and leads to the usual expression of the thermodynamical potential of non-interacting bosons or fermions. The calculation is detailed in Appendix 1.F

The difficulties encountered in the continuum time limit of the coherent-state functional integral are very similar to those that appear in the path integral formulation of a quantum particle in a magnetic field (Sec. 1.1.1). In the formal continuum limit, the ordering of the operators in the Hamiltonian is lost, which results in ambiguities or ill-defined quantities. In practice, however, these difficulties seldom occur and can be fixed by introducing the convergence factor $e^{i\omega_n \eta}$.²⁷

1.5 Perturbation theory and Feynman diagrams

Interacting systems are described by non-Gaussian actions so that the functional integral cannot in general be calculated exactly. When the interactions between particles are “weak” (in a sense that is to be explained), they can be perturbatively taken into account wrt the kinetic energy. Perturbation theory in many-body systems is based on Wick’s theorem (Sec. 1.5.1) and is formulated in terms of Feynman diagrams (Secs. 1.5.2-1.5.4).

²⁶See Appendix 1.F.

²⁷There are essentially two instances where the convergence factor $e^{i\omega_n \eta}$ is necessary: when calculating the thermodynamic potential and when computing boson/fermion loops in perturbation theory (Sec. 1.5)

1.5.1 Wick's theorem

We consider the partition function of a non-interacting system,

$$Z_0[J^*, J] = \int \mathcal{D}[\psi^*, \psi] \exp \left\{ -S_0[\psi^*, \psi] + \int_0^\beta d\tau \sum_\alpha [J_\alpha^*(\tau) \psi_\alpha(\tau) + \text{c.c.}] \right\}, \quad (1.294)$$

$$S_0[\psi^*, \psi] = - \int_0^\beta d\tau d\tau' \sum_{\alpha\alpha'} \psi_\alpha^*(\tau) G_0^{-1}(\alpha\tau, \alpha'\tau') \psi_{\alpha'}(\tau').$$

J and J^* are external “sources” that couple linearly to the fields ψ^* and ψ . They are c-numbers for bosons and Grassmann variables for fermions. $Z_0[J^*, J]$ can be calculated exactly using the results (1.860) for Gaussian integrals,

$$Z_0[J^*, J] = Z_0 \exp \left\{ - \int_0^\beta d\tau d\tau' \sum_{\alpha, \alpha'} J_\alpha^*(\tau) G_0(\alpha\tau, \alpha'\tau') J_{\alpha'}(\tau') \right\}, \quad (1.295)$$

where $Z_0 = Z_0[0, 0]$ is the non-interacting partition function for vanishing sources.

Let us now consider the average $\langle \psi_{\alpha_1}(\tau_1) \cdots \psi_{\alpha_n}(\tau_n) \psi_{\alpha'_n}^*(\tau'_n) \cdots \psi_{\alpha'_1}^*(\tau'_1) \rangle_0$ where

$$\langle \cdots \rangle_0 = \frac{1}{Z_0} \int \mathcal{D}[\psi^*, \psi] (\cdots) e^{-S_0[\psi^*, \psi]}. \quad (1.296)$$

This average can be expressed as the functional derivative

$$\frac{1}{Z_0} \frac{\zeta^n \delta^{(2n)} Z_0[J^*, J]}{\delta J_{\alpha_1}^*(\tau_1) \cdots \delta J_{\alpha_n}^*(\tau_n) \delta J_{\alpha'_n}(\tau'_n) \cdots \delta J_{\alpha'_1}(\tau'_1)} \Big|_{J^*=J=0}. \quad (1.297)$$

This leads to (see (1.866) in Appendix 1.E)

$$\begin{aligned} & \langle \psi_{\alpha_1}(\tau_1) \cdots \psi_{\alpha_n}(\tau_n) \psi_{\alpha'_n}^*(\tau'_n) \cdots \psi_{\alpha'_1}^*(\tau'_1) \rangle_0 \\ &= (-1)^n \sum_{p \in S_n} \zeta^p G_0(\alpha_n \tau_n, \alpha'_{p(n)} \tau'_{p(n)}) \cdots G_0(\alpha_1 \tau_1, \alpha'_{p(1)} \tau'_{p(1)}), \end{aligned} \quad (1.298)$$

where the sum is over all permutations p of $\{1, \dots, n\}$. The average $\langle \psi_\alpha(\tau) \psi_{\alpha'}^*(\tau') \rangle_0$ is often called a contraction and denoted by

$$-G_0(\alpha\tau, \alpha'\tau') = \langle \psi_\alpha(\tau) \psi_{\alpha'}^*(\tau') \rangle_0 = \overline{\psi_\alpha(\tau) \psi_{\alpha'}^*(\tau')}. \quad (1.299)$$

Wick's theorem states that the average of a product of fields with the Gaussian action S_0 is given by the sum of all complete contractions [Eq. (1.298)],

$$\langle \psi_{\alpha_1}(\tau_1) \cdots \psi_{\alpha_n}(\tau_n) \psi_{\alpha'_n}^*(\tau'_n) \cdots \psi_{\alpha'_1}^*(\tau'_1) \rangle_0 = \sum \text{all complete contractions}. \quad (1.300)$$

A complete contraction is a configuration in which each ψ is contracted with a ψ^* and the overall sign is specified by $(-1)^n \zeta^p$ where p is the permutation such that ψ_{α_i} is contracted with $\psi_{\alpha_{p(i)}}^*$. Note that (1.300) also holds when the numbers of ψ and ψ^*

differ. In this case any complete contraction involves either $\overline{\psi\psi}$ or $\overline{\psi^*\psi^*}$ and vanishes since

$$\begin{aligned}\overline{\psi_\alpha(\tau)\psi_{\alpha'}(\tau')} &= \langle \psi_\alpha(\tau)\psi_{\alpha'}(\tau') \rangle_0 = \frac{1}{Z_0} \frac{\delta^{(2)} Z_0[J^*, J]}{\delta J_\alpha^*(\tau) J_{\alpha'}^*(\tau')} \Big|_{J^*=J=0} = 0, \\ \overline{\psi_\alpha^*(\tau)\psi_{\alpha'}^*(\tau')} &= \langle \psi_\alpha^*(\tau)\psi_{\alpha'}^*(\tau') \rangle_0 = \frac{1}{Z_0} \frac{\delta^{(2)} Z_0[J^*, J]}{\delta J_\alpha(\tau) J_{\alpha'}(\tau')} \Big|_{J^*=J=0} = 0.\end{aligned}\quad (1.301)$$

An immediate consequence of Wick's theorem is that once we know the one-particle Green function G_0 , we also know the higher-order Green functions in a non-interacting system. For instance, the two-particle Green function reads²⁸

$$\begin{aligned}G_0^{(4)}(\alpha_1\tau_1, \alpha_2\tau_2; \alpha'_2\tau'_2, \alpha'_1\tau'_1) &= \langle \psi_{\alpha_1}(\tau_1)\psi_{\alpha_2}(\tau_2)\psi_{\alpha'_2}^*(\tau'_2)\psi_{\alpha'_1}^*(\tau'_1) \rangle_0 \\ &= \overbrace{\psi_{\alpha_1}(\tau_1)\psi_{\alpha_2}(\tau_2)\psi_{\alpha'_2}^*(\tau'_2)\psi_{\alpha'_1}^*(\tau'_1)} + \overbrace{\psi_{\alpha_1}(\tau_1)\psi_{\alpha_2}(\tau_2)\psi_{\alpha'_2}^*(\tau'_2)\psi_{\alpha'_1}^*(\tau'_1)} \\ &= G_0(\alpha_1\tau_1, \alpha'_1\tau'_1)G_0(\alpha_2\tau_2, \alpha'_2\tau'_2) + \zeta G_0(\alpha_1\tau_1, \alpha'_2\tau'_2)G_0(\alpha_2\tau_2, \alpha'_1\tau'_1).\end{aligned}\quad (1.302)$$

The two particles created in the states α_1 and α_2 at times τ_1 and τ_2 propagate independently. The second term in the rhs of (1.302) comes from the indiscernability of the particles with the factor ζ reflecting the bosonic or fermionic statistics. It is convenient to represent the propagator G_0 by a directed line,

$$G_0(\alpha\tau, \alpha'\tau') = \begin{array}{c} \alpha\tau \quad \longrightarrow \quad \alpha'\tau' \\ \hline \end{array}$$

which starts at (α', τ') (creation of a particle in the one-body state α' at time τ') and ends at (α, τ) (annihilation of a particle in the one-body state α at time τ). The two-particle Green function can be represented by the diagram

$$G_0^{(4)}(\alpha_1\tau_1, \alpha_2\tau_2; \alpha'_2\tau'_2, \alpha'_1\tau'_1) = \begin{array}{c} \alpha_1\tau_1 \longrightarrow \alpha'_1\tau'_1 \\ \alpha_2\tau_2 \longrightarrow \alpha'_2\tau'_2 \end{array} + \zeta \begin{array}{c} \alpha_1\tau_1 \longrightarrow \alpha'_2\tau'_2 \\ \alpha_2\tau_2 \longrightarrow \alpha'_1\tau'_1 \end{array}$$

Such a diagram is called a Feynman diagram. As we shall see in the next sections, Feynman diagrams play an essential role in the perturbation theory of many-body systems.

1.5.2 Partition function and thermodynamic potential

We consider a many-body system with a two-body interaction,

$$\begin{aligned}Z &= \int \mathcal{D}[\psi^*, \psi] e^{-S_0[\psi^*, \psi] - S_{\text{int}}[\psi^*, \psi]}, \\ S_{\text{int}}[\psi^*, \psi] &= \frac{1}{2} \int_0^\beta d\tau \sum_{\alpha_1, \alpha_2, \alpha'_1, \alpha'_2} (\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2) \psi_{\alpha_1}^*(\tau)\psi_{\alpha_2}^*(\tau)\psi_{\alpha'_2}(\tau)\psi_{\alpha'_1}(\tau).\end{aligned}\quad (1.303)$$

²⁸Recall that the superscript (4) denotes the number of fields appearing in the definition of $G^{(4)}$. It also corresponds to the number of external “legs” in the Feynman diagrams representing $G^{(4)}$.

The perturbation expansion of the partition function Z is obtained by expanding $e^{-S_{\text{int}}}$ in powers of the two-body interaction v ,

$$\frac{Z}{Z_0} = \langle e^{-S_{\text{int}}} \rangle_0 = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \langle S_{\text{int}}^n \rangle_0 \quad (1.304)$$

where

$$\begin{aligned} \frac{(-1)^n}{n!} \langle S_{\text{int}}^n \rangle_0 &= \frac{(-1)^n}{2^n n!} \sum_{\alpha_1, \beta_2, \gamma_2, \delta_2} \cdots \sum_{\alpha_n, \beta_n, \gamma_n, \delta_n} (\alpha_1 \beta_1 | \hat{v} | \gamma_1 \delta_1) \cdots (\alpha_n \beta_n | \hat{v} | \gamma_n \delta_n) \\ &\times \int_0^\beta d\tau_1 \cdots d\tau_n \langle \psi_{\alpha_1}^*(\tau_1) \psi_{\beta_1}^*(\tau_1) \psi_{\delta_1}(\tau_1) \psi_{\gamma_1}(\tau_1) \cdots \\ &\cdots \psi_{\alpha_n}^*(\tau_n) \psi_{\beta_n}^*(\tau_n) \psi_{\delta_n}(\tau_n) \psi_{\gamma_n}(\tau_n) \rangle_0. \end{aligned} \quad (1.305)$$

The averages $\langle \cdots \rangle_0$ in (1.305) can be evaluated using Wick's theorem. For the $\mathcal{O}(v)$ term, one obtains

$$\begin{aligned} &-\frac{1}{2} \sum_{\alpha_1 \cdots \alpha'_2} (\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2) \int_0^\beta d\tau \langle \psi_{\alpha_1}^*(\tau^+) \psi_{\alpha_2}^*(\tau^+) \psi_{\alpha'_2}(\tau) \psi_{\alpha'_1}(\tau) \rangle_0 \\ &= -\frac{1}{2} \sum_{\alpha_1 \cdots \alpha'_2} (\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2) \int_0^\beta d\tau [G_0(\alpha'_1 \tau, \alpha_1 \tau^+) G_0(\alpha'_2 \tau, \alpha_2 \tau^+) \\ &\quad + \zeta G_0(\alpha'_1 \tau, \alpha_2 \tau^+) G_0(\alpha'_2 \tau, \alpha_1 \tau^+)], \end{aligned} \quad (1.306)$$

where the equal-time propagator $G_0(\alpha\tau, \alpha'\tau)$ is interpreted as $G_0(\alpha\tau, \alpha'\tau^+)$ in agreement with the proper time ordering in the interaction term (see the discussion after (1.259)). Both contractions can be represented by the two Feynman diagrams

$$\begin{aligned} &-\frac{1}{2} \sum_{\alpha_1 \cdots \alpha'_2} (\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2) \int_0^\beta d\tau G_0(\alpha'_1 \tau, \alpha_1 \tau^+) G_0(\alpha'_2 \tau, \alpha_2 \tau^+) = \text{Diagram 1} \\ &-\frac{\zeta}{2} \sum_{\alpha_1 \cdots \alpha'_2} (\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2) \int_0^\beta d\tau G_0(\alpha'_1 \tau, \alpha_2 \tau^+) G_0(\alpha'_2 \tau, \alpha_1 \tau^+) = \text{Diagram 2} \end{aligned}$$

where each propagator is represented as a directed line (see preceding section) and each interaction as a vertex with two incoming and two outgoing lines corresponding to $\psi_{\alpha'_1} \psi_{\alpha'_2}$ and $\psi_{\alpha_1}^* \psi_{\alpha_2}^*$, respectively,

$$(\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2) = \text{Diagram 3}$$

Note that unless otherwise specified we do not write explicitly the sign and prefactor when drawing a Feynman diagram.

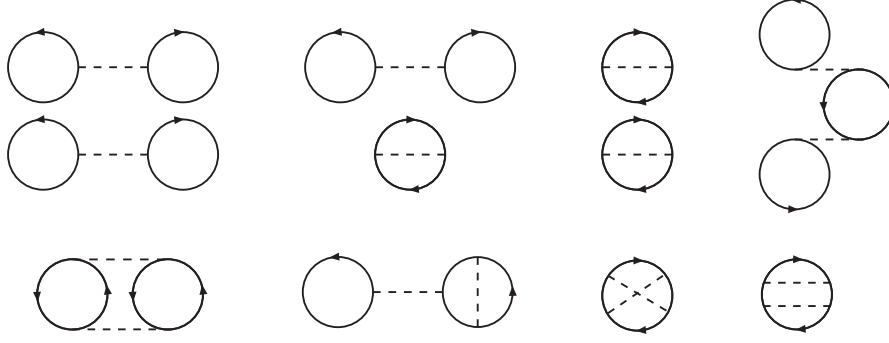


Figure 1.2: Diagrams contributing to Z/Z_0 to second order. The first three diagrams are made of two disconnected pieces.

All terms appearing in the perturbation expansion of the partition function can be represented by Feynman diagrams. These diagrams are often referred to as vacuum fluctuation graphs since in field theory they first arose in the “vacuum to vacuum transition” amplitude $\langle \text{vac} | e^{-i\hat{H}t} | \text{vac} \rangle$. The $\mathcal{O}(v^2)$ term

$$\frac{1}{2!2^2} \sum_{\alpha_1, \dots, \delta_2} (\alpha_1 \beta_1 | \hat{v} | \gamma_1 \delta_1) (\alpha_2 \beta_2 | \hat{v} | \gamma_2 \delta_2) \times \int_0^\beta d\tau_1 d\tau_2 \langle \psi_{\alpha_1}^*(\tau_1) \cdots \psi_{\gamma_1}(\tau_1) \psi_{\alpha_2}^*(\tau_2) \cdots \psi_{\gamma_2}(\tau_2) \rangle_0 \quad (1.307)$$

yields the diagrams shown in figure 1.2. What is interesting here is that the $4! = 24$ contractions arising from (1.307) are represented by only 8 diagrams. The number of diagrams even reduces to 5 for the thermodynamic potential (see below). Rather than starting from (1.305) and considering all possible contractions, it is therefore easier to draw all diagrams to a given order in v and compute each of these diagrams. Since we already know that to each line is associated a propagator G_0 and to each vertex a matrix element $(\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2)$, our remaining task is to determine the combinatorial factor and sign of a diagram.

Let us start with the first of the first-order diagram shown after (1.306). Schematically, this diagram is obtained from

$$-\frac{1}{2} \langle \text{---} \rangle_0 \rightarrow \text{---}$$

There is only one contraction that leads to the diagram so that the overall factor is $1/2$. Consider now the following second-order diagram



It is obtained from

$$\frac{1}{2!2^2} \langle \text{---} \text{---} \rangle_0$$

always even, a diagram with n interaction lines and n_L closed loops will have the overall sign $(-1)^n \zeta^{n_L}$ where the factor $(-1)^n$ simply comes from the expansion of $e^{-S_{\text{int}}}$ to n th order.

The diagrammatic rules for calculating the n th order contribution to Z/Z_0 are therefore the following:

1. Draw all distinct diagrams with n vertices connected by directed lines.
2. To each directed line, associate $G_0(\alpha\tau, \alpha'\tau'^+)$. (An equal-time propagator, with both ends connected to the same vertex, should be interpreted as $G_0(\alpha\tau, \alpha'\tau^+)$.)
3. To each vertex, associate $(\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2)$.
4. Sum over all indices α and integrate over all times τ .
5. Multiply the result by the combinatorial factor times $(-1)^n \zeta^{n_L}$ where n_L is the number of closed loops.

It is possible to write the diagrams directly in terms of the propagators $G_0(\alpha, \alpha'; i\omega_n)$. In frequency space, the interaction action (1.303) becomes

$$S_{\text{int}} = \frac{1}{2\beta} \sum_{\substack{\alpha_1, \alpha_2, \alpha'_1, \alpha'_2 \\ \omega_n, \omega'_n, \omega_\nu}} (\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2) \psi_{\alpha_1}^*(i\omega_n + i\omega_\nu) \psi_{\alpha_2}^*(i\omega'_n - i\omega_\nu) \psi_{\alpha'_2}(i\omega'_n) \psi_{\alpha'_1}(i\omega_n). \quad (1.313)$$

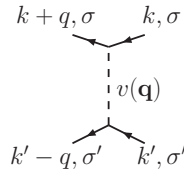
The sum of the frequencies associated with the propagators entering the vertex is conserved in the interaction process (frequency conservation). The preceding diagrammatic rules should therefore be modified as

- 2'. To each directed line, associate $G_0(\alpha, \alpha'; i\omega_n)$ while satisfying frequency conservation at each vertex. For a propagator with both ends connected to the same vertex (loop), multiply the propagator by $e^{i\omega_n\eta}$.
- 4'. Sum over all indices α and Matsubara frequencies ω_n .
- 6'. Multiply the result by $\frac{1}{\beta^n}$ where n is the number of vertices.

In translation invariant systems, it is also convenient to use the momentum basis $\{|\mathbf{k}, \sigma\rangle\}$ where σ denotes the spin of the particle (as well as other internal indices if any). For particles interacting via a two-body interaction $v(\mathbf{r} - \mathbf{r}')$, one has

$$S_{\text{int}} = \frac{1}{2\beta V} \sum_{\substack{k, k', q \\ \omega_n, \omega'_n, \omega_\nu}} v(\mathbf{q}) \psi_\sigma^*(k+q) \psi_{\sigma'}^*(k'-q) \psi_{\sigma'}(k') \psi_\sigma(k) \quad (1.314)$$

where $v(\mathbf{q})$ is the Fourier transform of $v(\mathbf{r})$ (see Sec. 1.2.2), and the interaction vertex assumes the diagrammatic representation



The modifications of the previous diagrammatic rules are straightforward:

- 2". To each directed line, associate $G_{0,\sigma}(\mathbf{k}, i\omega_n)$ while satisfying momentum, frequency and spin conservation at each vertex. For a propagator with both ends connected to the same vertex (loop), multiply the propagator by $e^{i\omega_n\eta}$.
- 3". To each vertex, associate $v(\mathbf{q})$ where \mathbf{q} is the transferred momentum in the interaction process.
- 4". Sum over all momenta and Matsubara frequencies.
- 6". Multiply the result by $\frac{1}{(\beta V)^n}$ where n is the number of vertices.

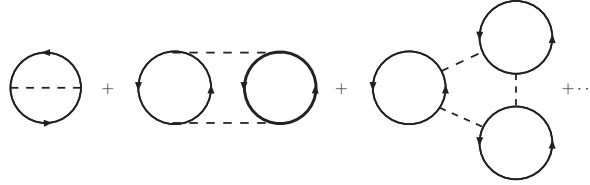
With these rules, the first-order correction to the partition function Z/Z_0 reads

$$\begin{aligned}
& -\frac{1}{2\beta V} v(\mathbf{q}=0) \sum_{k,k',\sigma,\sigma'} G_{0,\sigma}(k) G_{0,\sigma'}(k') e^{i(\omega_n+\omega'_n)\eta} \\
& -\frac{\zeta}{2\beta V} \sum_{k,k',\sigma} v(\mathbf{k}-\mathbf{k}') G_{0,\sigma}(k) G_{0,\sigma}(k') e^{i(\omega_n+\omega'_n)\eta}
\end{aligned} \tag{1.315}$$

and agrees with our previous result (1.306).

In practice, computing Feynman diagrams beyond the first or second order becomes rapidly cumbersome. However, as will become clear in the following chapters, the diagrammatic representation of the perturbation expansion often brings a physical interpretation which in turn suggests a resummation (to infinite order) of a subclass of diagrams.

One of the most familiar examples is the the random-phase approximation which amounts to summing the bubble (or ring) diagrams³⁰



Making use of the diagrammatic rules, we obtain

$$\begin{aligned}
\left(\frac{Z}{Z_0}\right)_{\text{bubble graphs}} &= -\frac{\zeta}{2} \text{Tr}(v G_0 G_0) + \frac{1}{4} \text{Tr}(v G_0 G_0)^2 - \frac{\zeta}{6} \text{Tr}(v G_0 G_0)^3 + \dots \\
&= -\frac{1}{2} \text{Tr} \ln(1 + \zeta v G_0 G_0),
\end{aligned} \tag{1.316}$$

where Tr stands for summation over internal indices. For a translation invariant system, this gives

$$\left(\frac{Z}{Z_0}\right)_{\text{bubble graphs}} = -\frac{1}{2} \sum_{\mathbf{q}, \omega_\nu} \ln [1 - \zeta v(\mathbf{q}) \Pi_0(\mathbf{q}, i\omega_\nu)] \tag{1.317}$$

where

$$\Pi_0(\mathbf{q}, i\omega_\nu) = -\frac{1}{\beta V} \sum_{\mathbf{k}, \omega_n, \sigma} G_{0,\sigma}(\mathbf{k}, i\omega_n) G_{0,\sigma}(\mathbf{k} + \mathbf{q}, i\omega_n + i\omega_\nu) \tag{1.318}$$

³⁰Depending on the context, the random-phase approximation sums up bubble (chapter 5) or ladder (chapter 6) diagrams.

Since $\Pi_0(\mathbf{q}, \tau) \propto \sum_{\mathbf{k}} G_{0,\sigma}(\mathbf{k}, \tau) G_{0,\sigma}(\mathbf{k} + \mathbf{q}, -\tau)$, it describes the propagation of a particle and a hole (see Sec. 1.2.3) and is therefore called a particle-hole propagator.

Linked cluster theorem and thermodynamic potential

To obtain the thermodynamics we need to compute $\ln(Z)$ rather than Z . The linked cluster theorem states that $\ln(Z/Z_0)$ is given by the sum of the connected graphs contributing to Z/Z_0 . A graph is said to be connected if it consists of only one piece. To derive this theorem, we use

$$\ln \frac{Z}{Z_0} = \lim_{R \rightarrow 0} \frac{d}{dR} \exp[R \ln(Z/Z_0)] = \lim_{R \rightarrow 0} \frac{d}{dR} \left(\frac{Z}{Z_0} \right)^R. \quad (1.319)$$

To compute $(Z/Z_0)^R$, we consider R replicas of the system and introduce a set of fields $\{\psi_{r,\alpha}^*, \psi_{r,\alpha}\}$ for the r th copy ($r \in [1, R]$),

$$\left(\frac{Z}{Z_0} \right)^R = \frac{1}{Z_0^R} \int \prod_{r=1}^R \mathcal{D}[\psi_r^*, \psi_r] \exp \left\{ - \sum_{r=1}^R S[\psi_r^*, \psi_r] \right\}. \quad (1.320)$$

The rules for calculating $(Z/Z_0)^R$ are the same as before except than each propagator $G_{0,r}(\alpha\tau, \alpha'\tau')$ now carries a replica index r . Since all fields attached to a given vertex share the same replica index, all propagators joining at this vertex must also share the same replica index. It follows that each connected part of a diagram carries a single index r , which yields a factor R when summed from 1 to R . A graph with n_c connected parts is therefore proportional to R^{n_c} and the graphs proportional to R are fully connected. From (1.319), we then deduce

$$\ln \frac{Z}{Z_0} = \sum \text{connected graphs} \quad (1.321)$$

and

$$\Omega = \Omega_0 - \frac{1}{\beta} \sum \text{connected graphs}, \quad (1.322)$$

where $\Omega_0 = -\frac{1}{\beta} \ln Z_0$ is the thermodynamic potential of the non-interacting system.

1.5.3 Green functions

Green functions can be calculated perturbatively in a similar manner and the various terms in the expansion can be represented by Feynman diagrams. Let us start with the one-particle Green function

$$G(\alpha_1\tau_1, \alpha_2\tau_2) = -\langle \psi_{\alpha_1}(\tau_1) \psi_{\alpha_2}^*(\tau_2) \rangle = -\frac{Z_0}{Z} \langle \psi_{\alpha_1}(\tau_1) \psi_{\alpha_2}^*(\tau_2) e^{-S_{\text{int}}} \rangle_0. \quad (1.323)$$

To compute G to a given order in the interaction, one should expand both Z and the average $\langle \cdots \rangle_0$ in (1.323). To first order, we use the expression (1.306) for Z/Z_0 and

$$-\langle \psi_{\alpha_1}(\tau_1) \psi_{\alpha_2}^*(\tau_2) e^{-S_{\text{int}}} \rangle_0 = G_0(\alpha_1\tau_1, \alpha_2\tau_2) + \langle \psi_{\alpha_1}(\tau_1) \psi_{\alpha_2}^*(\tau_2) S_{\text{int}} \rangle_0 \quad (1.324)$$

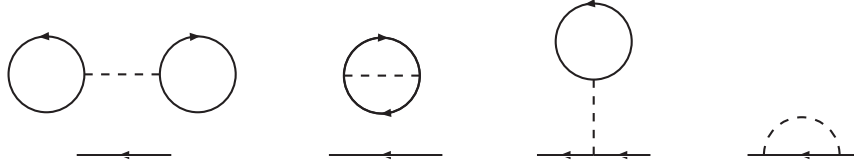
with

$$\begin{aligned} \langle \psi_{\alpha_1}(\tau_1) \psi_{\alpha_2}^*(\tau_2) S_{\text{int}} \rangle_0 &= \frac{1}{2} \sum_{\gamma_1, \dots, \gamma'_2} (\gamma_1 \gamma_2 | \hat{v} | \gamma'_1 \gamma'_2) \\ &\times \int_0^\beta d\tau \langle \psi_{\alpha_1}(\tau_1) \psi_{\alpha_2}^*(\tau_2) \psi_{\gamma_1}^*(\tau) \psi_{\gamma_2}^*(\tau) \psi_{\gamma'_2}(\tau) \psi_{\gamma'_1}(\tau) \rangle_0. \end{aligned} \quad (1.325)$$

Using Wick's theorem, we obtain for the last term

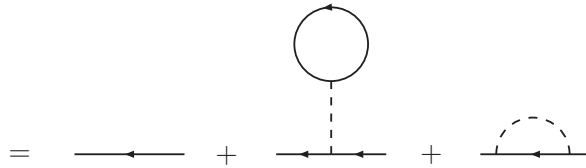
$$\begin{aligned} - \sum_{\gamma_1, \dots, \gamma'_2} (\gamma_1 \gamma_2 | \hat{v} | \gamma'_1 \gamma'_2) \int_0^\beta d\tau \left\{ \frac{1}{2} G_0(\alpha_1 \tau_1, \alpha_2 \tau_2) [G_0(\gamma'_1 \tau, \gamma_1 \tau) G_0(\gamma'_2 \tau, \gamma_2 \tau) \right. \\ \left. + \zeta G_0(\gamma'_1 \tau, \gamma_2 \tau) G_0(\gamma'_2 \tau, \gamma_1 \tau)] + G_0(\alpha_1 \tau_1, \gamma_1 \tau) [\zeta G_0(\gamma'_1 \tau, \alpha_2 \tau_2) G_0(\gamma'_2 \tau, \gamma_2 \tau) \right. \\ \left. + G_0(\gamma'_2 \tau, \alpha_2 \tau_2) G_0(\gamma'_1 \tau, \gamma_2 \tau)] \right\}, \end{aligned} \quad (1.326)$$

which can be represented by the following 4 diagrams



The diagrams for the one-particle Green function have two external lines (or legs) which carry the indices $(\alpha_1 \tau_1)$ (outgoing line) and $(\alpha_2 \tau_2)$ (incoming line). Only the indices carried by the internal lines are summed over. Combining (1.326) with the $\mathcal{O}(v)$ correction to Z/Z_0 , we obtain

$$\begin{aligned} G(\alpha_1 \tau_1, \alpha_2 \tau_2) &= G_0(\alpha_1 \tau_1, \alpha_2 \tau_2) - \sum_{\gamma_1, \dots, \gamma'_2} (\gamma_1 \gamma_2 | \hat{v} | \gamma'_1 \gamma'_2) \int_0^\beta d\tau G_0(\alpha_1 \tau_1, \gamma_1 \tau) \\ &\times [\zeta G_0(\gamma'_1 \tau, \alpha_2 \tau_2) G_0(\gamma'_2 \tau, \gamma_2 \tau) + G_0(\gamma'_2 \tau, \alpha_2 \tau_2) G_0(\gamma'_1 \tau, \gamma_2 \tau)] \end{aligned} \quad (1.327)$$



The $\mathcal{O}(v)$ correction to G_0 is given by the connected diagrams that contribute to $-\langle \psi_{\alpha_1}(\tau_1) \psi_{\alpha_2}^*(\tau_2) e^{-S_{\text{int}}} \rangle_0$; the vacuum fluctuation graphs factorize out in the numerator and denominator of (1.323).

This is a general result: the Green function is given by the sum of all connected graphs. Let us prove this result for the n -particle Green function

$$G^{(2n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n; \alpha'_n \tau'_n, \dots, \alpha'_1 \tau'_1) = (-1)^n \langle \psi_{\alpha_1}(\tau_1) \dots \psi_{\alpha'_1}^*(\tau'_1) \rangle. \quad (1.328)$$

We introduce R replicas of the system and consider the correlation function

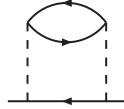
$$\begin{aligned}
 G_R^{(2n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n; \alpha'_n \tau'_n, \dots, \alpha'_1 \tau'_1) \\
 &= (-1)^n \int \prod_{r=1}^R \mathcal{D}[\psi_r^*, \psi_r] \psi_{1,\alpha_1}(\tau_1) \cdots \psi_{1,\alpha'_1}^*(\tau'_1) e^{-\sum_{r=1}^R S[\psi_r^*, \psi_r]} \\
 &= (-1)^n Z^{R-1} \int \mathcal{D}[\psi_1^*, \psi_1] \psi_{1,\alpha_1}(\tau_1) \cdots \psi_{1,\alpha'_1}^*(\tau'_1) e^{-S[\psi_1^*, \psi_1]}, \quad (1.329)
 \end{aligned}$$

where the last line is obtained by integrating out the fields ψ_r^*, ψ_r with $r \geq 2$. Thus $G^{(2n)}$ can be formally obtained from $G_R^{(2n)}$ in the limit $R = 0$. The perturbation expansion for $G_R^{(2n)}$ is obtained as before by expanding $e^{-S_{\text{int}}}$. The Feynman diagrams involve propagators carrying a replica index $r \in [1, R]$. All propagators attached to the same vertex share the same value of the replica index. Those corresponding to the external lines $\alpha_1 \cdots \alpha'_1$ have $r = 1$. Since the r index in the interaction vertex is summed over, a diagram with p disconnected parts, i.e. p parts that are not connected to the external legs, is proportional to R^p and vanishes in the limit $R = 0$ when $p \geq 1$. For the connected diagrams ($p = 0$), the integration of the fields $\psi_r^{(*)}$ with $r \in [2, R]$ in (1.329) gives a factor Z_0^{R-1} so that we finally obtain

$$\begin{aligned}
 G^{(2n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n; \alpha'_n \tau'_n, \dots, \alpha'_1 \tau'_1) \\
 = \frac{(-1)^n}{Z_0} \int \mathcal{D}[\psi^*, \psi] \psi_{\alpha_1}(\tau_1) \cdots \psi_{\alpha'_1}^*(\tau'_1) e^{-S[\psi^*, \psi]} \Big|_{\text{connected diagrams}} \quad (1.330)
 \end{aligned}$$

where only the connected diagrams, i.e. with all parts connected to the external lines, should be retained.

The combinatorial factor of a diagram can be computed, as for the partition function, by a direct evaluation of the number of contractions leading to that diagram. Let us consider for instance the following second-order diagram contributing to the one-particle Green function,



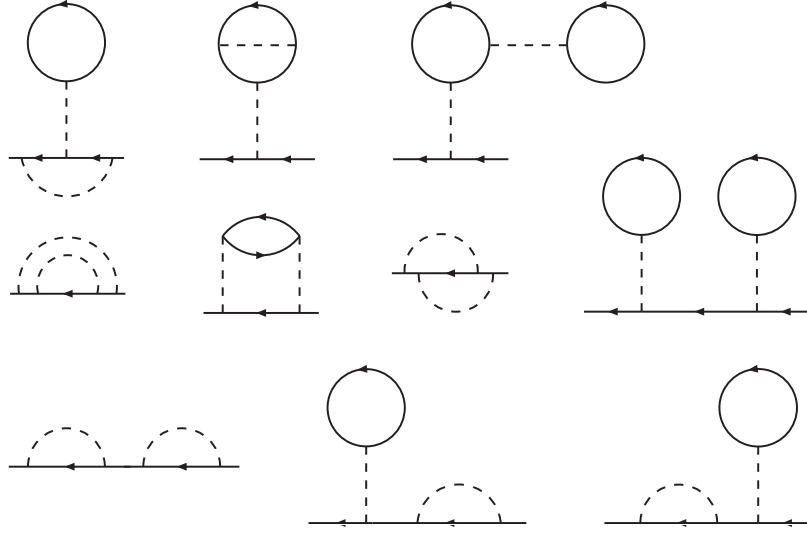
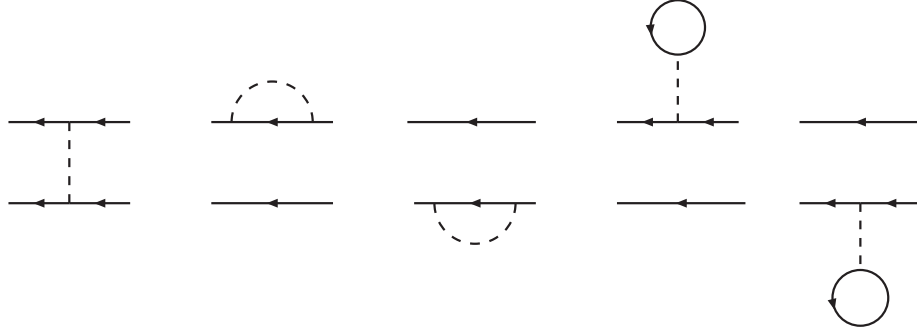
which is obtained from

$$\frac{1}{2!2^2} \langle \text{---} \text{---} \text{---} \rangle_0$$

The combinatorial factor reads

$$\frac{1}{2!2^2} \times \underbrace{2!}_{\text{interchange of vertices}} \times \underbrace{2}_{\text{connection of outgoing line to vertex}} \times \underbrace{2}_{\text{connection of incoming line to vertex}} = 1. \quad (1.331)$$

It turns out that the combinatorial factor is always unity for the n -particle Green function. One can easily convince oneself by working out a few examples. A proof can be found in Ref. [9].

Figure 1.3: Second-order diagrams for the one-particle Green function $G^{(2)} = G$.Figure 1.4: First-order diagrams for the two-particle Green function $G^{(4)}$.

The sign of a diagram can be obtained from (1.330) and a particular contraction leading to that diagram. As for the partition function, it is also given by the number n_L of closed loops. For the one-particle Green function, the sign of a diagram with l vertices is simply given by $(-1)^l \zeta^{n_L}$. (The proof is similar to that given for the partition function.) In the case of fermions, a diagram for the n -particle Green function takes the additional factor ζ^p where ζ^p is the signature of the permutation such that the incoming line $(\alpha'_i \tau'_i)$ joins the outgoing line $(\alpha_{p(i)} \tau_{p(i)})$.³¹

The diagrammatic rules for calculating the l th order contribution to the n -particle Green function $G^{(2n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n; \alpha'_n \tau'_n, \dots, \alpha'_1 \tau'_1)$ are the following:

1. Draw all distinct connected diagrams with n incoming lines $(\alpha'_n \tau'_n \dots \alpha'_1 \tau'_1)$, n outgoing lines $(\alpha_1 \tau_1 \dots \alpha_n \tau_n)$, and l interaction vertices.
2. To each directed line, associate $G_0(\alpha \tau, \alpha' \tau'^+)$.

³¹For a simple example, consider the non-interacting two-particle Green function [Eq. (1.302)].

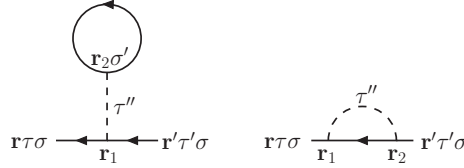
3. To each vertex, associate $(\alpha\alpha'|\hat{v}|\gamma\gamma')$.
4. Sum over all internal indices α and integrate over all internal times τ . (The indices $(\alpha'_i\tau'_i)$ and $(\alpha_i\tau_i)$ of incoming and outgoing lines should be held fixed.)
5. Multiply the result by the factor $(-1)^l\zeta^{n_L+p}$ where n_L is the number of closed loops and p the permutation such that each incoming line $(\alpha'_i\tau'_i)$ terminates at $(\alpha_{p(i)}\tau_{p(i)})$.

As an example, the second-order diagrams for the one-particle Green function are shown in figure 1.3 and the first-order diagrams for the two-particle Green functions in figure 1.4.

Let us illustrate the various ways to calculate a diagram with the example of a system with the following action,

$$\begin{aligned}
 S_0 &= - \int_0^\beta d\tau d\tau' \int d^d r d^d r' \sum_\sigma \psi_\sigma^*(\mathbf{r}, \tau) G_{0,\sigma}^{-1}(\mathbf{r}, \tau; \mathbf{r}', \tau') \psi_\sigma(\mathbf{r}', \tau'), \\
 S_{\text{int}} &= \frac{1}{2} \int_0^\beta d\tau \int d^d r d^d r' \sum_{\sigma, \sigma'} v(\mathbf{r} - \mathbf{r}') \psi_\sigma^*(\mathbf{r}, \tau) \psi_{\sigma'}^*(\mathbf{r}', \tau) \psi_{\sigma'}(\mathbf{r}', \tau) \psi_\sigma(\mathbf{r}, \tau).
 \end{aligned}
 \tag{1.332}$$

The first-order correction to $G_{0,\sigma}(\mathbf{r}, \tau; \mathbf{r}', \tau')$ is obtained from the diagrams



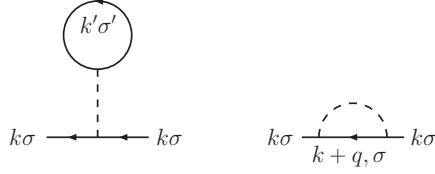
and is given by

$$\begin{aligned}
 & - \zeta \int_0^\beta d\tau'' \int d^d r_1 d^d r_2 \sum_{\sigma'} v(\mathbf{r}_1 - \mathbf{r}_2) G_{0,\sigma}(\mathbf{r}, \tau; \mathbf{r}_1, \tau'') G_{0,\sigma}(\mathbf{r}_1, \tau''; \mathbf{r}', \tau') \\
 & \quad \times G_{0,\sigma'}(\mathbf{r}_2, \tau''; \mathbf{r}_2, \tau''^+) \\
 & - \int_0^\beta d\tau'' \int d^d r_1 d^d r_2 v(\mathbf{r}_1 - \mathbf{r}_2) G_{0,\sigma}(\mathbf{r}, \tau; \mathbf{r}_1, \tau'') \\
 & \quad \times G_{0,\sigma}(\mathbf{r}_1, \tau''; \mathbf{r}_2, \tau''^+) G_{0,\sigma}(\mathbf{r}_2, \tau''; \mathbf{r}', \tau').
 \end{aligned}
 \tag{1.333}$$

When the system is translation invariant, it is convenient to start from

$$\begin{aligned}
 S_0 &= - \sum_{k,\sigma} \psi_\sigma^*(k) G_{0,\sigma}^{-1}(k) \psi_\sigma(k), \\
 S_{\text{int}} &= \frac{1}{2\beta V} \sum_{\substack{k,k',q \\ \sigma,\sigma'}} v(\mathbf{q}) \psi_\sigma^*(k+q) \psi_{\sigma'}^*(k'-q) \psi_{\sigma'}(k') \psi_\sigma(k).
 \end{aligned}
 \tag{1.334}$$

The first-order correction to $G_{0,\sigma}(k)$ is represented by the two diagrams



and reads

$$\begin{aligned}
 & -\frac{\zeta}{\beta V} \sum_{k', \sigma'} v(0) G_{0, \sigma}(k)^2 G_{0, \sigma'}(k') e^{i\omega'_n \eta} \\
 & -\frac{1}{\beta V} \sum_q v(\mathbf{q}) G_{0, \sigma}(k)^2 G_{0, \sigma}(k+q) e^{i\omega_{n+\nu} \eta}, \quad (1.335)
 \end{aligned}$$

where $q = (\mathbf{q}, i\omega_\nu)$. This result can also be obtained from the Fourier transform of (1.333).

1.5.4 Symmetrized vertices

Perturbation theory can be formulated in terms of the symmetrized vertex introduced in Sec. 1.2 [Eq. (1.165)]. One then starts from the action

$$S_{\text{int}}[\psi^*, \psi] = \frac{1}{4} \int_0^\beta d\tau \sum_{\alpha_1, \alpha_2, \alpha'_1, \alpha'_2} \{\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2\} \psi_{\alpha_1}^*(\tau) \psi_{\alpha_2}^*(\tau) \psi_{\alpha'_2}(\tau) \psi_{\alpha'_1}(\tau) \quad (1.336)$$

with a vertex which is (anti)symmetrized under the exchange of the two incoming or outgoing particles,

$$\{\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2\} = \zeta \{\alpha_1 \alpha_2 | \hat{v} | \alpha'_2 \alpha'_1\} = \zeta \{\alpha_2 \alpha_1 | \hat{v} | \alpha'_1 \alpha'_2\}. \quad (1.337)$$

Since this vertex no longer distinguishes between direct and exchange scatterings of the two incoming particles, it should be graphically represented by a dot,

$$\{\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2\} = \begin{array}{c} \alpha_1 \quad \alpha'_1 \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ \alpha_2 \quad \alpha'_2 \end{array} = \begin{array}{c} \leftarrow \quad \leftarrow \\ | \\ \leftarrow \quad \leftarrow \end{array} + \zeta \begin{array}{c} \leftarrow \quad \leftarrow \\ \diagdown \quad \diagup \\ \leftarrow \quad \leftarrow \end{array}$$

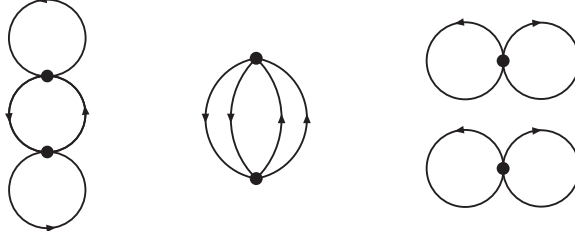
(we write explicitly that the second diagram comes with a sign ζ).

As previously, perturbation theory is obtained by expanding $e^{-S_{\text{int}}}$. Using Wick's theorem, we can again express the results by diagrams made of (anti)symmetrized vertices connected by propagators. Because we do not longer distinguish between the two incoming and outgoing lines of a vertex, the number of diagrams is considerably reduced. For instance, the $\mathcal{O}(v)$ correction to Z/Z_0 ,

$$-\frac{1}{2} \sum_{\alpha_1, \alpha_2, \alpha'_1, \alpha'_2} \{\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2\} \int_0^\beta d\tau G_0(\alpha'_1 \tau, \alpha_1 \tau^+) G_0(\alpha'_2 \tau, \alpha_2 \tau^+) \quad (1.338)$$

is represented by a single diagram:

$$\begin{array}{c} \text{Two circles sharing a central dot} \end{array} = \begin{array}{c} \text{Two circles connected by a dashed line} \end{array} + \begin{array}{c} \text{A circle with a dashed line through its center} \end{array}$$

Figure 1.5: Second-order diagrams contributing to the partition function Z/Z_0 .

To second order, there are only 3 different diagrams (Fig. 1.5) instead of the 8 to be considered when working with non-(anti)symmetrized vertices (Fig. 1.2).

The combinatorial factor is determined as before. (Note that the action S_{int} is now defined with a factor $\frac{1}{4}$.) For instance, the second of the three diagrams shown in figure 1.5 is obtained from

$$\frac{1}{2!4^2} \langle \text{diagram 1} \text{ diagram 2} \rangle_0 \rightarrow \text{diagram 2}$$

and has a combinatorial factor

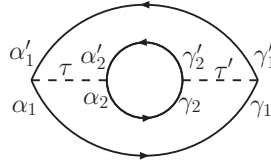
$$\frac{1}{2!4^2} \times 4 = \frac{1}{8}. \quad (1.339)$$

The factor 4 in the lhs comes from the 4 ways to connect the two vertices in a way consistent with the topology of the diagram.

As for the sign of the diagram, it can be determined as before from a particular contraction. One may also use the fact that the diagram should have the same sign as the one obtained *via* the replacement $\{\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2\} \rightarrow (\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2)$. For instance, if we write the preceding diagram as

$$\begin{aligned} \text{diagram} &= \text{sign} \times \frac{1}{8} \sum_{\alpha_1 \dots \gamma'_2} \{\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2\} \{\gamma_1\gamma_2|\hat{v}|\gamma'_2\gamma'_1\} \int_0^\beta d\tau d\tau' \\ &\quad \times G_0(\gamma_1\tau', \alpha_1\tau) G_0(\gamma_2\tau', \alpha_2\tau) G_0(\alpha'_2\tau, \gamma'_2\tau') G_0(\alpha'_1\tau, \gamma'_1\tau'), \end{aligned}$$

the replacement $\{\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2\} \rightarrow (\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2)$ gives



and the sign is therefore $(-1)^2\zeta^2$ since there are two vertices and two closed loops. Note that the sign of the diagram can be unambiguously defined only once we have its expression in terms of the vertices. For instance, we could write $\{\alpha_2\alpha_1|\hat{v}|\alpha'_1\alpha'_2\}$ instead $\{\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2\}$ in the preceding equation and the diagram would then have a negative sign.

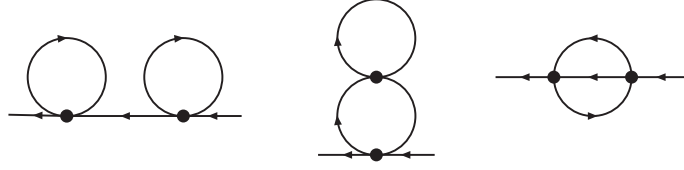


Figure 1.6: Second-order diagrams with symmetrized vertices contributing to the one-particle Green function.

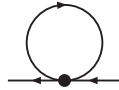
The diagrammatic rules for calculating a diagram are therefore the following:

1. To each directed line, associate $G_0(\alpha\tau, \alpha'\tau'^+)$.
2. To each vertex, associate $\{\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2\}$.
3. Sum over all one-particle indices α and integrate all times τ over the interval $[0, \beta]$.
4. Multiply the diagram by the combinatorial factor and by $(-1)^l \zeta^{n_L}$ where l is the number of vertices and n_L the number of closed loops in the diagram obtained by replacing $\{\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2\}$ by $(\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2)$ in each vertex.

When considering the perturbative expansion of the n -particle Green function $G^{(2n)}(\alpha_1\tau_1, \dots, \alpha'_1\tau'_1)$, the last 2 rules should be replaced by

- 3'. Sum over all indices α and integrate all times τ over the interval $[0, \beta]$, while holding fixed the indices $(\alpha_i\tau_i)$ and $(\alpha'_i\tau'_i)$ of the external lines.
- 4'. Multiply by the combinatorial factor and by $(-1)^l \zeta^{n_L} \zeta^p$ where l is the number of vertices, n_L the number of closed loops in the diagram obtained by replacing all vertices $\{\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2\}$ by $(\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2)$, and p the permutation of the incoming and outgoing lines.

For example, the first-order contribution to the one-particle Green function $G_0(\alpha\tau, \alpha'\tau')$ is given by the diagram



$$= -\zeta \int_0^\beta d\tau'' \sum_{\alpha_1 \dots \alpha_4} \{\alpha_1\alpha_2|\hat{v}|\alpha_4\alpha_3\} G_0(\alpha\tau, \alpha_1\tau'') G_0(\alpha_3\tau'', \alpha_2\tau'') G_0(\alpha_4\tau'', \alpha'\tau'). \quad (1.340)$$

The second-order diagrams are shown in figure 1.6.

Fully symmetrized vertices

We define a new field

$$\psi_{\tilde{\alpha}}(\tau) = \begin{cases} \psi_{\alpha}(\tau) & \text{if } c = -, \\ \psi_{\alpha}^*(\tau) & \text{if } c = +, \end{cases} \quad (1.341)$$

where $\tilde{\alpha} = (\alpha, c)$ with $c = \pm$ a “charge” index. $\psi_{\alpha+}$ creates a particle whereas $\psi_{\alpha-}$ creates a hole (i.e. removes a particle from the system). The action can be written as

$$S_0[\psi] = \frac{1}{2} \int_0^\beta d\tau d\tau' \sum_{\tilde{\alpha}, \tilde{\alpha}'} \psi_{\tilde{\alpha}}(\tau) G_0^{-1}(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') \psi_{\tilde{\alpha}'}(\tau'), \quad (1.342)$$

$$S_{\text{int}}[\psi] = \frac{1}{4!} \int_0^\beta d\tau \sum_{\tilde{\alpha}_1, \dots, \tilde{\alpha}_4} v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_3 \tilde{\alpha}_4} \psi_{\tilde{\alpha}_1}(\tau) \psi_{\tilde{\alpha}_2}(\tau) \psi_{\tilde{\alpha}_3}(\tau) \psi_{\tilde{\alpha}_4}(\tau),$$

where the (anti)symmetric propagator G_0 is defined by

$$G_0(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') = \zeta G_0(\tilde{\alpha}'\tau', \tilde{\alpha}\tau) = \begin{cases} -G_0(\alpha\tau, \alpha'\tau') & \text{if } c = -c' = -, \\ 0 & \text{if } c = c'. \end{cases} \quad (1.343)$$

Note that in (1.342, 1.343), we use opposite sign conventions for $G_0(\tilde{\alpha}\tau, \tilde{\alpha}'\tau')$ and $G_0(\alpha\tau, \alpha'\tau')$. This choice turns out to be more convenient when dealing with the field $\psi_{\tilde{\alpha}}$ (in particular for the formal manipulations in section 1.6). The vertex $v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_3 \tilde{\alpha}_4}$ is (anti)symmetric under the exchange of any two of its arguments,

$$v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_3 \tilde{\alpha}_4} = \zeta v_{\tilde{\alpha}_2 \tilde{\alpha}_1 \tilde{\alpha}_3 \tilde{\alpha}_4} = \zeta v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_4 \tilde{\alpha}_3} = \zeta v_{\tilde{\alpha}_3 \tilde{\alpha}_2 \tilde{\alpha}_1 \tilde{\alpha}_4}, \quad (1.344)$$

and satisfies

$$v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_3 \tilde{\alpha}_4} = \begin{cases} \{\tilde{\alpha}_1 \tilde{\alpha}_2 | \hat{v} | \tilde{\alpha}_4 \tilde{\alpha}_3\} & \text{if } c_1 = c_2 = -c_3 = -c_4 = +, \\ 0 & \text{if } c_1 + c_2 + c_3 + c_4 \neq 0. \end{cases} \quad (1.345)$$

Note the position of $\tilde{\alpha}_3$ and $\tilde{\alpha}_4$ which follows from the definition (1.342) of $v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_3 \tilde{\alpha}_4}$. The Wick theorem now reads

$$\langle \psi_{\tilde{\alpha}_1}(\tau_1) \cdots \psi_{\tilde{\alpha}_n}(\tau_n) \rangle = \sum \text{all complete contractions} \quad (1.346)$$

and is a consequence of the results for Gaussian integration over complex or Grassman variables discussed in section 1.E.4. The various terms appearing in the perturbation expansion of the partition function can be represented by Feynman diagrams. Since we do not distinguish between ψ_{α} and ψ_{α}^* (the difference is encoded in the charge index c of $\psi_{\tilde{\alpha}}$), the propagator should be represented by a non-directed line

$$G_0(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') = \begin{array}{c} \tilde{\alpha}\tau \quad \tilde{\alpha}'\tau' \\ \hline \end{array}$$

and the vertex by a simple dot,

$$v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_3 \tilde{\alpha}_4} = \begin{array}{c} \tilde{\alpha}_1 \quad \tilde{\alpha}_4 \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ \tilde{\alpha}_2 \quad \tilde{\alpha}_3 \end{array}$$

The first-order correction to the partition function reads

$$\text{Diagram: two circles connected by a dot} = -\frac{1}{8} \int_0^\beta d\tau \sum_{\tilde{\alpha}_1 \dots \tilde{\alpha}_4} v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_3 \tilde{\alpha}_4} G_0(\tilde{\alpha}_1\tau, \tilde{\alpha}_4\tau) G_0(\tilde{\alpha}_2\tau, \tilde{\alpha}_3\tau), \quad (1.347)$$

where the combinatorial factor comes from the $1/4!$ in front of the interaction and

the 3 ways to pair the lines of the vertex. The sign is obtained from a particular contraction, e.g.

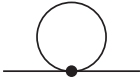
$$-\frac{1}{4!} \int_0^\beta d\tau \sum_{\tilde{\alpha}_1, \dots, \tilde{\alpha}_4} v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_3 \tilde{\alpha}_4} \overbrace{\psi_{\tilde{\alpha}_1}(\tau) \psi_{\tilde{\alpha}_2}(\tau) \psi_{\tilde{\alpha}_3}(\tau) \psi_{\tilde{\alpha}_4}(\tau)}^{(1.348)}. \quad (1.348)$$

Equation (1.347) gives

$$\begin{aligned} & -\frac{1}{8} \int_0^\beta d\tau \sum_{\substack{\alpha_1 \dots \alpha_4 \\ c, c' = \pm}} v_{\alpha_1 c, \alpha_2 c', \alpha_3 \bar{c}', \alpha_4 \bar{c}} G_0(\alpha_1, c, \tau; \alpha_4, \bar{c}, \tau) G_0(\alpha_2, c', \tau; \alpha_3, \bar{c}', \tau) \\ & = -\frac{1}{2} \int_0^\beta d\tau \sum_{\alpha_1 \dots \alpha_4} v_{\alpha_1 +, \alpha_2 +, \alpha_3 -, \alpha_4 -} G_0(\alpha_4, -, \tau; \alpha_1, +, \tau^+) G_0(\alpha_3, -, \tau; \alpha_2, +, \tau^+) \end{aligned} \quad (1.349)$$

(with $\bar{c} = -c$) and therefore reproduces (1.338). In equation (1.349) we have interpreted the equal time propagator $G_0(\alpha\tau, \alpha'\tau)$ as $G_0(\alpha\tau, \alpha'\tau^+)$ for reasons already discussed. Note that $G_0(\tilde{\alpha}\tau, \tilde{\alpha}'\tau)$ corresponds to $G_0(\tilde{\alpha}\tau, \tilde{\alpha}'\tau^+)$ if $c' = -c = +$ and to $G_0(\tilde{\alpha}\tau^+, \tilde{\alpha}'\tau)$ if $c = -c' = +$.

Similarly, for the first-order correction to the Green function $G(\tilde{\alpha}\tau, \tilde{\alpha}'\tau')$ one obtains



$$= -\frac{1}{2} \int_0^\beta d\tau'' \sum_{\tilde{\alpha}_1 \dots \tilde{\alpha}_4} v_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\alpha}_3 \tilde{\alpha}_4} G(\tilde{\alpha}\tau, \tilde{\alpha}_1\tau'') G(\tilde{\alpha}_2\tau'', \tilde{\alpha}_3\tau'') G(\tilde{\alpha}_4\tau'', \tilde{\alpha}'\tau'), \quad (1.350)$$

which can be shown to be equivalent to (1.340) when $\tilde{\alpha} = (\alpha, -)$ and $\tilde{\alpha}' = (\alpha', +)$.

One should be careful about the time ordering of the fields when using this formalism. To illustrate this point, let us consider non-interacting particles and express the action

$$S[\Psi^\dagger, \Psi] = \frac{1}{2} \sum_{\omega_n} \Psi^\dagger(i\omega_n) \mathcal{G}^{-1}(i\omega_n) \Psi(i\omega_n) \quad (1.351)$$

in terms of the two-component field

$$\Psi(\tau) = \begin{pmatrix} \psi(\tau) \\ \psi^*(\tau) \end{pmatrix}, \quad \Psi(i\omega_n) = \begin{pmatrix} \psi(i\omega_n) \\ \psi^*(-i\omega_n) \end{pmatrix}. \quad (1.352)$$

For simplicity, we consider a single one-body state with energy $\epsilon = \xi + \mu$. In frequency space, the propagator \mathcal{G} is a 2×2 matrix defined by

$$\mathcal{G}^{-1}(i\omega_n) = \begin{pmatrix} -i\omega_n + \xi & 0 \\ 0 & \zeta(i\omega_n + \xi) \end{pmatrix}. \quad (1.353)$$

The functional integral gives

$$Z_0 = \int \mathcal{D}[\psi^*, \psi] e^{-S[\Psi^\dagger, \Psi]} = \prod_{\omega_n} [\mathcal{G}_{11}(i\omega_n) \mathcal{G}_{22}(i\omega_n)]^{\zeta/2} \quad (1.354)$$

and

$$\Omega_0 = -\frac{\zeta}{2\beta} \sum_{\omega_n} \ln[\mathcal{G}_{11}(i\omega_n)\mathcal{G}_{22}(i\omega_n)]. \quad (1.355)$$

If now one introduces the convergence factor $e^{i\omega_n\eta}$, one obtains (see Appendix 1.F)³²

$$\frac{\zeta}{2\beta} \sum_{\omega_n} \ln(\omega_n^2 + \xi^2) e^{i\omega_n\eta} = \frac{\zeta}{\beta} \ln(1 - \zeta e^{-\beta\xi}) + \zeta \frac{\xi}{2}, \quad (1.356)$$

which differs from the exact result by $\zeta\xi/2$.

The reason for this apparent difficulty is that if we permute creation and annihilation fields, which is what we have done when writing

$$\begin{aligned} \psi^*(\tau)G_0(\tau - \tau')\psi(\tau') &= \zeta\psi(\tau')G_0(-\tau' + \tau)\psi^*(\tau) \\ &\equiv \Psi_2^\dagger(\tau')\mathcal{G}_{22}(\tau' - \tau)\Psi_2(\tau), \end{aligned} \quad (1.357)$$

one should then interpret the equal time propagator $\mathcal{G}_{22}(0)$ as $\mathcal{G}_{22}(0^+)$ rather than $\mathcal{G}_{22}(0^-)$. Accordingly, we should use the convergence factor $e^{-i\omega_n\eta}$ for the (22) component of the propagator. Thus the correct expression of the thermodynamic potential is

$$\begin{aligned} \Omega_0 &= -\frac{\zeta}{2\beta} \sum_{\omega_n} \left\{ \ln[\mathcal{G}_{11}(i\omega_n)]e^{i\omega_n\eta} + \ln[\mathcal{G}_{22}(i\omega_n)]e^{-i\omega_n\eta} \right\} \\ &= -\frac{\zeta}{\beta} \sum_{\omega_n} \ln[\mathcal{G}_{11}(i\omega_n)]e^{i\omega_n\eta}, \end{aligned} \quad (1.358)$$

in agreement with (1.293). The mean particle number $N = -\partial\Omega_0/\partial\mu$ is then given by

$$\begin{aligned} N &= \frac{\zeta}{2\beta} \sum_{\omega_n} \left[\mathcal{G}_{11}(i\omega_n)e^{i\omega_n\eta} + \zeta\mathcal{G}_{22}(i\omega_n)e^{-i\omega_n\eta} \right] \\ &= -\frac{\zeta}{\beta} \sum_{\omega_n} \frac{e^{i\omega_n\eta}}{i\omega_n - \xi}, \end{aligned} \quad (1.359)$$

which coincides with (1.291).

In formal manipulations of the functional integral as well as in some practical calculations, it is sometimes convenient to use the field $\psi_{\tilde{\alpha}}$ rather than ψ_{α} and ψ_{α}^* . This is particularly true when one has to deal with superfluid or superconducting systems where the (global) gauge symmetry is broken.³³ In these systems, the one-particle Green function $G(\tilde{\alpha}\tau, \tilde{\alpha}'\tau')$ has both “normal” ($G(\alpha, c, \tau; \alpha', -c, \tau')$) and “anomalous” ($G(\alpha, c, \tau; \alpha', c, \tau')$) components and can be represented as a 2×2 matrix

$$G(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') = \begin{pmatrix} G(\alpha, +, \tau; \alpha', +, \tau') & G(\alpha, +, \tau; \alpha', -, \tau') \\ G(\alpha, -, \tau; \alpha', +, \tau') & G(\alpha, -, \tau; \alpha', -, \tau') \end{pmatrix} \quad (1.360)$$

³²For fermions, the Matsubara frequencies appear in pairs $(\omega_n, \omega_{-n-1} = -\omega_n)$ so that $\det[\mathcal{G}^{-1}(i\omega_n)\mathcal{G}^{-1}(-i\omega_n)] = (\omega_n^2 + \xi^2)^2$ and $\det \mathcal{G}^{-1} = \prod_{\omega_n} (\omega_n^2 + \xi^2)$.

³³The (global) gauge invariance, i.e. the invariance of the action in the transformation $\psi_{\sigma}(\mathbf{r}, \tau) \rightarrow \psi_{\sigma}(\mathbf{r}, \tau)e^{i\Lambda}$ and $\psi_{\sigma}^*(\mathbf{r}, \tau) \rightarrow \psi_{\sigma}^*(\mathbf{r}, \tau)e^{-i\Lambda}$, is related to the conservation of the number of particles (Sec. 2.2.7). Broken gauge symmetry in superfluid and superconducting systems is discussed in chapter 6, while the concept of spontaneously broken symmetry is introduced in chapters 2 and 3.

$$= \left(\begin{array}{c} \overleftrightarrow{\hspace{1.5cm}} \\ \overleftarrow{\hspace{1.5cm}} \end{array} \quad \begin{array}{c} \overleftrightarrow{\hspace{1.5cm}} \\ \overleftarrow{\hspace{1.5cm}} \end{array} \right).$$

Moreover, in bosonic superfluid systems, the Green functions $G^{(2n+1)}$ with an odd number of legs do not vanish, and $G^{(1)}(\tilde{\alpha}, \tau) = \langle \psi_{\tilde{\alpha}}(\tau) \rangle$ is the order parameter of the superfluid phase (see chapter 6).³⁴ Superfluid or superconducting systems cannot be described within a perturbation expansion starting from the non-interacting limit. As for any system where a symmetry is spontaneously broken, it is necessary to reorganize the perturbation theory about a broken-symmetry state. The perturbation expansion in bosonic superfluid systems is explained in detail in section 1.7. Superconductors (i.e. superfluid fermion systems) are discussed in chapter 6.

1.6 Generating functionals

In this section, we define connected Green functions, one-particle (1PI) and two-particle (2PI) irreducible vertices. 1PI and 2PI vertices allow to reformulate and simplify the perturbation expansion discussed in section 1.5. Furthermore, we shall see in forthcoming chapters that the corresponding generating functionals enable to set up non-perturbative approaches to strongly correlated quantum systems (chapters ?? and 7).

1.6.1 Connected Green functions

In this section we define the connected Green functions and their generating functional. We first consider normal systems where global gauge invariance is not broken³³ before discussing the general case where we allow the system to be superfluid.

Normal systems

We consider the partition function in the presence of external sources,

$$Z[J^*, J] = \int \mathcal{D}[\psi^*, \psi] \exp \left\{ -S[\psi^*, \psi] + \int_0^\beta d\tau \sum_\alpha [J_\alpha^*(\tau) \psi_\alpha(\tau) + \text{c.c.}] \right\}, \quad (1.361)$$

where J^*, J are c-numbers for bosons and anticommuting variables for fermions. The Green functions

$$\begin{aligned} G^{(2n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n; \alpha'_n \tau'_n, \dots, \alpha'_1 \tau'_1) \\ = (-1)^n \langle \psi_{\alpha_1}(\tau_1) \dots \psi_{\alpha_n}(\tau_n) \psi_{\alpha'_n}^*(\tau'_n) \dots \psi_{\alpha'_1}^*(\tau'_1) \rangle \\ = (-\zeta)^n \frac{\delta^{(2n)} \mathcal{G}[J^*, J]}{\delta J_{\alpha_1}^*(\tau_1) \dots \delta J_{\alpha_n}^*(\tau_n) \delta J_{\alpha'_n}(\tau'_n) \dots \delta J_{\alpha'_1}(\tau'_1)} \Big|_{J^*=J=0} \end{aligned} \quad (1.362)$$

can be obtained from the generating functional

$$\mathcal{G}[J^*, J] = \frac{Z[J^*, J]}{Z[0, 0]}, \quad (1.363)$$

³⁴In fermion systems, $\langle \psi_{\tilde{\alpha}}(\tau) \rangle$ always vanishes in the absence of external Grassmannian sources ($J^* = J = 0$). In superfluid fermion systems, the broken gauge symmetry manifests itself by non-zero averages $\langle \psi_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}'}^*(\tau') \rangle$ and $\langle \psi_{\tilde{\alpha}}^*(\tau) \psi_{\tilde{\alpha}'}(\tau') \rangle$ (chapter 6).

where $Z[0,0] = Z$ is the partition function in the absence of external sources. In a normal system, the only non-vanishing Green functions are of the type (1.362) with n incoming particles and n outgoing particles. ^g

In Sec. 1.5, we showed that the Green function $G^{(2n)}$ can be obtained from the sum of all Feynman diagrams that are connected to the external legs. However, these diagrams need not be fully connected.³⁵ As the disconnected diagrams can be expressed in terms of lower-order Green functions ($G^{(2n-2)}$, $G^{(2n-4)}$, etc.), it is useful to deal with the “connected” Green functions $G_c^{(2n)}$ defined as the sum of all fully connected diagrams. The corresponding generating functional is $W[J^*, J] = \ln Z[J^*, J]$. This can be shown using the replica method as in the derivation of the linked cluster theorem (Sec. 1.5.2). The generating functional $(\mathcal{G}[J^*, J])^R$ of the Green functions of R replica of the systems can be written as a functional integral over R distinct fields. The connected diagrams are proportional to R (Sec. 1.5.2), while a diagram with n disconnected pieces is of order R^n . The connected diagrams can therefore be obtained from the functional

$$\lim_{R \rightarrow 0} \frac{\partial}{\partial R} (\mathcal{G}[J^*, J])^R = \ln \mathcal{G}[J^*, J] = \ln Z[J^*, J] - \ln Z[0, 0], \quad (1.364)$$

or more simply $W[J^*, J] = \ln Z[J^*, J]$ since $\ln Z[0, 0]$ is independent of the external sources.

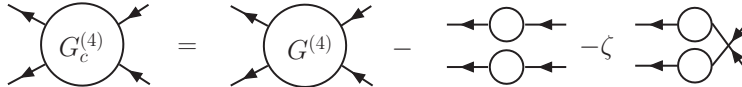
A direct calculation gives

$$G_c(\alpha_1 \tau_1, \alpha'_1 \tau'_1) = -\zeta \frac{\delta^{(2)} W[J^*, J]}{\delta J_{\alpha_1}^*(\tau_1) \delta J_{\alpha'_1}(\tau'_1)} \Big|_{J^*=J=0} = G(\alpha_1 \tau_1, \alpha'_1 \tau'_1) \quad (1.365)$$

and

$$\begin{aligned} G_c^{(4)}(\alpha_1 \tau_1, \alpha_2 \tau_2; \alpha'_2 \tau'_2, \alpha'_1 \tau'_1) &= \frac{\delta^{(4)} W[J^*, J]}{\delta J_{\alpha_1}^*(\tau_1) \delta J_{\alpha_2}^*(\tau_2) \delta J_{\alpha'_2}(\tau'_2) \delta J_{\alpha'_1}(\tau'_1)} \Big|_{J^*=J=0} \\ &= G^{(4)}(\alpha_1 \tau_1, \alpha_2 \tau_2; \alpha'_2 \tau'_2, \alpha'_1 \tau'_1) \\ &\quad - G(\alpha_1 \tau_1, \alpha'_1 \tau'_1) G(\alpha_2 \tau_2, \alpha'_2 \tau'_2) \\ &\quad - \zeta G(\alpha_1 \tau_1, \alpha'_2 \tau'_2) G(\alpha_2 \tau_2, \alpha'_1 \tau'_1) \end{aligned} \quad (1.366)$$

in a normal system where $\langle \psi_\alpha(\tau) \rangle = 0$. The last equation can be graphically represented as



(writing explicitly the sign of the diagrams), where the empty circles stand for the one-particle Green function $G \equiv G^{(2)}$. Clearly, $G_c^{(4)}$ is given by the sum of all fully connected diagrams.

The connected diagrams are analog to the cumulants of a probability function $P(x)$ with generating function

$$Z(j) = \int_{-\infty}^{\infty} dx P(x) e^{jx} = \sum_{n=0}^{\infty} \frac{j^n}{n!} \langle x^n \rangle. \quad (1.367)$$

³⁵For instance, in a non-interacting system, none of the diagrams contributing to $G^{(4)}$ are fully connected [Eq. (1.302) and corresponding figure].

The n th-order cumulant $\langle x^n \rangle_c$ is defined by

$$\begin{aligned}\langle x^n \rangle_c &= \frac{\partial^n}{\partial j^n} W(j) \Big|_{j=0}, \\ W(j) &= \ln Z(j) = \sum_{n=1}^{\infty} \frac{j^n}{n!} \langle x^n \rangle_c.\end{aligned}\tag{1.368}$$

One easily finds

$$\begin{aligned}\langle x \rangle_c &= \langle x \rangle, \\ \langle x^2 \rangle_c &= \langle x^2 \rangle - \langle x \rangle^2 = \langle (x - \langle x \rangle)^2 \rangle, \\ \langle x^3 \rangle_c &= \langle x^3 \rangle - 3\langle x^2 \rangle \langle x \rangle + 2\langle x \rangle^3 = \langle (x - \langle x \rangle)^3 \rangle, \\ \langle x^4 \rangle_c &= \langle (x - \langle x \rangle)^4 \rangle - 3\langle (x - \langle x \rangle)^2 \rangle^2.\end{aligned}\tag{1.369}$$

For a Gaussian distribution function $P(x) = (a/2\pi)^{1/2} e^{-(x-x_0)^2/2a}$,

$$W(j) = \ln \left\{ \sqrt{\frac{a}{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2a}(x-x_0)^2 + jx} \right\} = \frac{1}{2} aj^2 + jx_0,\tag{1.370}$$

so that $\langle x \rangle_c = x_0$, $\langle x^2 \rangle_c = a$, and $\langle x^n \rangle_c = 0$ for $n \geq 3$. By inverting (1.369), one can express all averages $\langle x^n \rangle$ in terms of the average value x_0 and the second-order cumulant $\langle x^2 \rangle_c$ (which is nothing but Wick's theorem). The analog result for a many-particle system is that when the action $S[\psi^*, \psi]$ is Gaussian (non-interacting particles), the only non-vanishing connected Green function is $G_c^{(2)}$ (when $G^{(1)} = 0$), and all higher-order Green functions $G^{(n \geq 4)}$ are entirely determined by $G_c^{(2)}$.

General case

As pointed out in section 1.5.4, in superfluid systems the Green functions take a more general form where the number of outgoing particles may differ from that of incoming particles. The total number of fields can even be odd in (bosonic) superfluid systems. It is then convenient to use the field $\psi_{\tilde{\alpha}}(\tau)$ (with $\tilde{\alpha} = (\alpha, c)$ and $c = \pm$ a charge index) introduced in Sec. 1.5.4 and define the Green functions as³⁶

$$G^{(n)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_n \tau_n) = \langle \psi_{\tilde{\alpha}_1}(\tau_1) \cdots \psi_{\tilde{\alpha}_n}(\tau_n) \rangle = \frac{\delta^{(n)} \mathcal{G}[J]}{\delta J_{\tilde{\alpha}_1}(\tau_1) \cdots \delta J_{\tilde{\alpha}_n}(\tau_n)} \Big|_{J=0}.\tag{1.371}$$

This definition will be used from now on whenever we will be working with the field $\psi_{\tilde{\alpha}}$. The generating functional is given by

$$\begin{aligned}\mathcal{G}[J] &= \frac{1}{Z[0]} \int \mathcal{D}[\psi] \exp \left\{ -S[\psi] + \int_0^\beta d\tau \sum_{\tilde{\alpha}} J_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}}(\tau) \right\} \\ &= 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^\beta d\tau_1 \cdots d\tau_n \sum_{\tilde{\alpha}_1 \cdots \tilde{\alpha}_n} G^{(n)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_n \tau_n) J_{\tilde{\alpha}_n}(\tau_n) \cdots J_{\tilde{\alpha}_1}(\tau_1).\end{aligned}\tag{1.372}$$

³⁶The sign convention in (1.371) agrees with that of (1.343).

Similarly, the connected Green functions and their generating functional $W[J] = \ln Z[J]$ are defined by

$$W[J] = \ln Z + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^\beta d\tau_1 \cdots d\tau_n \sum_{\tilde{\alpha}_1 \cdots \tilde{\alpha}_n} G_c^{(n)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_n \tau_n) J_{\tilde{\alpha}_n}(\tau_n) \cdots J_{\tilde{\alpha}_1}(\tau_1) \quad (1.373)$$

and

$$G_c^{(n)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_n \tau_n) = \left. \frac{\delta^{(n)} W[J]}{\delta J_{\tilde{\alpha}_1}(\tau_1) \cdots \delta J_{\tilde{\alpha}_n}(\tau_n)} \right|_{J=0}. \quad (1.374)$$

For the lowest-order Green functions one finds

$$\begin{aligned} G_c^{(1)}(\tilde{\alpha} \tau) &= G^{(1)}(\tilde{\alpha} \tau) = \langle \psi_{\tilde{\alpha}}(\tau) \rangle, \\ G_c^{(2)}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}_2 \tau_2) &= G^{(2)}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}_2 \tau_2) - \langle \psi_{\tilde{\alpha}_1}(\tau_1) \rangle \langle \psi_{\tilde{\alpha}_2}(\tau_2) \rangle \end{aligned} \quad (1.375)$$

and

$$\begin{aligned} G_c^{(3)}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}_2 \tau_2, \tilde{\alpha}_3 \tau_3) &= G^{(3)}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}_2 \tau_2, \tilde{\alpha}_3 \tau_3) - \langle \psi_{\tilde{\alpha}_1}(\tau_1) \rangle G_c^{(2)}(\tilde{\alpha}_2 \tau_2, \tilde{\alpha}_3 \tau_3) \\ &\quad - \langle \psi_{\tilde{\alpha}_2}(\tau_2) \rangle G_c^{(2)}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}_3 \tau_3) - \langle \psi_{\tilde{\alpha}_3}(\tau_3) \rangle G_c^{(2)}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}_2 \tau_2) \\ &\quad - \langle \psi_{\tilde{\alpha}_1}(\tau_1) \rangle \langle \psi_{\tilde{\alpha}_2}(\tau_2) \rangle \langle \psi_{\tilde{\alpha}_3}(\tau_3) \rangle. \end{aligned} \quad (1.376)$$

For a fermion system, all Green functions with an odd number of legs vanish.

Equations of motion

The Green functions $G^{(n)}$ are not independent but are related by “equations of motion” (Schwinger-Dyson equations).³⁷ Let us consider the generating functional $\mathcal{G}[J]$ [Eq. (1.372)]. The change of variables $\psi_{\tilde{\alpha}}(\tau) \rightarrow \psi_{\tilde{\alpha}}(\tau) + \epsilon f_{\tilde{\alpha}}(\tau)$, with $\epsilon \rightarrow 0$ and $f_{\tilde{\alpha}}(\tau)$ a complex of Grassmannian field, has a unit Jacobian and gives

$$\mathcal{G}[J] = \frac{1}{Z[0]} \int \mathcal{D}[\psi] e^{-S[\psi + \epsilon f] + \int_0^\beta d\tau \sum_{\tilde{\alpha}} J_{\tilde{\alpha}}(\tau) [\psi_{\tilde{\alpha}}(\tau) + \epsilon f_{\tilde{\alpha}}(\tau)]}. \quad (1.377)$$

Expanding to first order in ϵ , one finds

$$\frac{1}{Z[0]} \int \mathcal{D}[\psi] e^{-S[\psi] + \int_0^\beta d\tau \sum_{\tilde{\alpha}} J_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}}(\tau)} \int_0^\beta d\tau \sum_{\tilde{\alpha}} f_{\tilde{\alpha}}(\tau) \left[\zeta \frac{\delta S}{\delta \psi_{\tilde{\alpha}}(\tau)} - J_{\tilde{\alpha}}(\tau) \right] = 0 \quad (1.378)$$

(for Grassmann variables we use the chain rule (1.226) for derivation) and, since the function $f_{\tilde{\alpha}}(\tau)$ is arbitrary

$$\frac{1}{Z[0]} \int \mathcal{D}[\psi] e^{-S[\psi] + \int_0^\beta d\tau \sum_{\tilde{\alpha}} J_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}}(\tau)} \left[\zeta \frac{\delta S}{\delta \psi_{\tilde{\alpha}}(\tau)} - J_{\tilde{\alpha}}(\tau) \right] = 0. \quad (1.379)$$

³⁷In the operator formalism, the equations of motion are obtained by calculating $\partial_{\tau_1} G^{(n)}(\tilde{\alpha}_1 \tau_1 \cdots \tilde{\alpha}_n \tau_n) = \partial_{\tau_1} \langle T_\tau \hat{\psi}_{\tilde{\alpha}_1}(\tau_1) \cdots \hat{\psi}_{\tilde{\alpha}_n}(\tau_n) \rangle$ making use of $\partial_\tau \hat{\psi}_{\tilde{\alpha}}(\tau) = [\hat{H}, \hat{\psi}_{\tilde{\alpha}}(\tau)]$.

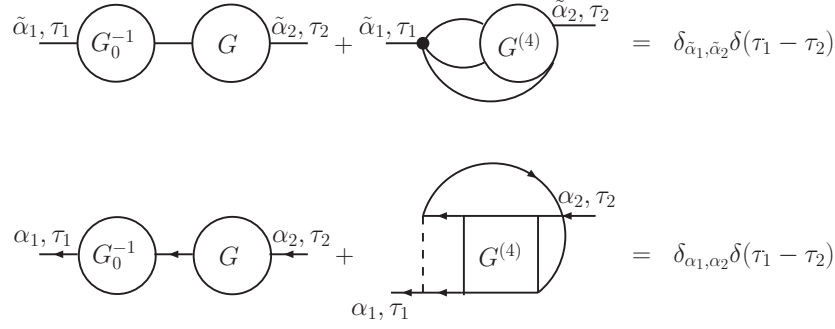


Figure 1.7: Diagrammatic representation of the equation of motion for $G = G^{(2)}$ in the general case [Eq. (1.382)] and for a normal system [Eq. (1.383)].

If we write the action as in (1.342), equation (1.379) gives

$$\begin{aligned} \frac{1}{Z[0]} \int \mathcal{D}[\psi] e^{-S[\psi] + \int_0^\beta d\tau \sum_{\tilde{\alpha}} J_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}}(\tau)} & \left[\int_0^\beta d\tau'_1 \sum_{\tilde{\alpha}'_1} G_0^{-1}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}'_1 \tau'_1) \psi_{\tilde{\alpha}'_1}(\tau'_1) \right. \\ & \left. + \frac{1}{3!} \sum_{\tilde{\alpha}'_2, \tilde{\alpha}'_3, \tilde{\alpha}'_4} v_{\tilde{\alpha}_1 \tilde{\alpha}'_2 \tilde{\alpha}'_3 \tilde{\alpha}'_4} \psi_{\tilde{\alpha}'_2}(\tau_1) \psi_{\tilde{\alpha}'_3}(\tau_1) \psi_{\tilde{\alpha}'_4}(\tau_1) - \zeta J_{\tilde{\alpha}_1}(\tau_1) \right] = 0. \quad (1.380) \end{aligned}$$

The equation of motion for the Green function $G^{(n)}$ is obtained by taking the $(n-1)$ th-order functional derivative wrt J and setting $J = 0$ in the end,

$$\begin{aligned} & \int_0^\beta d\tau'_1 \sum_{\tilde{\alpha}'_1} G_0^{-1}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}'_1 \tau'_1) G^{(n)}(\tilde{\alpha}_n \tau_n, \dots, \tilde{\alpha}_2 \tau_2, \tilde{\alpha}'_1 \tau'_1) \\ & + \frac{1}{3!} \sum_{\tilde{\alpha}'_2, \tilde{\alpha}'_3, \tilde{\alpha}'_4} v_{\tilde{\alpha}_1 \tilde{\alpha}'_2 \tilde{\alpha}'_3 \tilde{\alpha}'_4} G^{(n+2)}(\tilde{\alpha}_n \tau_n, \dots, \tilde{\alpha}_2 \tau_2, \tilde{\alpha}'_2 \tau_1, \tilde{\alpha}'_3 \tau_1, \tilde{\alpha}'_4 \tau_1) \\ & = \zeta \sum_{i=2}^n \delta_{\tilde{\alpha}_i, \tilde{\alpha}_1} \delta(\tau_i - \tau_1) G^{(n-2)}(\tilde{\alpha}_n \tau_n, \dots, \tilde{\alpha}_{i+1} \tau_{i+1}, \tilde{\alpha}_{i-1} \tau_{i-1}, \dots, \tilde{\alpha}_2 \tau_2). \quad (1.381) \end{aligned}$$

The equation of motion for $G^{(2)} = G$,

$$\begin{aligned} & \int_0^\beta d\tau'_1 \sum_{\tilde{\alpha}'_1} G_0^{-1}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}'_1 \tau'_1) G(\tilde{\alpha}'_1 \tau'_1, \tilde{\alpha}_2 \tau_2) \\ & + \frac{1}{3!} \sum_{\tilde{\alpha}'_2, \tilde{\alpha}'_3, \tilde{\alpha}'_4} v_{\tilde{\alpha}_1 \tilde{\alpha}'_2 \tilde{\alpha}'_3 \tilde{\alpha}'_4} G^{(4)}(\tilde{\alpha}'_2 \tau_1, \tilde{\alpha}'_3 \tau_1, \tilde{\alpha}'_4 \tau_1, \tilde{\alpha}_2 \tau_2) = \delta_{\tilde{\alpha}_1, \tilde{\alpha}_2} \delta(\tau_1 - \tau_2) \quad (1.382) \end{aligned}$$

is represented diagrammatically in figure 1.7. For a normal system, one finds (with

$\tilde{\alpha}_1 = (\alpha_1, +)$ and $\tilde{\alpha}_2 = (\alpha_2, +)$

$$\begin{aligned} & \int_0^\beta d\tau'_1 \sum_{\alpha'_1} G_0^{-1}(\alpha_1 \tau_1, \alpha'_1 \tau'_1) G(\alpha'_1 \tau'_1, \alpha_2 \tau_2) \\ & + \sum_{\alpha'_2, \alpha'_3, \alpha'_4} (\alpha_1 \alpha'_2 |\hat{v}| \alpha'_4 \alpha'_3) G^{(4)}(\alpha'_3 \tau_1, \alpha'_4 \tau_1, \alpha'_2 \tau_1, \alpha_2 \tau_2) = \delta_{\alpha_1, \alpha_2} \delta(\tau_1 - \tau_2) \end{aligned} \quad (1.383)$$

(see Fig. 1.7).

1.6.2 Effective action and 1PI vertices

In this section, we introduce the effective action and the 1PI vertices considering again first normal systems before discussing the general case. The effective action is further discussed in section 1.7 and plays a fundamental role in the non-perturbative renormalization group approach (chapter 7).

Normal systems

In presence of external sources, the fields $\psi_\alpha, \psi_\alpha^*$ acquire non-zero expectation values,

$$\begin{aligned} \phi_\alpha(\tau) &= \langle \psi_\alpha(\tau) \rangle_{J^*, J} = \frac{\delta W[J^*, J]}{\delta J_\alpha^*(\tau)}, \\ \phi_\alpha^*(\tau) &= \langle \psi_\alpha^*(\tau) \rangle_{J^*, J} = \zeta \frac{\delta W[J^*, J]}{\delta J_\alpha(\tau)}, \end{aligned} \quad (1.384)$$

where $\langle \dots \rangle_{J^*, J}$ denotes an average value in the presence of the external sources. ϕ_α and ϕ_α^* are c-numbers for bosonic fields and Grassmann variables for fermionic fields.

The effective action $\Gamma[\phi^*, \phi]$ is defined as the Legendre transform of $\ln Z[J^*, J]$,

$$\Gamma[\phi^*, \phi] = -\ln Z[J^*, J] + \int_0^\beta d\tau \sum_\alpha [J_\alpha^*(\tau) \phi_\alpha(\tau) + \text{c.c.}]. \quad (1.385)$$

In (1.385), $J_\alpha(\tau)$ and $J_\alpha^*(\tau)$ should be considered as functionals of $\phi_\alpha(\tau)$ and $\phi_\alpha^*(\tau)$ obtained by inverting (1.384). $\Gamma[\phi^*, \phi]$ satisfies³⁸

$$\begin{aligned} \frac{\delta \Gamma[\phi^*, \phi]}{\delta \phi_\alpha(\tau)} &= - \int_0^\beta d\tau' \sum_{\alpha'} \left(\frac{\delta J_{\alpha'}(\tau')}{\delta \phi_\alpha(\tau)} \frac{\delta W[J^*, J]}{\delta J_{\alpha'}(\tau')} + \frac{\delta J_{\alpha'}^*(\tau')}{\delta \phi_\alpha(\tau)} \frac{\delta W[J^*, J]}{\delta J_{\alpha'}^*(\tau')} \right) \\ &+ \int_0^\beta d\tau' \sum_{\alpha'} \left(\frac{\delta J_{\alpha'}^*(\tau')}{\delta \phi_\alpha(\tau)} \phi_{\alpha'}(\tau') + \zeta \frac{\delta J_{\alpha'}(\tau')}{\delta \phi_\alpha(\tau)} \phi_{\alpha'}^*(\tau') \right) + \zeta J_\alpha^*(\tau) \\ &= \zeta J_\alpha^*(\tau) \end{aligned} \quad (1.386)$$

and the companion equation

$$\frac{\delta \Gamma[\phi^*, \phi]}{\delta \phi_\alpha^*(\tau)} = J_\alpha(\tau). \quad (1.387)$$

³⁸In the case of Grassmann variables, we use the chain rule (1.226) for derivation.

The effective action is analog to the Gibbs free energy introduced in statistical mechanics. Let us consider for instance a classical spin system with partition function

$$Z(\mathbf{h}) = e^{-\beta F(\mathbf{h})} = \int \mathcal{D}[\mathbf{S}] \delta(\mathbf{S}(\mathbf{r})^2 - 1) e^{-\beta \int d^d r [\mathcal{H}(\mathbf{S}(\mathbf{r})) - \mathbf{h} \cdot \mathbf{S}(\mathbf{r})]}, \quad (1.388)$$

where $\mathcal{H}(\mathbf{S}(\mathbf{r}))$ is the Hamiltonian density and \mathbf{h} an external field. The magnetization of the system is given by

$$\mathbf{M} = \int d^d r \langle \mathbf{S}(\mathbf{r}) \rangle = \frac{1}{\beta} \frac{1}{\partial \mathbf{h}} \ln Z(\mathbf{h}) = -\frac{\partial F(\mathbf{h})}{\partial \mathbf{h}}. \quad (1.389)$$

The Gibbs free energy is defined as the Legendre transform of the Helmholtz free energy $F(\mathbf{h})$,

$$G(\mathbf{M}) = F(\mathbf{h}) + \mathbf{M} \cdot \mathbf{h}, \quad (1.390)$$

and satisfies

$$\frac{\partial G(\mathbf{M})}{\partial \mathbf{M}} = \mathbf{h}. \quad (1.391)$$

$F(\mathbf{h})$ and $G(\mathbf{M})$ contain the same physical information. In the absence of an external field, the magnetization of the system at thermodynamic equilibrium is obtained by requiring the Gibbs free energy to be stationary. Note that $G(\mathbf{M})$ (if calculated exactly) includes all effects of thermal fluctuations.

More generally, one can consider a spatially varying field $\mathbf{h}(\mathbf{r})$ giving rise to a non uniform magnetization $\mathbf{M}(\mathbf{r}) = \langle \mathbf{S}(\mathbf{r}) \rangle$. $F[\mathbf{h}]$ and $G[\mathbf{M}]$ are then functionals of $\mathbf{h}(\mathbf{r})$ and $\mathbf{M}(\mathbf{r})$, respectively. $F[\mathbf{h}]$ is the generating functional of the connected correlation functions of the spin density field $\mathbf{S}(\mathbf{r})$ whereas $G[\mathbf{M}]$ is the generating functional of the 1PI vertices (see below).

Self-energy and Dyson equation

The one-particle irreducible (1PI) vertices³⁹ are defined as the functional derivatives of the effective action,

$$\begin{aligned} \Gamma^{(2n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n; \alpha'_n \tau'_n, \dots, \alpha'_1 \tau'_1) \\ = \frac{\delta^{(2n)} \Gamma[\phi^*, \phi]}{\delta \phi_{\alpha'_1}(\tau'_1) \dots \delta \phi_{\alpha'_n}(\tau'_n) \delta \phi_{\alpha_n}^*(\tau_n) \dots \delta \phi_{\alpha_1}^*(\tau_1)} \Big|_{\phi^* = \phi = 0}. \end{aligned} \quad (1.392)$$

Inverting (1.392), one obtains

$$\begin{aligned} \Gamma[\phi^*, \phi] &= \Gamma[0, 0] \\ &+ \sum_{n=1}^{\infty} \frac{1}{(n!)^2} \int_0^\beta d\tau_1 \dots d\tau'_1 \sum_{\alpha_1 \dots \alpha'_1} \Gamma^{(2n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n; \alpha'_n \tau'_n, \dots, \alpha'_1 \tau'_1) \\ &\quad \times \phi_{\alpha_1}^*(\tau_1) \dots \phi_{\alpha_n}^*(\tau_n) \phi_{\alpha'_n}(\tau'_n) \dots \phi_{\alpha'_1}(\tau'_1), \end{aligned} \quad (1.393)$$

where $\Gamma[0, 0] = -W[0, 0] = \beta\Omega$.

³⁹The reason for this terminology is explained below.

Taking the functional derivatives of the first of equations (1.384) wrt $\phi_{\alpha'}(\tau')$, one obtains

$$\begin{aligned}\delta_{1,2} &= \frac{\delta\phi_1}{\delta\phi_2} \\ &= \sum_3 \left(\frac{\delta J_3}{\delta\phi_2} \frac{\delta^{(2)}W[J^*, J]}{\delta J_3 \delta J_1^*} + \frac{\delta J_3^*}{\delta\phi_2} \frac{\delta^{(2)}W[J^*, J]}{\delta J_3^* \delta J_1^*} \right) \\ &= \sum_3 \left(\frac{\delta^{(2)}\Gamma[\phi^*, \phi]}{\delta\phi_2 \delta\phi_3^*} \frac{\delta^{(2)}W[J^*, J]}{\delta J_3 \delta J_1^*} + \zeta \frac{\delta^{(2)}\Gamma[\phi^*, \phi]}{\delta\phi_2 \delta\phi_3} \frac{\delta^{(2)}W[J^*, J]}{\delta J_3^* \delta J_1^*} \right),\end{aligned}\quad (1.394)$$

where we use the short-hand notation $i \equiv (\alpha_i, \tau_i)$, $\delta_{i,j} = \delta_{\alpha_i, \alpha_j} \delta(\tau_i - \tau_j)$, and $\sum_i = \int_0^\beta d\tau_i \sum_{\alpha_i}$. By considering the functional derivatives of (1.384) wrt both $\phi_{\alpha'}(\tau')$ and $\phi_{\alpha'}^*(\tau')$, one obtains four equations that can be cast in the form

$$\sum_3 \begin{pmatrix} \frac{\delta^{(2)}\Gamma}{\delta\phi_2 \delta\phi_3^*} & \zeta \frac{\delta^{(2)}\Gamma}{\delta\phi_2 \delta\phi_3} \\ \frac{\delta^{(2)}\Gamma}{\delta\phi_2^* \delta\phi_3^*} & \frac{\delta^{(2)}\Gamma}{\delta\phi_2^* \delta\phi_3} \end{pmatrix} \begin{pmatrix} \frac{\delta^{(2)}W}{\delta J_3 \delta J_1^*} & \frac{\delta^{(2)}W}{\delta J_3^* \delta J_1} \\ \frac{\delta^{(2)}W}{\delta J_3 \delta J_1} & \frac{\delta^{(2)}W}{\delta J_3^* \delta J_1} \end{pmatrix} = \delta_{1,2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (1.395)$$

In a normal system, the matrices in (1.395) become diagonal for $J^* = J = 0$ and one obtains

$$- \int_0^\beta d\tau_3 \sum_{\alpha_3} G_c^{(2)}(\alpha_1 \tau_1, \alpha_3 \tau_3) \Gamma^{(2)}(\alpha_3 \tau_3, \alpha_2 \tau_2) = \delta_{\alpha_1, \alpha_2} \delta(\tau_1 - \tau_2), \quad (1.396)$$

i.e.

$$\Gamma^{(2)} = -G_c^{(2)-1} = -G^{(2)-1} \quad (1.397)$$

in a matrix sense (recall that $G_c^{(2)} = G^{(2)}$ in the absence of broken symmetry).

It is conventional to express $\Gamma^{(2)}$ in terms of the self-energy Σ defined by $\Gamma^{(2)} = -G_0^{-1} + \Sigma$ or $G^{-1} = G_0^{-1} - \Sigma$ (with $G \equiv G^{(2)}$). This equation can be rewritten as

$$G = G_0 + G_0 \Sigma G \quad (1.398)$$

or, more explicitly,

$$\begin{aligned}G(\alpha\tau, \alpha'\tau') &= G_0(\alpha\tau, \alpha'\tau') \\ &+ \int_0^\beta d\tau_1 d\tau_2 \sum_{\alpha_1, \alpha_2} G_0(\alpha\tau, \alpha_1\tau_1) \Sigma(\alpha_1\tau_1, \alpha_2\tau_2) G(\alpha_2\tau_2, \alpha'\tau').\end{aligned}\quad (1.399)$$

Equation (1.398) is known as the Dyson equation. For a translation invariant system, we obtain the simple expression

$$G(\mathbf{k}, i\omega_n) = \frac{1}{G_0^{-1}(\mathbf{k}, i\omega_n) - \Sigma(\mathbf{k}, i\omega_n)} = \frac{1}{i\omega_n - \xi_{\mathbf{k}} - \Sigma(\mathbf{k}, i\omega_n)} \quad (1.400)$$

(neglecting for simplicity internal degrees of freedom such as the spin of the particle), where $\Sigma(\mathbf{k}, i\omega_n)$ is the Fourier transform of $\Sigma(\mathbf{r}, \tau; \mathbf{r}', \tau') = \Sigma(\mathbf{r} - \mathbf{r}', \tau - \tau')$. The

Dyson equation can be graphically represented as

$$\begin{aligned}
 \text{thick line} &= \text{thin line} + \text{thin line} \circlearrowleft \Sigma \text{thick line} \\
 &= \text{thin line} + \text{thin line} \circlearrowleft \Sigma \text{thin line} + \text{thin line} \circlearrowleft \Sigma \text{thin line} \circlearrowleft \Sigma \text{thin line} + \dots
 \end{aligned}$$

where the thick line stands for G and the thin one for G_0 .

Let us introduce two definitions. i) A diagram is n -particle irreducible if it cannot be separated into two or more disconnected pieces by cutting n internal lines. ii) An amputated diagram has no propagator attached to the external legs ($\alpha_i \tau_i$); the latter connect directly to an interaction vertex. With these definitions, it is easy to see that the self-energy is given by the sum of one-particle irreducible (1PI) amputated diagrams. One easily verifies that all diagrams for the Green function G are indeed obtained from the Dyson equation. For instance, the self-energy diagram

$$\Sigma = \text{thin line} \circlearrowleft \text{circle} \text{thin line}$$

generates an infinite number of diagrams for the Green function,

$$G = \text{thin line} + \text{thin line} \circlearrowleft \text{circle} \text{thin line} + \text{thin line} \circlearrowleft \text{circle} \text{thin line} \circlearrowleft \text{circle} \text{thin line} + \dots$$

Note that it should be understood that the external legs in the self-energy diagrams are not part of the self-energy even though they are often drawn for clarity.

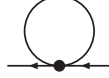
The diagrammatic rules for the self-energy follow directly from those corresponding to the one-particle Green function. To calculate the n th order contribution to the self-energy:

1. Draw all distinct 1PI amputated connected (2-leg) diagrams with n interaction vertices.
2. To each directed line, associate $G_0(\alpha\tau, \alpha', \tau'^+)$.
3. To each vertex, associate $(\gamma_1\gamma_2|\hat{v}|\gamma'_1\gamma'_2)$.
4. Sum over all internal indices α and integrate over all internal times τ .
5. Multiply the result by the factor $(-1)^n \zeta^{n_L}$ where n_L is the number of closed loops. Note that the combinatorial factor is unity since we use non-(anti)symmetrized vertices.

The two first-order diagrams contributing to the self-energy $\Sigma(\alpha_1\tau_1, \alpha'_1\tau'_1)$ are

$$\begin{aligned}
\text{Diagram 1: A circle with a dashed vertical line connecting its bottom to a horizontal line with two arrows pointing left.} &= -\zeta\delta(\tau_1 - \tau_1'^+) \sum_{\alpha_2, \alpha_2'} (\alpha_1 \alpha_2 |\hat{v}| \alpha_1' \alpha_2') G_0(\alpha_2' \tau_1, \alpha_2 \tau_1'^+) \\
\text{Diagram 2: A horizontal line with two arrows pointing left, with a dashed semi-circle above it.} &= -\delta(\tau_1 - \tau_1'^+) \sum_{\alpha_2, \alpha_2'} (\alpha_1 \alpha_2 |\hat{v}| \alpha_2' \alpha_1') G_0(\alpha_2' \tau_1, \alpha_2 \tau_1'^+)
\end{aligned}$$

The first-order self-energy correction can also be represented by the diagram



The second-order diagrams are given by those of figure 1.3 (with amputated legs) except the last four that are not 1PI. They are also given by the last two diagrams (with amputated legs) of figure 1.6.

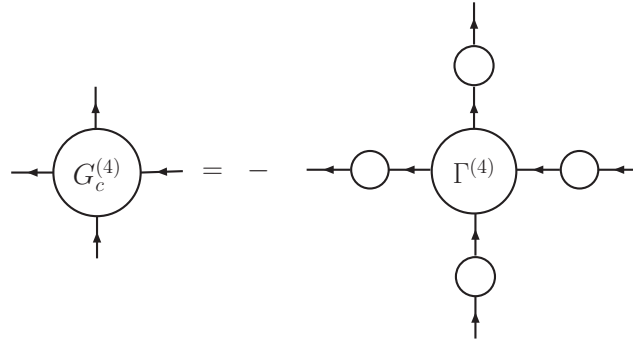
In perturbation theory, one always computes the self-energy rather than directly the one-particle Green function. Any finite order calculation of Σ leads (*via* the Dyson equation) to the summation of an infinite number of diagrams for the Green function. Moreover, a perturbative calculation of G to finite order would violate basic properties of the Green function such as causality, etc. (see Sec. 3.5).

Higher-order vertices

By taking functional derivatives of (1.395) with respect to J^* and J , one can relate the higher-order connected Green functions $G_c^{(n)}$ ($n \geq 4$) to the 1PI vertices. After a little algebra, one finds

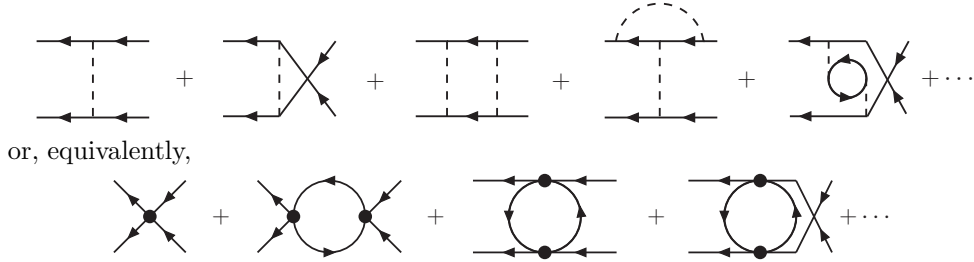
$$\begin{aligned}
G_c^{(4)}(\alpha_1 \tau_1, \alpha_2 \tau_2; \alpha_2' \tau_2', \alpha_1' \tau_1') &= - \int_0^\beta du_1 du_2 du_2' du_1' \sum_{\gamma_1, \gamma_2, \gamma_2', \gamma_1'} G(\alpha_1 \tau_1, \gamma_1 u_1) \\
&\times G(\alpha_2 \tau_2, \gamma_2 u_2) \Gamma^{(4)}(\gamma_1 u_1, \gamma_2 u_2; \gamma_2' u_2', \gamma_1' u_1') G(\gamma_2' u_2', \alpha_2' \tau_2') G(\gamma_1' u_1', \alpha_1' \tau_1'). \quad (1.401)
\end{aligned}$$

This expression can be graphically represented as



(writing explicitly the sign of the diagrams), where the empty circle stands for the

one-particle Green function G , and identifies $\Gamma^{(4)}(\alpha_1\tau_1, \alpha_2\tau_2; \alpha'_2\tau'_2, \alpha'_1\tau'_1)$ as the 4-leg (or two-particle) 1PI vertex. $\Gamma^{(4)}$ can be seen as the effective interaction vertex between two particles. To lowest order, it is given by the bare vertex $\{\alpha_1\alpha_2|\hat{v}|\alpha'_1\alpha'_2\}$, and its perturbation expansion can be represented by diagrams,



or, equivalently,



where the lines may contain any self-energy corrections. Since $\Gamma^{(4)}$ shares the same symmetry properties as $G_c^{(4)}$ [Eq. (1.401)], it is (anti)symmetric under the exchange of the two incoming or outgoing particles,

$$\begin{aligned}\Gamma^{(4)}(\alpha_1\tau_1, \alpha_2\tau_2; \alpha'_2\tau'_2, \alpha'_1\tau'_1) &= \zeta\Gamma^{(4)}(\alpha_2\tau_2, \alpha_1\tau_1; \alpha'_2\tau'_2, \alpha'_1\tau'_1) \\ &= \zeta\Gamma^{(4)}(\alpha_1\tau_1, \alpha_2\tau_2; \alpha'_1\tau'_1, \alpha'_2\tau'_2).\end{aligned}\quad (1.402)$$

General case

It is possible to define fully symmetric 1PI vertices starting from the partition function

$$Z[J] = \int \mathcal{D}[\psi] \exp\left\{-S[\psi] + \int_0^\beta d\tau \sum_{\tilde{\alpha}} J_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}}(\tau)\right\} \quad (1.403)$$

and the effective action $\Gamma[\phi]$ defined as the Legendre transform

$$\begin{aligned}\phi_{\tilde{\alpha}}(\tau) &= \langle \psi_{\tilde{\alpha}}(\tau) \rangle_J = \frac{\delta W[J]}{\delta J_{\tilde{\alpha}}(\tau)}, \\ \Gamma[\phi] &= -W[J] + \int_0^\beta d\tau \sum_{\tilde{\alpha}} J_{\tilde{\alpha}}(\tau) \phi_{\tilde{\alpha}}(\tau),\end{aligned}\quad (1.404)$$

where $W[J] = \ln Z[J]$. $\Gamma[\phi]$ satisfies

$$\frac{\delta \Gamma[\phi]}{\delta \phi_{\tilde{\alpha}}(\tau)} = \zeta J_{\tilde{\alpha}}(\tau). \quad (1.405)$$

In the absence of external sources ($J = 0$), the effective action is stationary. If the stationary value $\bar{\phi}$ is non-zero, the gauge symmetry is broken.⁴⁰

The 1PI vertices in the state $\bar{\phi}$ are defined by⁴¹

$$\Gamma^{(n)}(\tilde{\alpha}_1\tau_1, \dots, \tilde{\alpha}_n\tau_n) = \left. \frac{\delta^{(n)}\Gamma[\phi]}{\delta \phi_{\tilde{\alpha}_n}(\tau_n) \cdots \delta \phi_{\tilde{\alpha}_1}(\tau_1)} \right|_{\phi=\bar{\phi}} \quad (1.406)$$

⁴⁰See footnote 34 page 72.

⁴¹The 1PI vertices can also be defined wrt the state $\phi = 0$, i.e. by expanding the effective action $\Gamma[\phi]$ about $\phi = 0$. In fermion systems, this is the only possibility since $\phi = 0$ in the physical state.

or the inverse relation

$$\Gamma[\phi] = \Gamma[\bar{\phi}] + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^\beta d\tau_1 \cdots d\tau_n \sum_{\tilde{\alpha}_1, \dots, \tilde{\alpha}_n} \Gamma^{(n)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_n \tau_n) \times [\phi_{\tilde{\alpha}_1}(\tau_1) - \bar{\phi}_{\tilde{\alpha}_1}(\tau_1)] \cdots [\phi_{\tilde{\alpha}_n}(\tau_n) - \bar{\phi}_{\tilde{\alpha}_n}(\tau_n)]. \quad (1.407)$$

They are (anti)symmetric under the exchange of two particles,

$$\Gamma^{(n)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_i \tau_i, \dots, \tilde{\alpha}_j \tau_j, \dots, \tilde{\alpha}_n \tau_n) = \zeta \Gamma^{(n)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_j \tau_j, \dots, \tilde{\alpha}_i \tau_i, \dots, \tilde{\alpha}_n \tau_n). \quad (1.408)$$

From the first of equations (1.404), one easily deduces⁴²

$$\frac{\delta^{(2)} \Gamma[\phi]}{\delta \phi \delta \phi} = \zeta \left(\frac{\delta^{(2)} W[J]}{\delta J \delta J} \right)^{-1} \quad (1.409)$$

and, for $J = 0$ and $\phi = \bar{\phi}$,

$$\Gamma^{(2)} = G_c^{(2)-1}. \quad (1.410)$$

The self-energy is defined as $\Gamma^{(2)} = G_0^{-1} + \Sigma$,⁴³ i.e.

$$G_c^{-1} = G_0^{-1} + \Sigma, \quad (1.411)$$

and has a 2×2 matrix structure wrt the charge index c ,

$$\Sigma(\alpha\tau, \alpha'\tau') = \begin{pmatrix} \Sigma(\alpha, +, \tau; \alpha', +, \tau') & \Sigma(\alpha, +, \tau; \alpha', -, \tau') \\ \Sigma(\alpha, -, \tau; \alpha', +, \tau') & \Sigma(\alpha, -, \tau; \alpha', -, \tau') \end{pmatrix} \quad (1.412)$$

$$= \begin{pmatrix} \begin{array}{c} \leftarrow \bigcirc \rightarrow \\ \rightarrow \bigcirc \rightarrow \end{array} & \begin{array}{c} \leftarrow \bigcirc \leftarrow \\ \rightarrow \bigcirc \leftarrow \end{array} \end{pmatrix}.$$

Equation (1.411) is a generalization of the Dyson equation to systems with broken gauge symmetry. It is known as the Dyson-Beliaev equation. The perturbative expansion of $\Sigma(\tilde{\alpha}\tau, \tilde{\alpha}'\tau')$ in boson systems will be discussed in section 1.7.

From (1.409) and using the relations

$$\begin{aligned} \frac{\delta}{\delta J_{\tilde{\alpha}_{n+1}}(\tau_{n+1})} G_c^{(n)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_n \tau_n) &= \zeta^n G_c^{(n+1)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_{n+1} \tau_{n+1}), \\ \frac{\delta}{\delta J_{\tilde{\alpha}_{n+1}}(\tau_{n+1})} \Gamma^{(n)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_n \tau_n) &= \int_0^\beta d\tau \sum_{\tilde{\alpha}} G_c^{(2)}(\tilde{\alpha}_{n+1} \tau_{n+1}, \tilde{\alpha} \tau) \\ &\quad \times \Gamma^{(n+1)}(\tilde{\alpha}_1 \tau_1, \dots, \tilde{\alpha}_n \tau_n, \tilde{\alpha} \tau), \end{aligned} \quad (1.413)$$

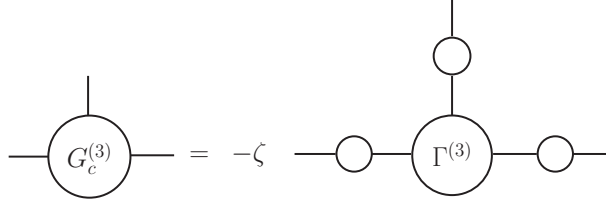
⁴²The sign difference between (1.397) and (1.410) comes from the sign convention for the Green function $G^{(2)}(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') = +\langle \psi_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}'}(\tau') \rangle$ (see Sec. 1.6.1).

⁴³Given the definition of the Green function $G^{(2)}$,⁴² the self-energy Σ in (1.411) is defined with the same sign convention as the one introduced for normal systems.

one can express higher-order Green functions $G_c^{(n)}$ in terms of $\Gamma^{(m \leq n)}$ and $G_c^{(m < n)}$. For instance, one finds

$$G_c^{(3)}(\tilde{\alpha}_1\tau_1, \tilde{\alpha}_2\tau_2, \tilde{\alpha}_3\tau_3) = -\zeta \int_0^\beta du_1 du_2 du_3 \sum_{\tilde{\gamma}_1, \tilde{\gamma}_2, \tilde{\gamma}_3} G_c(\tilde{\alpha}_1\tau_1, \tilde{\gamma}_1 u_1) \\ \times G_c(\tilde{\alpha}_2\tau_2, \tilde{\gamma}_2 u_2) G_c(\tilde{\alpha}_3\tau_3, \tilde{\gamma}_3 u_3) \Gamma^{(3)}(\tilde{\gamma}_1 u_1, \tilde{\gamma}_2 u_2, \tilde{\gamma}_3 u_3). \quad (1.414)$$

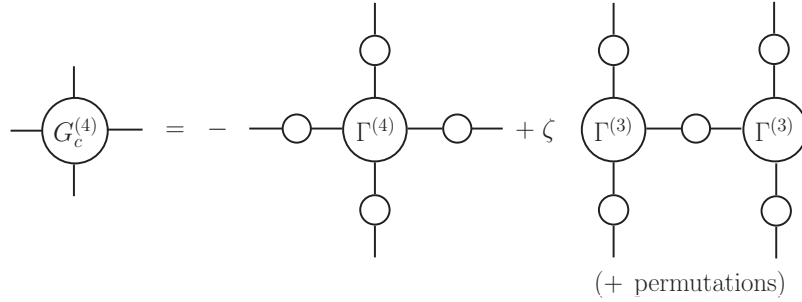
This relation can be graphically represented as



(the empty circles stand for the connected one-particle Green function) and identifies $\Gamma^{(3)}$ as the 3-leg 1PI vertex. To the next order, we obtain the equation

$$G_c^{(4)}(\tilde{\alpha}_1\tau_1, \tilde{\alpha}_2\tau_2, \tilde{\alpha}_3\tau_3, \tilde{\alpha}_4\tau_4) \\ = - \int_0^\beta du_1 du_2 du_3 du_4 \sum_{\tilde{\gamma}_1, \dots, \tilde{\gamma}_4} G_c(\tilde{\alpha}_1\tau_1, \tilde{\gamma}_1 u_1) G_c(\tilde{\alpha}_2\tau_2, \tilde{\gamma}_2 u_2) \\ \times G_c(\tilde{\alpha}_3\tau_3, \tilde{\gamma}_3 u_3) G_c(\tilde{\alpha}_4\tau_4, \tilde{\gamma}_4 u_4) \Gamma^{(4)}(\tilde{\gamma}_1 u_1, \tilde{\gamma}_2 u_2, \tilde{\gamma}_3 u_3, \tilde{\gamma}_4 u_4) \\ - \int_0^\beta du_1 du_2 du_3 \sum_{\tilde{\gamma}_1, \tilde{\gamma}_2, \tilde{\gamma}_3} \Gamma^{(3)}(\tilde{\gamma}_1 u_1, \tilde{\gamma}_2 u_2, \tilde{\gamma}_3 u_3) \\ \times \left[G_c^{(3)}(\tilde{\alpha}_1\tau_1, \tilde{\gamma}_1 u_1, \tilde{\alpha}_4\tau_4) G_c(\tilde{\alpha}_2\tau_2, \tilde{\gamma}_2 u_2) G_c(\tilde{\alpha}_3\tau_3, \tilde{\gamma}_3 u_3) \right. \\ + G_c(\tilde{\alpha}_1\tau_1, \tilde{\gamma}_1 u_1) G_c^{(3)}(\tilde{\alpha}_2\tau_2, \tilde{\gamma}_2 u_2, \tilde{\alpha}_4\tau_4) G_c(\tilde{\alpha}_3\tau_3, \tilde{\gamma}_3 u_3) \\ \left. + G_c(\tilde{\alpha}_1\tau_1, \tilde{\gamma}_1 u_1) G_c(\tilde{\alpha}_2\tau_2, \tilde{\gamma}_2 u_2) G_c^{(3)}(\tilde{\alpha}_3\tau_3, \tilde{\gamma}_3 u_3, \tilde{\alpha}_4\tau_4) \right]. \quad (1.415)$$

Combining (1.414) and (1.415), we finally obtain the following diagrammatic representation of $G_c^{(4)}$



The last diagram represents the contribution to $G_c^{(4)}$ which is one-particle reducible. It vanishes in a normal system where $\Gamma^{(3)} = 0$.

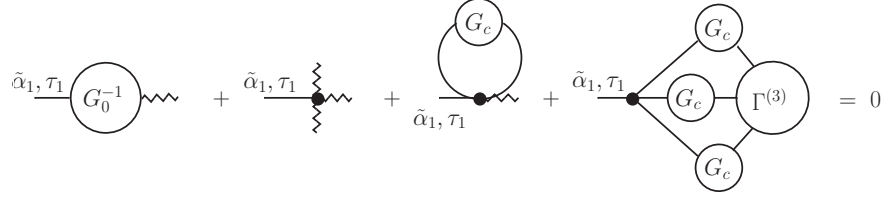


Figure 1.8: Diagrammatic representation of equation (1.420) with $\delta\Gamma/\delta\phi = 0$. The zigzag line stands for the order parameter $\bar{\phi}_{\tilde{\alpha}}(\tau)$.

Equations of motion

The equations of motion of the Green functions imply relations between the 1PI vertices. Equation (1.380) can be rewritten as

$$\sum_{1'} G_0^{-1}(1, 1') \phi_{1'} + \frac{1}{3!} \sum_{2', 3', 4'} v_{12'3'4'} \mathcal{G}^{(3)}(2', 3', 4') - \frac{\delta\Gamma}{\delta\phi_1} = 0, \quad (1.416)$$

where we use the shorthand notation $i \equiv (\tilde{\alpha}_i, \tau_i)$ and $\sum_i \equiv \int_0^\beta d\tau_i \sum_{\tilde{\alpha}_i}$, and

$$\mathcal{G}^{(3)}(2', 3', 4') = \frac{\delta^{(3)} \mathcal{G}[J]}{\delta J_{2'} \delta J_{3'} \delta J_{4'}}. \quad (1.417)$$

$\mathcal{G}[J] = Z[J]/Z[0]$ is the generating functional of the Green functions [Eq. (1.377)]. Using

$$\begin{aligned} \mathcal{G}^{(3)}(2', 3', 4') &= W^{(3)}(2', 3', 4') + \phi_2 W^{(2)}(3', 4') + \zeta \phi_{3'} W^{(2)}(2', 4') \\ &\quad + \phi_{4'} W^{(2)}(2', 3') + \phi_2 \phi_{3'} \phi_{4'} \end{aligned} \quad (1.418)$$

(see equation (1.376)) and

$$W^{(3)}(2', 3', 4') = -\zeta \sum_{2'', 3'', 4''} W^{(2)}(2', 2'') W^{(2)}(3', 3'') W^{(2)}(4', 4'') \Gamma^{(3)}(2'', 3'', 4''), \quad (1.419)$$

one finds

$$\begin{aligned} &\sum_{1'} G_0^{-1}(1, 1') \phi_{1'} - \frac{\delta\Gamma}{\delta\phi_1} \\ &+ \frac{1}{3!} \sum_{2', 3', 4'} v_{12'3'4'} \left[-\zeta \sum_{2'', 3'', 4''} W^{(2)}(2', 2'') W^{(2)}(3', 3'') W^{(2)}(4', 4'') \Gamma^{(3)}(2'', 3'', 4'') \right. \\ &\quad \left. + \phi_2 W^{(2)}(3', 4') + \zeta \phi_{3'} W^{(2)}(2', 4') + \phi_{4'} W^{(2)}(2', 3') + \phi_2 \phi_{3'} \phi_{4'} \right] = 0. \end{aligned} \quad (1.420)$$

If we consider this equation in the physical state, where $\delta\Gamma/\delta\phi = 0$ and $W^{(2)} = G_c$, we obtain an equation for the order parameter $\bar{\phi}_{\tilde{\alpha}}(\tau) = \langle \psi_{\tilde{\alpha}}(\tau) \rangle$ which is diagrammatically represented in figure 1.8.

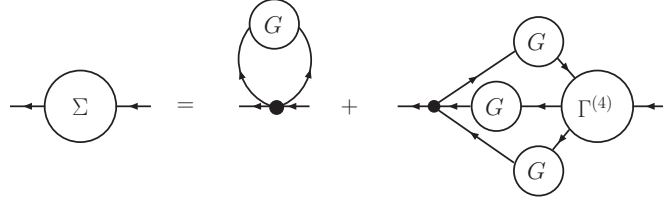


Figure 1.9: Diagrammatic representation of equation (1.422) in a normal system.

Equation (1.420) is also the starting point for deriving the equations of motion satisfied by the 1PI vertices. If we take the functional derivative wrt ϕ_2 , we obtain

$$\begin{aligned}
 \Sigma(1, 2) = & -\frac{\zeta}{3!} \sum_{2' \dots 4''} v_{1,2',3',4'} G_c(2', 2'') G_c(3', 3'') G_c(4', 4'') \Gamma^{(4)}(2'', 3'', 4'', 2) \\
 & + \frac{\zeta}{2} \sum_{2' \dots 4''} v_{1,2',3',4'} (G_c \Gamma^{(3)}(2) G_c)(2', 2'') G_c(3', 3'') G_c(4', 4'') \Gamma^{(3)}(2'', 3'', 4'') \\
 & - \frac{\zeta}{2} \sum_{2',3',4'} v_{1,2',3',4'} \phi_{2'} (G_c \Gamma^{(3)}(2) G_c)(3', 4') \\
 & + \frac{1}{2} \sum_{3',4'} v_{1,2,3',4'} [G_c(3', 4') + \phi_{3'} \phi_{4'}]. \tag{1.421}
 \end{aligned}$$

For a normal system ($\phi = 0$), the self-energy reads

$$\begin{aligned}
 \Sigma(1, 2) = & \sum_{3',4'} \{1, 3' | \hat{v} | 4', 2\} G(4', 3') \\
 & - \frac{1}{2} \sum_{2' \dots 4''} \{1, 2' | \hat{v} | 4', 3'\} G(2'', 2') G(3', 3'') G(4', 4'') \Gamma^{(4)}(3'', 4'', 2'', 2) \tag{1.422}
 \end{aligned}$$

and is shown diagrammatically in figure 1.9.

1.6.3 Luttinger-Ward functional and 2PI vertices

In this section, we introduce the Luttinger-Ward functional and the 2PI vertices. The Luttinger-Ward functional is used to set up “conserving” approximations, i.e. approximations that satisfy conservation laws, as well as non-perturbative approaches (chapter ??).

Normal systems

We consider the partition function in the presence of a bilinear source which couples to a particle-hole pair operator,

$$Z[J] = \int \mathcal{D}[\psi^*, \psi] \exp \left\{ -S[\psi^*, \psi] + \int_0^\beta d\tau d\tau' \sum_{\alpha, \alpha'} J_{\alpha\alpha'}(\tau, \tau') \psi_\alpha^*(\tau) \psi_{\alpha'}(\tau') \right\}. \tag{1.423}$$

By taking the functional derivative wrt the source, we obtain the one-particle Green function

$$G(\alpha\tau, \alpha'\tau') = -\zeta \frac{\delta \ln Z[J]}{\delta J_{\alpha'\alpha}(\tau', \tau)}. \quad (1.424)$$

The Legendre transform of $-\ln Z[J]$ is a functional of the propagator G ,

$$\Gamma[G] = -\ln Z[J] - \zeta \int_0^\beta d\tau d\tau' \sum_{\alpha, \alpha'} J_{\alpha\alpha'}(\tau, \tau') G(\alpha'\tau', \alpha\tau) \quad (1.425)$$

(with J a functional of G defined by (1.424)), which satisfies

$$\frac{\delta \Gamma[G]}{\delta G(\alpha\tau, \alpha'\tau')} = -\zeta J_{\alpha'\alpha}(\tau', \tau). \quad (1.426)$$

The actual Green function \bar{G} , obtained for vanishing external sources, corresponds to the stationary value of the functional $\Gamma[G]$.

For a non-interacting system, $\Gamma[G]$ can be calculated exactly since the action is Gaussian. The partition function reads⁴⁴

$$Z[J] = \det(-G_0^{-1} - J)^{-\zeta} = \exp[-\zeta \text{Tr} \ln(-G_0^{-1} - J)], \quad (1.427)$$

and (1.424) then gives $G = (G_0^{-1} + J)^{-1}$. We deduce

$$\Gamma[G] = -\zeta \text{Tr} \ln(-G) + \zeta \text{Tr}(G_0^{-1}G - 1). \quad (1.428)$$

For an interacting system, we write the functional Γ as

$$\Gamma[G] = -\zeta \text{Tr} \ln(-G) + \zeta \text{Tr}(G_0^{-1}G - 1) + \Phi[G], \quad (1.429)$$

where $\Phi[G]$ is referred to as the Luttinger-Ward functional. Equation (1.426) then gives

$$-\zeta G^{-1}(\alpha'\tau', \alpha\tau) + \zeta G_0^{-1}(\alpha'\tau', \alpha\tau) + \frac{\delta \Phi[G]}{\delta G(\alpha\tau, \alpha'\tau')} = -\zeta J_{\alpha'\alpha}(\tau', \tau), \quad (1.430)$$

which is nothing but the Dyson equation $G^{-1} = G_0^{-1} - \Sigma$ [Eq. (1.398)]. For $J = 0$, the self-energy is given by the first-order functional derivative of the Luttinger-Ward functional,

$$\Sigma(\alpha\tau, \alpha'\tau') = -\zeta \frac{\delta \Phi[G]}{\delta G(\alpha'\tau', \alpha\tau)} \Big|_{G=\bar{G}}, \quad (1.431)$$

where \bar{G} is the solution of the equation $\delta \Gamma / \delta G = 0$. Equation (1.431) can be used to find a diagrammatic interpretation of $\Phi[G]$. The perturbation expansion of Σ wrt G_0 (Sec. 1.6.2) can be rewritten as an expansion wrt the full propagator G ,⁴⁵

⁴⁴We use equation (1.863).

⁴⁵We assume that the particles interact *via* a two-body interaction \hat{v} .

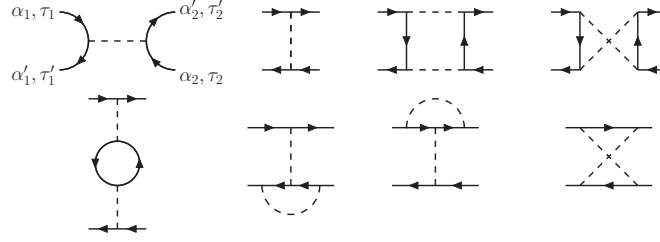


Figure 1.10: Diagrams contributing to the 2PI vertex $\Phi^{(2)}$ to second-order in the interaction.

Since Σ is defined as the functional derivative of the Luttinger-Ward functional $\Phi[G]$ [Eq. (1.431)], we deduce that $\Phi[G]$ is given by the sum of the 2PI Feynman diagrams defined as the graphs that cannot be separated into two disconnected pieces by cutting one or two lines:⁴⁶

$$\Phi[G] = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \dots$$

Since the functional derivation wrt G amounts to removing a propagator G from the diagrams contributing to the Luttinger-Ward functional, the diagrammatic definition of $\Phi[G]$ reproduces the expansion of Σ in terms of G . Note that a two-particle reducible diagram for $\Phi[G]$ would give a contribution to the self-energy which is not 1PI. The diagrammatic rules for $\Phi[G]$ are the same as those for $-\ln Z$. One can check that they are consistent with the diagrammatic rules for the self-energy. For instance, to first-order $\Phi[G]$ is given by

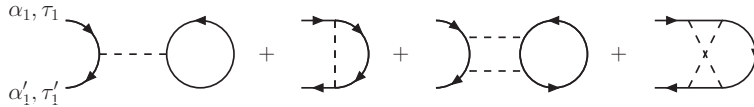
$$\begin{aligned} \Phi[G] = & \frac{1}{2} \sum_{\alpha_1 \dots \alpha'_2} (\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2) \int_0^\beta d\tau G(\alpha'_1 \tau, \alpha_1 \tau^+) G(\alpha'_2 \tau, \alpha_2 \tau^+) \\ & + \frac{\zeta}{2} \sum_{\alpha_1 \dots \alpha'_2} (\alpha_1 \alpha_2 | \hat{v} | \alpha'_1 \alpha'_2) \int_0^\beta d\tau G(\alpha'_1 \tau, \alpha_2 \tau^+) G(\alpha'_2 \tau, \alpha_1 \tau^+), \end{aligned} \quad (1.432)$$

and the first-order functional derivative $\Phi^{(1)}$ reproduces the lowest-order contribution to the self-energy with G_0 replaced by G (see page 81).

The 2PI vertices $\Phi^{(n)}$ are defined by

$$\Phi^{(n)}(\alpha_1 \tau_1, \alpha'_1 \tau'_1; \dots; \alpha_n \tau_n, \alpha'_n \tau'_n) = \frac{(-\zeta)^n \delta^{(n)} \Phi[G]}{\delta G(\alpha_1 \tau_1, \alpha'_1 \tau'_1) \dots \delta G(\alpha_n \tau_n, \alpha'_n \tau'_n)} \Big|_{G=\bar{G}}. \quad (1.433)$$

$\Phi^{(n)}$ is a vertex with n external “bosonic” legs $(\alpha_i \tau_i, \alpha'_i \tau'_i)$. For example, to second-order $\Phi[G]$ is defined by the four diagrams of the preceding figure, so that $\Phi^{(1)}$ is given by the (amputated) diagrams



⁴⁶The 2PI diagrams are also called skeleton diagrams as they do not contain self-energy insertions.

where the external legs $(\alpha_i \tau_i)$ and $(\alpha'_i \tau'_i)$ are drawn nearby so that they can be seen as a single bosonic (particle-hole) leg $(\alpha_i \tau_i, \alpha'_i \tau'_i)$. The diagrams contributing to $\Phi^{(2)}$ to $\mathcal{O}(v^2)$ are shown in figure 1.10. It is clear that $\Phi^{(1)}$, $\Phi^{(2)}$ and more generally all vertices obtained from $\Phi[G]$ are 2PI: they cannot be separated into two disconnected pieces by cutting only two internal lines if one consider each external bosonic leg as a single piece. Since the leg $(\alpha_i \tau_i, \alpha'_i \tau'_i)$ corresponds to a particle-hole pair, the vertices $\Phi^{(n)}$ are said to be irreducible in the particle-hole channel. This, of course, follows from our choice of $J_{\alpha\alpha'}(\tau, \tau')$ as an external source that couples to a particle-hole pair. We shall see in the next section that it is also possible to define irreducible vertices in the particle-particle channel.

In the 2PI formalism, the Green functions are naturally defined by

$$W^{(n)}(\alpha_1 \tau_1, \alpha'_1 \tau'_1; \dots; \alpha_n \tau_n, \alpha'_n \tau'_n) = \frac{(-\zeta)^n \delta^{(n)} \ln Z[J]}{\delta J_{\alpha'_1 \alpha_1}(\tau'_1, \tau_1) \dots \delta J_{\alpha'_n \alpha_n}(\tau'_n, \tau_n)} \Big|_{J=0}. \quad (1.434)$$

One easily verifies that⁴⁷

$$\begin{aligned} W^{(1)}(\alpha_1 \tau_1, \alpha'_1 \tau'_1) &= G^{(2)}(\alpha_1 \tau_1, \alpha'_1 \tau'_1) \equiv G(\alpha_1 \tau_1, \alpha'_1 \tau'_1), \\ W^{(2)}(\alpha_1 \tau_1, \alpha'_1 \tau'_1; \alpha_2 \tau_2, \alpha'_2 \tau'_2) &= G^{(4)}(\alpha_1 \tau_1, \alpha_2 \tau_2; \alpha'_2 \tau'_2, \alpha'_1 \tau'_1) \\ &\quad - G(\alpha_1 \tau_1, \alpha'_1 \tau'_1) G(\alpha_2 \tau_2, \alpha'_2 \tau'_2). \end{aligned} \quad (1.435)$$

$W^{(2)}$ is a “connected” Green function wrt the external bosonic legs $(\alpha_1 \tau_1, \alpha'_1 \tau'_1)$ and $(\alpha_2 \tau_2, \alpha'_2 \tau'_2)$. It plays a role similar to that of the connected Green function $G_c^{(4)}$ introduced in the 1PI formalism (Sec. 1.6.2).⁴⁸ By taking a functional derivative wrt J in (1.426), one obtains the relation

$$W^{(2)} = \left(\frac{\delta \Gamma}{\delta G \delta G} \right)^{-1}, \quad (1.436)$$

where the inverse should be understood in a bosonic matrix sense, the multiplication being defined by

$$(AB)_{\gamma_1 \gamma_2} = \sum_{\gamma_3} A_{\gamma_1 \gamma_3} B_{\gamma_3 \gamma_2}, \quad (1.437)$$

with the short-hand notation

$$\gamma = (\alpha \tau, \alpha' \tau'), \quad \sum_{\gamma} = \int_0^\beta d\tau d\tau' \sum_{\alpha, \alpha'}. \quad (1.438)$$

Using

$$\frac{\delta^{(2)}}{\delta G_{\gamma_1} \delta G_{\gamma_2}} = \Pi_{\gamma_1 \gamma_2}^{-1} + \Phi_{\gamma_1 \gamma_2}^{(2)} \quad (1.439)$$

(which follows from (1.429)), where

$$\Pi_{\gamma_1 \gamma_2} = \zeta G(\alpha_1 \tau_1, \alpha'_2 \tau'_2) G(\alpha_2 \tau_2, \alpha'_1 \tau'_1) \quad (1.440)$$

⁴⁷In Eq. (1.435) and below, it is implicitly assumed that we consider the physical state, i.e. $J = 0$, $G = \bar{G}$, etc.

⁴⁸Note that for a non-interacting system, one has $W^{(2)}(\alpha_1 \tau_1, \alpha'_1 \tau'_1; \alpha_2 \tau_2, \alpha'_2 \tau'_2) = \zeta G_0(\alpha_1 \tau_1, \alpha'_2 \tau'_2) G_0(\alpha_2 \tau_2, \alpha'_1 \tau'_1)$ while $G_c^{(4)}(\alpha_1 \tau_1, \alpha'_1 \tau'_1; \alpha_2 \tau_2, \alpha'_2 \tau'_2) = 0$.

is the particle-hole propagator, we can rewrite (1.436) as

$$W^{(2)} = (\Pi^{-1} + \Phi^{(2)})^{-1} = \Pi - \Pi\Phi^{(2)}W^{(2)}. \quad (1.441)$$

Equation (1.441) is known as the Bethe-Salpether equation and relates the two-particle Green function $W^{(2)}$ to the 2PI vertex $\Phi^{(2)}$:

It is similar to the Dyson equation (1.398) with $\Phi^{(2)}$ and Π playing the role of the self-energy Σ and the non-interacting propagator G_0 , respectively.

Making use of the relation between $W^{(2)}$ and $G_c^{(4)}$,

$$W_{\gamma_1\gamma_2}^{(2)} = G_c^{(4)}(\alpha_1\tau_1, \alpha_2\tau_2; \alpha'_2\tau'_2, \alpha'_1\tau'_1) + \zeta G(\alpha_1\tau_1, \alpha'_2\tau'_2)G(\alpha_2\tau_2, \alpha'_1\tau'_1) \quad (1.442)$$

(which follows from (1.435)) and the relation (1.401) between $G_c^{(4)}$ and the 1PI vertex $\Gamma^{(4)}$, we also obtain a relation between $\Gamma^{(4)}$ and $\Phi^{(2)}$,

$$\Gamma^{(4)}(\alpha_1\tau_1, \alpha_2\tau_2; \alpha'_2\tau'_2, \alpha'_1\tau'_1) = [\Phi^{(2)}(1 + \Pi\Phi^{(2)})^{-1}] (\alpha'_1\tau'_1, \alpha_1\tau_1; \alpha'_2\tau'_2, \alpha_2\tau_2), \quad (1.443)$$

which takes the diagrammatic form

General case

We can generalize the preceding analysis by considering the action

$$S[\psi] - \frac{1}{2} \int_0^\beta d\tau d\tau' \sum_{\tilde{\alpha}, \tilde{\alpha}'} J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau') \psi_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}'}(\tau'), \quad (1.444)$$

where $J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau') = \zeta J_{\tilde{\alpha}'\tilde{\alpha}}(\tau', \tau)$ is an (anti)symmetric source. With our sign convention for the Green function (Sec. 1.6.1),

$$G(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') = \langle \psi_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}'}(\tau') \rangle = \frac{\delta \ln Z[J]}{\delta J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau')}. \quad (1.445)$$

The Legendre transform is now defined as

$$\begin{aligned} \Gamma[G] &= -\ln Z[J] + \frac{1}{2} \int_0^\beta d\tau d\tau' \sum_{\tilde{\alpha}, \tilde{\alpha}'} J_{\tilde{\alpha}, \tilde{\alpha}'}(\tau, \tau') G(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') \\ &= -\frac{\zeta}{2} \text{Tr} \ln(G) + \frac{\zeta}{2} \text{Tr}(G_0^{-1}G - 1) + \Phi[G] \end{aligned} \quad (1.446)$$

and satisfies

$$\frac{\delta \Gamma[G]}{\delta G_\gamma} = J_\gamma \quad (1.447)$$

| | $\Phi[G]$ | $\Phi_\gamma^{(1)}$ | $\Phi_{\gamma_1\gamma_2}^{(2)}$ | $\Phi_{\gamma_1\gamma_2\gamma_3}^{(3)}$ |
|--------------------|-----------|---------------------|---------------------------------|---|
| $\mathcal{O}(v)$ | | | | |
| $\mathcal{O}(v^2)$ | | | | |
| $\mathcal{O}(v^3)$ | | | | |

Figure 1.11: Diagrammatic representation of the Luttinger-Ward functional $\Phi[G]$ and the 2PI vertices $\Phi_\gamma^{(1)}$, $\Phi_{\gamma_1\gamma_2}^{(2)}$ and $\Phi_{\gamma_1\gamma_2\gamma_3}^{(3)}$ to third order in the interaction.

with the short-hand notation $\gamma = (\tilde{\alpha}\tau, \tilde{\alpha}'\tau')$. Equations (1.446) and (1.447) imply that for $J = 0$ the self-energy is defined by

$$\Sigma_\gamma = \left. \frac{\delta\Phi[G]}{\delta G_\gamma} \right|_{G=\bar{G}}, \quad (1.448)$$

where \bar{G} is solution of $\delta\Gamma/\delta G = 0$, and the Luttinger-Ward functional given by the sum of 2PI diagrams (Fig. 1.11).

The 2PI vertices are defined by

$$\Phi_{\gamma_1 \dots \gamma_n}^{(n)} = \left. \frac{\delta^{(n)}\Phi[G]}{\delta G_{\gamma_1} \dots \delta G_{\gamma_n}} \right|_{G=\bar{G}}. \quad (1.449)$$

$\Phi^{(n)}$ is a vertex with n external bosonic legs (Fig. 1.11). It is 2PI in the sense that it cannot be separated into two disconnected pieces by cutting only two internal lines. Note that an external leg $\gamma = (\tilde{\alpha}\tau, \tilde{\alpha}'\tau')$ corresponds to a particle-hole pair if $c = -c'$ and to a particle-particle pair if $c = c'$. Since G_γ is (anti)symmetric in the exchange $(\tilde{\alpha}\tau) \leftrightarrow (\tilde{\alpha}'\tau')$, $\Phi^{(n)}$ satisfies

$$\begin{aligned} \Phi_{\gamma_1 \dots \gamma_i \dots \gamma_j \dots \gamma_n}^{(n)} &= \Phi_{\gamma_1 \dots \gamma_j \dots \gamma_i \dots \gamma_n}^{(n)}, \\ \Phi_{\gamma_1 \dots \gamma_i \dots \gamma_n}^{(n)} &= \zeta \Phi_{\gamma_1 \dots \tilde{\gamma}_i \dots \gamma_n}^{(n)}, \end{aligned} \quad (1.450)$$

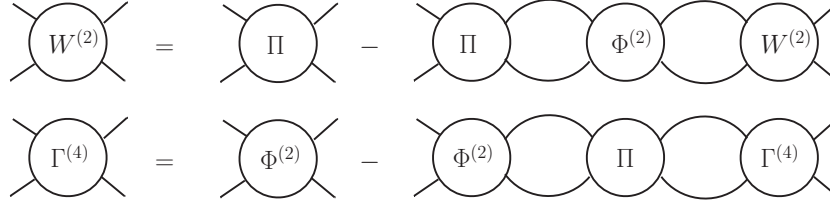


Figure 1.12: Diagrammatic representation of the Bethe-Salpeter equations relating $W^{(2)}$ to $\Phi^{(2)}$ [Eq. (1.457)] and the 1PI vertex $\Gamma^{(4)}$ to $\Phi^{(2)}$ [Eq. (1.458)].

where $\bar{\gamma}_i = (\tilde{\alpha}'_i \tau'_i, \tilde{\alpha}_i \tau_i)$.

The Green functions are defined by

$$W_{\gamma_1 \dots \gamma_n}^{(n)} = \frac{\delta^{(n)} \ln Z[J]}{\delta J_{\gamma_1} \dots \delta J_{\gamma_n}} \Big|_{J=0}. \quad (1.451)$$

To lowest-order they read

$$\begin{aligned} W_{\gamma}^{(1)} &= G_{\gamma}, \\ W_{\gamma_1 \gamma_2}^{(2)} &= G^{(4)}(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}'_1 \tau'_1, \tilde{\alpha}_2 \tau_2, \tilde{\alpha}'_2 \tau'_2) - G(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}'_1 \tau'_1) G(\tilde{\alpha}_2 \tau_2, \tilde{\alpha}'_2 \tau'_2). \end{aligned} \quad (1.452)$$

$W_{\gamma_1 \gamma_2}^{(2)}$ is given by the sum of diagrams that are fully connected to the external bosonic legs γ_1 and γ_2 . To relate $W^{(2)}$ to $\Phi^{(2)}$, we start from

$$W^{(2)} = \left(\frac{\delta^{(2)}}{\delta G \delta G} \right)^{-1}, \quad (1.453)$$

where the inverse should be understood in a bosonic matrix sense with the multiplication defined by

$$(AB)_{\gamma_1 \gamma_2} = \frac{1}{2} \sum_{\gamma_3} A_{\gamma_1 \gamma_3} B_{\gamma_3 \gamma_2} \quad (1.454)$$

and the identity matrix by

$$I_{\gamma_1 \gamma_2} = \delta_{\tilde{\alpha}_1, \tilde{\alpha}_2} \delta_{\tilde{\alpha}'_1, \tilde{\alpha}'_2} \delta(\tau_1 - \tau_2) \delta(\tau'_1 - \tau'_2) + \zeta \delta_{\tilde{\alpha}_1, \tilde{\alpha}'_2} \delta_{\tilde{\alpha}'_1, \tilde{\alpha}_2} \delta(\tau_1 - \tau'_2) \delta(\tau'_1 - \tau_2). \quad (1.455)$$

These definitions are consistent with the (anti)symmetry properties of the Green functions and vertices under the exchange $(\tilde{\alpha}_i \tau_i, \tilde{\alpha}'_i \tau'_i) \leftrightarrow (\tilde{\alpha}'_i \tau'_i, \tilde{\alpha}_i \tau_i)$ of the two particles in the bosonic external leg γ_i . Defining the particle-particle propagator as

$$\Pi_{\gamma_1 \gamma_2} = G(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}'_2 \tau'_2) G(\tilde{\alpha}'_1 \tau'_1, \tilde{\alpha}_2 \tau_2) + \zeta G(\tilde{\alpha}_1 \tau_1, \tilde{\alpha}_2 \tau_2) G(\tilde{\alpha}'_1 \tau'_1, \tilde{\alpha}'_2 \tau'_2), \quad (1.456)$$

we obtain the Bethe-Salpether equation relating $W^{(2)}$ to $\Phi^{(2)}$ (Fig. 1.12),

$$W^{(2)} = \left(\Pi^{-1} + \Phi^{(2)} \right)^{-1} = \Pi - \Pi \Phi^{(2)} W^{(2)}. \quad (1.457)$$

Similarly, we can derive a relation between $\Phi^{(2)}$ and the 1PI vertex $\Gamma^{(4)}$,

$$\Gamma^{(4)} = \left(\Phi^{(2)-1} + \Pi \right)^{-1} = \Phi^{(2)} - \Phi^{(2)} \Pi \Gamma^{(4)}, \quad (1.458)$$

with the definition $\Gamma_{\gamma_1\gamma_2}^{(4)} = \Gamma^{(4)}(\tilde{\alpha}_1\tau_1, \tilde{\alpha}'_1\tau'_1, \tilde{\alpha}_2\tau_2, \tilde{\alpha}'_2\tau'_2)$ (Fig. 1.12). In a normal system, $c_1 + c'_1 + c_2 + c'_2 = 0$, and the Bethe-Salpeter equation can be projected onto the particle-hole ($c_1 + c'_1 = c_2 + c'_2 = 0$) and particle-particle ($c_1 = c'_1 = -c_2 = -c'_2$) channels. The corresponding vertices, $\Phi_{\text{ph}}^{(2)}$ and $\Phi_{\text{pp}}^{(2)}$, are 2PI in the particle-hole and particle-particle channels, respectively.

When dealing with bosons, it appears natural to work with a functional $\Phi[G_c, \phi]$ of both the connected Green function G_c and the classical field $\phi = \langle \psi \rangle$. Let us consider the partition function with both linear and bilinear external sources,

$$Z[J, h] = \int \mathcal{D}[\psi] \exp \left\{ -S[\psi] + \frac{1}{2} \int_0^\beta d\tau d\tau' \sum_{\tilde{\alpha}, \tilde{\alpha}'} \psi_{\tilde{\alpha}}(\tau) J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau') \psi_{\tilde{\alpha}'}(\tau') \right. \\ \left. + \int_0^\beta d\tau \sum_{\tilde{\alpha}} h_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}}(\tau) \right\}, \quad (1.459)$$

where $J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau') = J_{\tilde{\alpha}'\tilde{\alpha}}(\tau', \tau)$ is symmetric. We have

$$\phi_{\tilde{\alpha}}(\tau) = \langle \psi_{\tilde{\alpha}}(\tau) \rangle = \frac{\delta \ln Z[J, h]}{\delta h_{\tilde{\alpha}}(\tau)}, \\ G_c(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') = \langle \psi_{\tilde{\alpha}}(\tau) \psi_{\tilde{\alpha}'}(\tau') \rangle - \langle \psi_{\tilde{\alpha}}(\tau) \rangle \langle \psi_{\tilde{\alpha}'}(\tau') \rangle \quad (1.460) \\ = \frac{\delta \ln Z[J, h]}{\delta J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau')} - \phi_{\tilde{\alpha}}(\tau) \phi_{\tilde{\alpha}'}(\tau').$$

The effective action is defined as a double Legendre transform,

$$\Gamma[G_c, \phi] = -\ln Z[J, h] + \int_0^\beta d\tau \sum_{\tilde{\alpha}} h_{\tilde{\alpha}}(\tau) \phi_{\tilde{\alpha}}(\tau) \\ + \frac{1}{2} \int_0^\beta d\tau d\tau' \sum_{\tilde{\alpha}, \tilde{\alpha}'} J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau') [G_c(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') + \phi_{\tilde{\alpha}}(\tau) \phi_{\tilde{\alpha}'}(\tau')], \quad (1.461)$$

and satisfies

$$\frac{\delta \Gamma[G_c, \phi]}{\delta \phi_{\tilde{\alpha}}(\tau)} = h_{\tilde{\alpha}}(\tau) + \int_0^\beta d\tau' \sum_{\tilde{\alpha}'} J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau') \phi_{\tilde{\alpha}'}(\tau'), \\ \frac{\delta \Gamma[G_c, \phi]}{\delta G_c(\tilde{\alpha}\tau, \tilde{\alpha}'\tau')} = J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau'). \quad (1.462)$$

It can be written as

$$\Gamma[G_c, \phi] = -\frac{1}{2} \text{Tr} \ln(G_c) + \frac{1}{2} \int_0^\beta d\tau d\tau' \phi_{\tilde{\alpha}}(\tau) G_0^{-1}(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') \phi_{\tilde{\alpha}'}(\tau') \\ + \frac{1}{2} \text{Tr}(G_0^{-1} G_c - 1) + \Phi[G_c, \phi], \quad (1.463)$$

where $\Phi[G_c, \phi]$ is the Luttinger-Ward functional. The equations of state (1.462) give

$$\int_0^\beta d\tau' \sum_{\tilde{\alpha}'} G_0^{-1}(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') \phi_{\tilde{\alpha}'}(\tau') + \frac{\delta \Phi[G_c, \phi]}{\delta \phi_{\tilde{\alpha}}(\tau)} \\ = h_{\tilde{\alpha}}(\tau) + \int_0^\beta d\tau' \sum_{\tilde{\alpha}'} J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau') \phi_{\tilde{\alpha}'}(\tau') \quad (1.464)$$

and

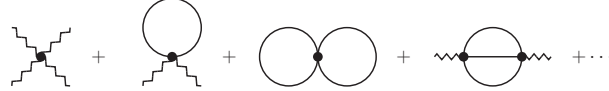
$$-G_c^{-1}(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') + G_0^{-1}(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') + \frac{\delta\Phi[G_c, \phi]}{\delta G_c(\tilde{\alpha}\tau, \tilde{\alpha}'\tau')} = J_{\tilde{\alpha}\tilde{\alpha}'}(\tau, \tau'). \quad (1.465)$$

The first equation is an equation for the order parameter $\phi_{\tilde{\alpha}}(\tau)$. The second one is Dyson's equation $G_c^{-1} = G_0^{-1} + \Sigma$ with the self-energy

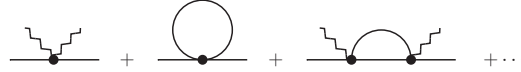
$$\Sigma(\tilde{\alpha}\tau, \tilde{\alpha}'\tau') = \frac{\delta\Phi[G_c, \phi]}{\delta G_c(\tilde{\alpha}\tau, \tilde{\alpha}'\tau')} \quad (1.466)$$

for vanishing external sources ($J = h = 0$).

The effective action $\Gamma[G_c, \phi]$ is given by the sum of the 2PI diagrams,



and the corresponding self-energy has the following diagrammatic expansion



The zigzag line in these diagrams stands for the order parameter $\phi_{\tilde{\alpha}}(\tau)$. The perturbation expansion (in the 1PI formalism) about a broken symmetry state ($\phi_{\tilde{\alpha}}(\tau) \neq 0$) in boson systems is discussed in detail in section 1.7.2.

1.7 Saddle-point approximation and loop expansion

In section 1.5.4, we have pointed out that the perturbation theory of interacting bosons about the non-interacting limit breaks down when the field takes a finite expectation value $\langle\psi_\alpha\rangle$ which breaks the gauge symmetry. In this section, we show how the stationary phase approximation allows us to reorganize the perturbation expansion as a “loop expansion” about a broken-symmetry state. We start by introducing the principle of the method on the simple example of a one-dimensional integral.

1.7.1 Steepest descent and stationary phase approximations

We consider the integral

$$I(l) = \int_{-\infty}^{\infty} dt e^{-lf(t)}, \quad (1.467)$$

where $f(t)$ is a real function with an absolute minimum at t_0 and look for an expansion in $1/l$. For large l , the integral is dominated by the vicinity of t_0 . Expanding $f(t)$ about t_0 and using $f'_0 \equiv f'(t_0) = 0$, we obtain

$$\begin{aligned} I(l) &= e^{-lf_0} \int_{-\infty}^{\infty} dt \exp\left\{-\frac{l}{2}f''_0(t-t_0)^2 - l \sum_{n=3}^{\infty} \frac{f_0^{(n)}}{n!}(t-t_0)^n\right\} \\ &= e^{-lf_0} \sqrt{\frac{2\pi}{f''_0 l}} \int_{-\infty}^{\infty} \frac{d\tau}{\sqrt{2\pi}} \exp\left\{-\frac{\tau^2}{2} - \sum_{n=3}^{\infty} \frac{\tau^n}{n!} \frac{f_0^{(n)}}{(f''_0)^{n/2} l^{n/2-1}}\right\}, \end{aligned} \quad (1.468)$$

where $\tau = \sqrt{f_0''}l(t - t_0)$. The integral can be calculated in powers of $1/l$ using Wick's theorem with the bare propagator

$$\frac{\square}{\tau\tau} = \int_{-\infty}^{\infty} \frac{d\tau}{\sqrt{2\pi}} \tau^2 e^{-\tau^2/2} = 1 \quad (1.469)$$

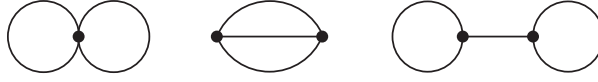
and the vertices

$$V_n = \frac{f_0^{(n)}}{(f_0'')^{n/2} l^{n/2-1}}. \quad (1.470)$$

By the linked cluster theorem (Sec. 1.5.2)

$$I(l) = e^{-lf_0} \sqrt{\frac{2\pi}{f_0''l}} \exp\left\{\sum \text{connected diagrams}\right\}. \quad (1.471)$$

Since $V_n = \mathcal{O}(l^{-n/2+1})$, the $\mathcal{O}(1/l)$ contribution is given by the three diagrams



with respective combinatorial factors $-1/8$, $1/12$ and $1/8$. We deduce

$$\ln I(l) = -lf_0 + \frac{1}{2} \ln\left(\frac{2\pi}{f_0''l}\right) - \frac{1}{8l} \frac{f_0^{(4)}}{f_0'^2} + \frac{5}{24l} \frac{(f_0^{(3)})^2}{f_0'^3} + \mathcal{O}(l^{-2}). \quad (1.472)$$

A similar analysis can be made when the function $f(t)$ is purely imaginary. In this case, for large l the integral is dominated by the vicinity of the point t_0 where the phase of the integrand is stationary ($f'(t_0) = 0$). The expansion (1.471) is then known as the stationary phase method. More generally, let us consider the integral

$$I(l) = \int_{(\mathcal{C})} dz e^{-lf(z)} \quad (1.473)$$

along a path (\mathcal{C}) in the complex plane. The complex function $f(z)$ is analytic along (\mathcal{C}) and vanishes at the end points. Since we can deform the integration contour in the domain of analyticity of $f(z)$, we deform (\mathcal{C}) into a new contour (\mathcal{C}') which satisfies the three conditions:

1. the endpoints of (\mathcal{C}') are the same as those of (\mathcal{C}) .
2. $\Re[f(z)]$ has a minimum at the point z_0 of (\mathcal{C}') .
3. $\Im[f(z)]$ is constant along (\mathcal{C}') near z_0 .

The last two conditions imply that z_0 is a stationary point of $f(z)$ ($f'(z_0) = 0$) and therefore a saddle point of $\Re[f(z)]$.⁴⁹ For large l , we expect the vicinity of z_0 to give the dominant contribution to $I(l)$ (condition (2)). The condition (3) ensures

⁴⁹Recall that an analytic complex function $f(z)$ satisfies the Cauchy-Riemann conditions $\partial_x \Re[f(z)] = \partial_y \Im[f(z)]$ and $\partial_x \Im[f(z)] = -\partial_y \Re[f(z)]$ (obtained by calculating $f'(z) = \lim_{dz \rightarrow 0} [f(z+dz) - f(z)]/dz$ with $dz = dx$ and $dz = idy$). The Cauchy-Riemann conditions imply $\nabla^2 \Re[f(z)] = \nabla^2 \Im[f(z)] = 0$, which prevents $\Re[f(z)]$ and $\Im[f(z)]$ to have an absolute minimum or maximum.

that $\Im[f(z)]$ does not give rise to rapid oscillations in the integrand as $l \rightarrow \infty$ which would suppress the contribution of the vicinity of z_0 . To calculate $I(l)$, we then write $z = z_0 + \rho e^{i\theta}$ and expand $f(z)$ about z_0 ,

$$f(z) = f(z_0) + \frac{1}{2}\rho^2|f_0''|e^{i(2\theta+\theta_0)} + \sum_{n=3}^{\infty} \frac{\rho^n e^{in\theta}}{n!} f_0^{(n)}, \quad (1.474)$$

where $f_0'' \equiv f''(z_0) = |f_0''|e^{i\theta_0}$. Condition (3) implies $2\theta + \theta_0 = 0$ or π , and the existence of a minimum of $\Re[f(z)]$ at z_0 selects the solution $2\theta + \theta_0 = 0$.⁵⁰ It is easy to see that (C') is then the path of steepest descents of $e^{-l\Re[f(z)]}$. The integral over ρ can be calculated as in the previous case using the linked cluster theorem.

1.7.2 Saddle-point approximation and loop expansion in field theory

We consider the partition function

$$Z[J^*, J] = \int \mathcal{D}[\psi^*, \psi] e^{-l(S[\psi^*, \psi] - \int_0^\beta d\tau \int d^d r [J^*(x)\psi(x) + \text{c.c.}])} \quad (1.475)$$

($x = (\mathbf{r}, \tau)$) describing a system of (spin-zero) bosons (ψ is a complex field). The factor l is introduced to organize the perturbation expansion and will be set to unity in the end. We assume that the bosons interact *via* a contact interaction,

$$S[\psi^*, \psi] = \int_0^\beta d\tau \int d^d r \left\{ \psi^*(x) \left(\partial_\tau - \mu - \frac{\nabla^2}{2m} \right) \psi(x) + \frac{g}{2} \psi^*(x) \psi^*(x) \psi(x) \psi(x) \right\} \quad (1.476)$$

($g > 0$).

Partition function and thermodynamic potential

Within a saddle-point approximation, the action reads

$$S_c = \beta V \left(-\mu |\psi_c|^2 + \frac{g}{2} |\psi_c|^4 \right) \quad (1.477)$$

where the “classical” field ψ_c (assumed to be time and space independent) is determined from the condition

$$\frac{\partial S_c}{\partial \psi_c} = \frac{\partial S_c}{\partial \psi_c^*} = 0 \quad (1.478)$$

in the absence of external sources ($J = J^* = 0$). When $\mu > 0$, the solution which minimizes the action is $|\psi_c| = \sqrt{\mu/g}$. As will be discussed in chapter 6, this solution corresponds to a superfluid system and $|\psi_c|^2$ determines the density of the Bose-Einstein condensate. Expanding about the saddle-point solution, $\psi = \psi_c + \chi/\sqrt{l}$, we obtain

$$lS[\chi^*, \chi] = lS_c + S^{(2)} + \mathcal{O}(l^{-1/2}), \quad (1.479)$$

⁵⁰The fact that the path of steepest descents of $e^{-l\Re[f(z)]}$ keeps $\Im[f(z)]$ constant near z_0 (stationary phase) is a consequence of the Cauchy-Riemann conditions.⁴⁹

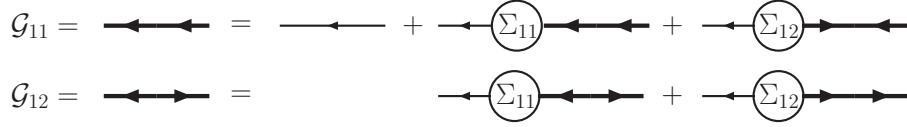


Figure 1.13: Diagrammatic representation of the Beliaev-Dyson equations (1.484). The thin line stands for G_0 and the thick one for \mathcal{G} .

where the Gaussian part of the action

$$S^{(2)} = -\frac{1}{2} \int_0^\beta d\tau \int d^d r (\chi^*(x), \chi(x)) \mathcal{G}_c^{-1}(x, x') \begin{pmatrix} \chi(x') \\ \chi^*(x') \end{pmatrix} \quad (1.480)$$

is defined by the inverse “classical” propagator

$$\mathcal{G}_c^{-1}(x, x') = -\delta(\tau - \tau') \delta(\mathbf{r} - \mathbf{r}') \times \begin{pmatrix} \partial_{\tau'} - \mu - \frac{\nabla_{\mathbf{r}'}^2}{2m} + 2g|\psi_c|^2 & g\psi_c^2 \\ g\psi_c^{*2} & -\partial_{\tau'} - \mu - \frac{\nabla_{\mathbf{r}'}^2}{2m} + 2g|\psi_c|^2 \end{pmatrix}. \quad (1.481)$$

In the superfluid phase ($|\psi_c| > 0$), the bosonic (connected) propagator \mathcal{G} becomes a 2×2 matrix,⁵¹

$$\mathcal{G}(x, x') = - \begin{pmatrix} \langle \psi(x) \psi^*(x') \rangle_c & \langle \psi(x) \psi(x') \rangle_c \\ \langle \psi^*(x) \psi^*(x') \rangle_c & \langle \psi^*(x) \psi(x') \rangle_c \end{pmatrix}. \quad (1.482)$$

where $\langle \psi(x) \psi^*(x') \rangle_c = \langle \psi(x) \psi^*(x') \rangle - \langle \psi(x) \rangle \langle \psi^*(x') \rangle$, etc. It satisfies the Beliaev-Dyson equation $\mathcal{G}^{-1}(k) = \mathcal{G}_0^{-1}(k) - \Sigma(k)$ where

$$\mathcal{G}_0(k) = \begin{pmatrix} G_0(k) & 0 \\ 0 & G_0(-k) \end{pmatrix} \quad (1.483)$$

($k = (\mathbf{k}, i\omega_n)$) is the non-interacting propagator and $\Sigma(k)$ the self-energy. More explicitly, the Beliaev-Dyson equations read

$$\begin{aligned} \mathcal{G}_{11}(k) &= G_0(k) + G_0(k) \Sigma_{11}(k) \mathcal{G}_{11}(k) + G_0(k) \Sigma_{12}(k) \mathcal{G}_{21}(k), \\ \mathcal{G}_{12}(k) &= G_0(k) \Sigma_{11}(k) \mathcal{G}_{12}(k) + G_0(k) \Sigma_{12}(k) \mathcal{G}_{22}(k), \end{aligned} \quad (1.484)$$

with $\mathcal{G}_{11}(k) = \mathcal{G}_{22}(-k) = -\langle \psi(k) \psi^*(k) \rangle$ and $\mathcal{G}_{12}(k) = \mathcal{G}_{21}^*(k) = -\langle \psi(k) \psi(-k) \rangle$ (Fig. 1.13). The classical propagator (1.481) corresponds to the self-energy

$$\begin{aligned} \Sigma_{11}(k) &= \Sigma_{22}(k) = 2g|\psi_c|^2, \\ \Sigma_{12}(k) &= \Sigma_{21}^*(k) = g\psi_c^2 \end{aligned} \quad (1.485)$$

(Fig. 1.14).

⁵¹In this section, \mathcal{G} denotes the connected propagator and the subscript “c” of \mathcal{G}_c stands for “classical”. Note the sign convention in the definition of \mathcal{G} [Eq. (1.480)].

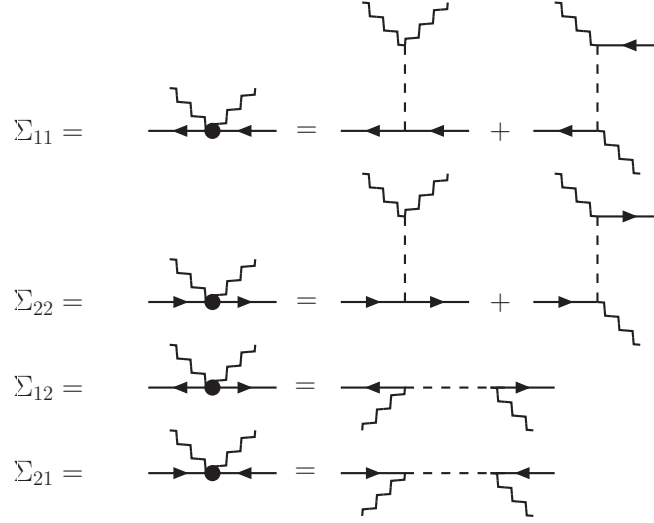


Figure 1.14: Diagrammatic representation of the self-energies (1.485). The zigzag line stands for ψ_c or ψ_c^* . One sometimes introduces a directed zigzag line to distinguish between ψ_c (incoming line) and ψ_c^* (outgoing line).

Since the action (1.479) is Gaussian (ignoring the $\mathcal{O}(l^{-1/2})$ terms), we can carry out the functional integral (see Appendix 1.E.4),⁵²

$$Z = e^{-lS_c} (\det \mathcal{G}_c^{-1})^{-1/2}, \quad (1.486)$$

and obtain the thermodynamic potential⁵³

$$\Omega = \frac{l}{\beta} S_c - \frac{1}{2\beta} \text{Tr} \ln \mathcal{G}_c + \mathcal{O}(l^{-1}). \quad (1.487)$$

Let us now consider the corrections to the Gaussian action (1.479),

$$lS[\chi^*, \chi] = lS_c + S^{(2)}[\chi^*, \chi] + \frac{1}{\sqrt{l}} S^{(3)}[\chi^*, \chi] + \frac{1}{l} S^{(4)}[\chi^*, \chi], \quad (1.488)$$

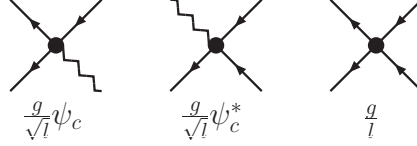
with

$$\begin{aligned} S^{(3)} &= g \int_0^\beta d\tau \int d^d r [\psi_c \chi^*(x) |\chi(x)|^2 + \text{c.c.}], \\ S^{(4)} &= \frac{g}{2} \int_0^\beta d\tau \int d^d r \chi^*(x) \chi^*(x) \chi(x) \chi(x). \end{aligned} \quad (1.489)$$

These corrections give rise to 3- and 4-leg vertices which can be represented by the following diagrams

⁵²Because of the 2×2 matrix structure of \mathcal{G}_c , $\det(-\mathcal{G}_c) = \det(\mathcal{G}_c)$.

⁵³We use $\ln \det \mathcal{G} = \text{Tr} \ln \mathcal{G}$ (see Appendix 1.E.4).



The partition function can be calculated treating $S^{(3)}$ and $S^{(4)}$ in perturbation and using the linked cluster theorem,

$$\begin{aligned} Z &= e^{-lS_c} \int \mathcal{D}[\chi^*, \chi] e^{-S^{(2)} - \frac{1}{\sqrt{l}} S^{(3)} - \frac{1}{l} S^{(4)}} \\ &= e^{-lS_c} (\det \mathcal{G}_c^{-1})^{-1/2} \exp \left\{ \sum \text{connected diagrams} \right\}. \end{aligned} \quad (1.490)$$

To order $1/l$, one finds that the partition function is given by the following diagrams,

$$\ln Z = -lS_c + \frac{1}{2} \text{Tr} \ln \mathcal{G}_c + \frac{1}{l} \left\{ \text{diagram 1} + \text{diagram 2} + \text{diagram 3} \right\},$$

where the lines in the diagrams should be drawn in all possible ways compatible with $S^{(3)}$, $S^{(4)}$, and the classical propagator \mathcal{G}_c . For example, the first diagram means



where the lines stand for the classical propagator \mathcal{G}_c .

The expansion in $1/l$ turns out to be an expansion in the number of loops. Consider a diagram with $n_V = n_V^{(3)} + n_V^{(4)}$ vertices, where $n_V^{(3)}$ ($n_V^{(4)}$) is the number of 3-leg (4-leg) vertices. Since the propagator \mathcal{G}_c is independent of l , the diagram is of order $l^{-n_V^{(4)} - n_V^{(3)}/2} = l^{-n_V + n_V^{(3)}/2}$. The number n_I of internal lines is given by

$$2n_I = 4n_V^{(4)} + 3n_V^{(3)} = 4n_V - n_V^{(3)} \quad (1.491)$$

(obtained by counting the total number of lines attached to the n_V vertices). Since each vertex has a momentum conservation, a diagram with n_V vertices has $n_V - 1$ momentum conservation constraints, so that the number of independent momentum loops is

$$n_M = n_I - (n_V - 1) = n_V - \frac{n_V^{(3)}}{2} + 1. \quad (1.492)$$

The order of the diagram, $l^{-n_V + n_V^{(3)}/2} = l^{-(n_M - 1)}$, is therefore given by the number of loops. In the absence of a condensate ($\psi_c = 0$), $n_V^{(3)} = 0$ and $\mathcal{G}_c = \mathcal{G}_0$, and a diagram with n_M loops is of order $g^{n_V} = g^{n_M - 1}$. The loop expansion then corresponds to the perturbation expansion about the non-interacting limit discussed in section 1.5. On the other hand, when $|\psi_c| > 0$, the classical propagator \mathcal{G}_c contains an infinite resummation of interaction terms and a diagram with n_M loops contains from $n_M - 1$ to $2(n_M - 1)$ vertices. To any order, the loop expansion then corresponds to an infinite resummation of perturbation theory.

Effective action and 1PI vertices

We now consider the effective action defined in section 1.6.2,

$$\Gamma[\phi^*, \phi] = -\frac{1}{l} \ln Z[J^*, J] + \int_0^\beta d\tau \int d^d r [J^*(x) \phi(x) + \text{c.c.}], \quad (1.493)$$

where

$$\phi(x) = \frac{1}{l} \frac{\delta \ln Z[J^*, J]}{\delta J^*(x)}, \quad \phi^*(x) = \frac{1}{l} \frac{\delta \ln Z[J^*, J]}{\delta J(x)} \quad (1.494)$$

(with $Z[J^*, J]$ given by (1.475)). For arbitrary external sources, the saddle point equations read

$$\left. \frac{\delta S[\psi^*, \psi]}{\delta \psi(x)} \right|_{\psi_c} = J^*(x), \quad \left. \frac{\delta S[\psi^*, \psi]}{\delta \psi^*(x)} \right|_{\psi_c} = J(x). \quad (1.495)$$

We expand about the classical state, $\psi(x) = \psi_c(x) + \frac{1}{\sqrt{l}} \chi(x)$, using

$$\begin{aligned} lS[\psi^*, \psi] - l \int_0^\beta d\tau \int d^d r [J^*(x) \psi(x) + \text{c.c.}] \\ = lS_c - l \int_0^\beta d\tau \int d^d r [J^*(x) \psi_c(x) + \text{c.c.}] + S^{(2)}[\chi^*, \chi] + \mathcal{O}(l^{-1/2}), \end{aligned} \quad (1.496)$$

where the Gaussian part $S^{(2)}$ of the action is defined by (1.480,1.481) with a time- and space-dependent classical field $\psi_c(x)$. From

$$\ln Z[J^*, J] = -lS_c + l \int_0^\beta d\tau \int d^d r [J^*(x) \psi_c(x) + \text{c.c.}] + \frac{1}{2} \text{Tr} \ln \mathcal{G}_c + \mathcal{O}(l^{-1}), \quad (1.497)$$

and (1.494,1.495), we deduce

$$\begin{aligned} \phi(x) &= -\frac{\delta S_c}{\delta J^*(x)} + \frac{\delta}{\delta J^*(x)} \int_0^\beta d\tau' \int d^d r' [J^*(x') \psi_c(x') + \text{c.c.}] + \mathcal{O}(l^{-1}) \\ &= \psi_c(x) + \mathcal{O}(l^{-1}) \end{aligned} \quad (1.498)$$

and $\phi^*(x) = \psi_c^*(x) + \mathcal{O}(l^{-1})$. This yields

$$\Gamma[\phi^*, \phi] = S_c + \int_0^\beta d\tau \int d^d r \{ J^*(x) [\phi(x) - \psi_c(x)] + \text{c.c.} \} + \frac{1}{2l} \text{Tr} \ln \mathcal{G}_c + \mathcal{O}(l^{-2}), \quad (1.499)$$

where the $\mathcal{O}(l^{-2})$ contribution comes from the 2-loop and higher-order diagrams. Noting that

$$\begin{aligned} S_c + \int_0^\beta d\tau \int d^d r \{ J^*(x) [\phi(x) - \psi_c(x)] + \text{c.c.} \} \\ = S_c + \int_0^\beta d\tau \int d^d r \left\{ \left. \frac{\delta S_c}{\delta \psi(x)} \right|_{\psi_c} [\phi(x) - \psi_c(x)] + \text{c.c.} \right\} \\ = S[\phi^*, \phi] + \mathcal{O}(l^{-2}), \end{aligned} \quad (1.500)$$

we finally deduce

$$\Gamma[\phi^*, \phi] = S[\phi^*, \phi] + \frac{1}{2l} \text{Tr} \ln \mathcal{G}_c + \mathcal{O}(l^{-2}), \quad (1.501)$$

where $\mathcal{G}_c \equiv \mathcal{G}_c[\phi^*, \phi]$ is obtained from (1.482) by replacing $\psi_c(x)$ by $\phi(x)$, i.e.

$$\mathcal{G}_c^{-1}(x, x') = - \begin{pmatrix} \frac{\delta^{(2)} S[\phi^*, \phi]}{\delta \phi^*(x) \delta \phi(x')} & \frac{\delta^{(2)} S[\phi^*, \phi]}{\delta \phi^*(x) \delta \phi^*(x')} \\ \frac{\delta^{(2)} S[\phi^*, \phi]}{\delta \phi(x) \delta \phi(x')} & \frac{\delta^{(2)} S[\phi^*, \phi]}{\delta \phi(x) \delta \phi^*(x')} \end{pmatrix}. \quad (1.502)$$

In (1.500) and (1.501), we have used the fact that $\phi(x) - \psi_c(x)$ is of order $1/l$.

To order $1/l$ and for vanishing external sources, the equations of state (1.386, 1.387) read

$$\begin{aligned} 0 &= \frac{\delta \Gamma}{\delta \phi^*(x)} = \frac{\delta S}{\delta \phi^*(x)} + \frac{1}{2l} \text{Tr} \left(\mathcal{G}_c \frac{\delta \Sigma}{\delta \phi^*(x)} \right), \\ 0 &= \frac{\delta \Gamma}{\delta \phi(x)} = \frac{\delta S}{\delta \phi(x)} + \frac{1}{2l} \text{Tr} \left(\mathcal{G}_c \frac{\delta \Sigma}{\delta \phi(x)} \right), \end{aligned} \quad (1.503)$$

where we have used $\mathcal{G}_c^{-1} = \mathcal{G}_0^{-1} - \Sigma$, with

$$\Sigma(x, x') = g \delta(\mathbf{r} - \mathbf{r}') \delta(\tau - \tau') \begin{pmatrix} 2|\phi(x)|^2 & \phi(x)^2 \\ \phi^*(x)^2 & 2|\phi(x)|^2 \end{pmatrix}. \quad (1.504)$$

We therefore obtain

$$\begin{aligned} & - \int_0^\beta d\tau' \int d^d r' G_0^{-1}(x, x') \phi(x') + g \phi^*(x) \phi(x)^2 \\ & + \frac{g}{l} \int_0^\beta d\tau \int d^d r \{ [\mathcal{G}_{c,11}(x, x) + \mathcal{G}_{c,22}(x, x)] \phi(x) + \mathcal{G}_{c,12}(x, x) \phi^*(x) \} = 0 \end{aligned} \quad (1.505)$$

and a similar equation with $\phi(x) \leftrightarrow \phi^*(x)$. Equation (1.505) can be diagrammatically represented as

and corresponds to a one-loop approximation to the exact result (1.420) (Fig. 1.8). Here the zigzag line stands for $\phi(x)$ or $\phi^*(x)$ and the solid one (in the loop) for the classical propagator $\mathcal{G}_c \equiv \mathcal{G}_c[\phi^*, \phi]$. The one-loop term in (1.505) gives the $\mathcal{O}(1/l)$ correction to the classical (saddle-point) result $|\phi(x)| = \sqrt{\mu/g}$. From (1.501), one can also obtain the two-point vertices

$$\begin{aligned} \Gamma_{11}^{(2)}(x, x') &= \frac{\delta^{(2)} \Gamma}{\delta \phi^*(x) \delta \phi(x')}, \\ \Gamma_{12}^{(2)}(x, x') &= \frac{\delta^{(2)} \Gamma}{\delta \phi^*(x) \delta \phi^*(x')}, \\ \Gamma_{22}^{(2)}(x, x') &= \frac{\delta^{(2)} \Gamma}{\delta \phi(x) \delta \phi^*(x')} \end{aligned} \quad (1.506)$$

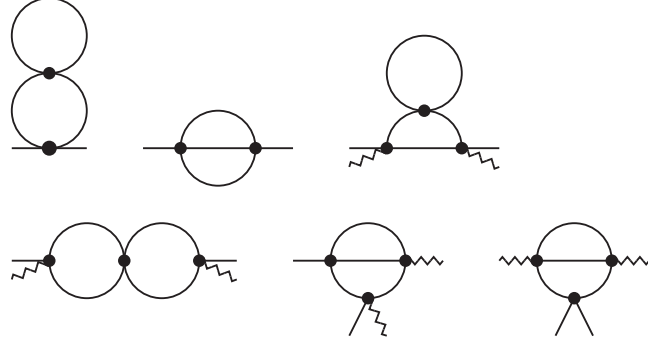
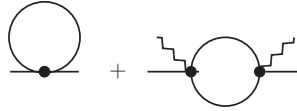


Figure 1.15: Two-loop corrections to the self-energy.

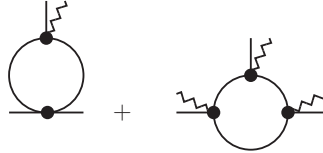
to order $1/l$. For instance, one finds

$$\Gamma_{11}^{(2)}(x, x') = -\mathcal{G}_{c,11}^{-1}(x, x') + \frac{1}{2l} \text{Tr} \left(\mathcal{G}_c \frac{\delta^{(2)} \Sigma}{\delta \phi^*(x) \delta \phi(x')} \right) + \frac{1}{2l} \text{Tr} \left(\mathcal{G}_c \frac{\delta \Sigma}{\delta \phi^*(x)} \mathcal{G}_c \frac{\delta \Sigma}{\delta \phi(x')} \right) \quad (1.507)$$

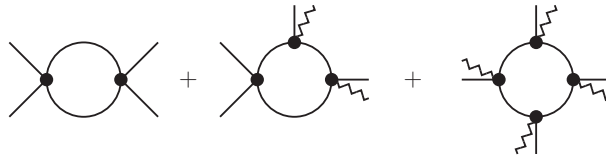
with Σ the classical self-energy (1.504). The $\mathcal{O}(1/l)$ correction to $-\mathcal{G}_{c,ij}^{-1}$ gives the one-loop self-energy. It can be diagrammatically represented as



Higher-order vertices are obtained by taking the functional derivative of $\Gamma^{(2)}$ wrt $\phi(x)$ or $\phi^*(x)$. The derivative of the (bare) 3-leg vertex $g\phi^{(*)}(x)$ gives the (bare) 4-leg vertex g . On the other hand, when acting on the classical propagator $\mathcal{G}_c = (\mathcal{G}_0^{-1} - \Sigma)^{-1}$, the functional derivative pulls out an external line attached to a 3-leg vertex. Thus we obtain diagrams of the type



(diagrams obtained by exchanging the external lines are not shown) for the one-loop correction to the 3-leg vertex $\Gamma^{(3)}$, and



for the 4-leg vertex.

A similar analysis can be carried out at order $1/l^2$. One finds that the effective action

$$\Gamma[\phi^*, \phi] = S[\phi^*, \phi] + \frac{1}{2l} \text{Tr} \ln \mathcal{G}_c + \frac{1}{l^2} \left(\text{diagram 1} + \text{diagram 2} \right), \quad (1.508)$$

to this order is given by the 1PI two-loop diagrams (see the calculation below). The two-loop order vertices are obtained from the functional derivatives of (1.508). For instance, the two-loop correction to the self-energy is given by the diagrams of figure 1.15. Note that the absence of one-particle reducible diagrams in the effective action is a necessary condition for the self-energy to be one-particle irreducible.

The effective action to two-loop order. Let us compute the effective action at order $1/l^2$. For simplicity, we consider a real field. The partition function reads

$$Z[J] = \int \mathcal{D}[\psi] \exp \left\{ -lS[\psi] + l \int dx J(x) \psi(x) \right\} \quad (1.509)$$

with the action

$$S[\psi] = -\frac{1}{2} \int dx dx' \psi(x) G_0^{-1}(x, x') \psi(x') + S_{\text{int}}[\psi]. \quad (1.510)$$

The saddle-point approximation gives

$$\left. \frac{\delta S[\psi]}{\delta \psi(x)} \right|_{\psi_c} = J(x). \quad (1.511)$$

Expanding about the classical field ψ_c , $\psi = \psi_c + \chi/\sqrt{l}$, we rewrite the action as

$$\begin{aligned} lS[\psi] - l \int dx J(x) \psi(x) &= lS[\psi_c] - l \int dx J(x) \psi_c(x) - \frac{1}{2} \int dx_1 dx_2 \chi(x_1) G_c^{-1}(x_1, x_2) \chi(x_2) \\ &\quad + \frac{1}{3! \sqrt{l}} \int dx_1 dx_2 dx_3 \chi(x_1) \chi(x_2) \chi(x_3) S_c^{(3)}(x_1, x_2, x_3) \\ &\quad + \frac{1}{4! l} \int dx_1 dx_2 dx_3 dx_4 \chi(x_1) \chi(x_2) \chi(x_3) \chi(x_4) S_c^{(4)}(x_1, x_2, x_3, x_4) \\ &\quad + \mathcal{O}(l^{-3/2}), \end{aligned} \quad (1.512)$$

where

$$S_c^{(n)}(x_1, \dots, x_n) = \left. \frac{\delta^{(n)} S[\psi]}{\delta \psi(x_1) \dots \delta \psi(x_n)} \right|_{\psi_c} \quad (1.513)$$

and $G_c^{-1}(x_1, x_2) = -S^{(2)}(x_1, x_2)$ is the inverse classical propagator. $Z[J]$ is calculated using the linked cluster theorem,

$$Z[J] = e^{-lS_c + l \int dx J(x) \psi_c(x)} [\det(-G_c^{-1})]^{-1/2} \exp \left\{ \sum \text{connected graphs} \right\}. \quad (1.514)$$

The $\mathcal{O}(1/l)$ contribution is given by the three two-loop diagrams shown after

(1.471), i.e.

$$\begin{aligned}
\ln Z[J] = & -lS_c + l \int dx J(x)\psi_c(x) - \frac{1}{2}\text{Tr} \ln(-G_c^{-1}) \\
& - \frac{1}{8l} \int dx_1 dx_2 dx_3 dx_4 G_c(x_1, x_2) G_c(x_3, x_4) S_c^{(4)}(x_1, x_2, x_3, x_4) \\
& - \frac{1}{l} \int dx_1 dx_2 dx_3 dy_1 dy_2 dy_3 S_c^{(3)}(x_1, x_2, x_3) S_c^{(3)}(y_1, y_2, y_3) \\
& \times \left[\frac{1}{12} G_c(x_1, y_1) G_c(x_2, y_2) G_c(x_3, y_3) \right. \\
& \left. + \frac{1}{8} G_c(x_1, x_2) G_c(y_1, y_2) G_c(x_3, y_3) \right] + \mathcal{O}(l^{-2}). \quad (1.515)
\end{aligned}$$

Equation (1.515) gives the thermodynamic potential to two-loop order.

We can now compute the effective action $\Gamma[\phi]$. We have

$$\begin{aligned}
\phi(x) &= \frac{1}{l} \frac{\delta \ln Z[J]}{\delta J(x)} \\
&= \psi_c(x) - \frac{\delta S_c}{\delta J(x)} + \int dx' J(x') \frac{\delta \psi_c(x')}{\delta J(x)} - \frac{1}{2l} \frac{\delta}{\delta J(x)} \text{Tr} \ln(-G_c^{-1}) + \mathcal{O}(l^{-2}) \\
&= \psi_c(x) - \frac{1}{2l} \frac{\delta}{\delta J(x)} \text{Tr} \ln(-G_c^{-1}) + \mathcal{O}(l^{-2}). \quad (1.516)
\end{aligned}$$

Using

$$\begin{aligned}
\frac{\delta}{\delta J(x)} \text{Tr} \ln(-G_c^{-1}) &= \frac{\delta}{\delta J(x)} \text{Tr} \ln S_c^{(2)} \\
&= \int dy \frac{\delta \psi_c(y)}{\delta J(x)} \text{Tr} \left[\frac{\delta S_c^{(2)}}{\delta \psi_c(y)} S_c^{(2)-1} \right], \quad (1.517)
\end{aligned}$$

with $\delta J(x)/\delta \psi_c(y) = -G_c^{-1}(x, y)$, we obtain

$$\begin{aligned}
\phi(x) &= \psi_c(x) - \frac{1}{2l} \int dy dy_1 dy_2 G_c(x, y) S_c^{(3)}(y, y_1, y_2) G_c(y_2, y_1) + \mathcal{O}(l^{-2}). \\
&= \psi_c(x) - \frac{1}{2l} \int dy dy_1 dy_2 G_c(x, y; \phi) S_c^{(3)}(y, y_1, y_2; \phi) G_c(y_2, y_1; \phi) + \mathcal{O}(l^{-2}), \quad (1.518)
\end{aligned}$$

where the last line is obtained by replacing G_c by $G_c(\phi) \equiv G_c[\phi]$ (and similarly $S_c^{(3)} \rightarrow S_c^{(3)}(\phi) \equiv S_c^{(3)}[\phi]$), which does not change the result to $\mathcal{O}(1/l)$. To obtain $\Gamma[\phi]$, we also need $J(x)$ to $\mathcal{O}(1/l)$,

$$\begin{aligned}
J(x) &= \frac{\delta S}{\delta \psi(x)} \Big|_{\phi} + \int dy \frac{\delta^{(2)} S}{\delta \psi(x) \delta \psi(y)} \Big|_{\phi} [\psi_c(y) - \phi(y)] + \mathcal{O}(l^{-2}) \\
&= \frac{\delta S}{\delta \phi(x)} - \frac{1}{2l} \int dy G_c^{-1}(x, y; \phi) \int dy_1 dy_2 dy_3 G_c(y, y_3; \phi) \\
&\quad \times S_c^{(3)}(y_1, y_2, y_3; \phi) G_c(y_2, y_1; \phi) + \mathcal{O}(l^{-2}) \\
&= \frac{\delta S}{\delta \phi(x)} - \frac{1}{2l} \int dy_1 dy_2 S_c^{(3)}(x, y_1, y_2; \phi) G_c(y_2, y_1; \phi) + \mathcal{O}(l^{-2}). \quad (1.519)
\end{aligned}$$

We deduce

$$\begin{aligned}\Gamma[\phi] &= -\frac{1}{l} \ln Z[J] + \int dx J(x) \phi(x) \\ &= S_c + \frac{1}{2l} \text{Tr} \ln(-G_c^{-1}(\phi)) + \int dx J(x) [\phi(x) - \psi_c(x)] \\ &\quad - (\text{2-loop diagrams}) + \mathcal{O}(l^{-3}),\end{aligned}\tag{1.520}$$

where the contribution of the three two-loop diagrams is given in (1.515) (up to a factor $1/l$). Using (1.518) we then find

$$\begin{aligned}\Gamma[\phi] &= S[\phi] + \frac{1}{2l} \text{Tr} \ln(-G_c^{-1}(\phi)) - (\text{2-loop diagrams}) \\ &\quad - \frac{1}{8l^2} \int dx_1 dx_2 dx_3 dy_1 dy_2 dy_3 G_c(x_3, y_3; \phi) G_c(x_1, x_2; \phi) G_c(y_1, y_2; \phi) \\ &\quad \times S_c^{(3)}(x_1, x_2, x_3; \phi) S_c^{(3)}(y_1, y_2, y_3; \phi) + \mathcal{O}(l^{-3}).\end{aligned}\tag{1.521}$$

The last term cancels the 2-loop diagram which is one-particle reducible and we finally obtain

$$\begin{aligned}\Gamma[\phi] &= S[\phi] + \frac{1}{2l} \text{Tr} \ln(-G_c^{-1}(\phi)) \\ &\quad + \frac{1}{8l^2} \int dx_1 dx_2 dx_3 dx_4 S_c^{(4)}(x_1, x_2, x_3, x_4; \phi) G_c(x_1, x_2; \phi) G_c(x_3, x_4; \phi) \\ &\quad + \frac{1}{12l^2} \int dx_1 dx_2 dx_3 dy_1 dy_2 dy_3 S_c^{(3)}(x_1, x_2, x_3; \phi) S_c^{(3)}(y_1, y_2, y_3; \phi) \\ &\quad \times G_c(x_1, y_1; \phi) G_c(x_2, y_2; \phi) G_c(x_3, y_3; \phi) + \mathcal{O}(l^{-3}),\end{aligned}\tag{1.522}$$

in agreement with (1.508).

1.8 Perturbation theory at zero temperature

In this section, we briefly discuss perturbation theory at zero temperature for systems having a fixed number of particles.⁵⁴ The advantage of this approach is that one works directly in real time and no analytic continuation is necessary, contrary to the finite temperature formalism in the grand canonical ensemble described in the previous sections. On the other hand, we shall see that the zero temperature approach suffers from some drawbacks and the finite temperature formalism is often preferable in practice.

We write the Hamiltonian of the N -particle system as $\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$, where \hat{H}_0 is the non-interacting Hamiltonian whose ground state $|\phi_0\rangle$ is known. If we let $|\phi_0\rangle$ evolve during a time T , we obtain

$$e^{-i\hat{H}T}|\phi_0\rangle = e^{-i\hat{H}T} \sum_n |n\rangle \langle n|\phi_0\rangle = \sum_n e^{-iE_n T} |n\rangle \langle n|\phi_0\rangle,\tag{1.523}$$

where $\{|n\rangle, E_n\}$ denotes an orthonormal basis of \hat{H} . Sending T to infinity with a (small) negative imaginary part, we project out the ground state $|0\rangle$ of \hat{H} ,

$$\lim_{T \rightarrow \infty(1-i\eta)} e^{-i\hat{H}T}|\phi_0\rangle = e^{-iE_0 T} |0\rangle \langle 0|\phi_0\rangle\tag{1.524}$$

⁵⁴A thorough discussion of perturbation theory at zero temperature can be found in chapter 3 of Ref. [9].

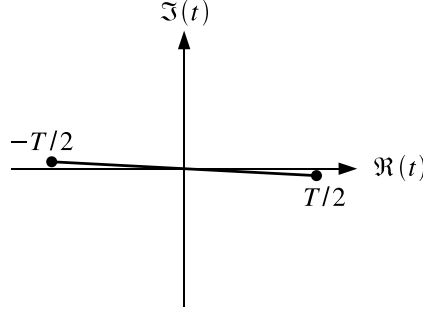


Figure 1.16: Contour in the complex t plane used in the definition of the functional integral at zero temperature.

($\eta = 0^+$), provided that $|0\rangle$ is non-degenerate and has a finite overlap with the non-interacting ground state $|\phi_0\rangle$. We deduce that the ground state energy of the interacting system can be obtained from

$$E_0 = \lim_{T \rightarrow \infty(1-i\eta)} \frac{i}{T} \ln \langle \phi_0 | e^{-i\hat{H}T} | \phi_0 \rangle. \quad (1.525)$$

Let us now consider the one-particle Green function⁵⁵

$$G(\alpha t, \alpha' t') = -i \langle 0 | T \hat{\psi}_\alpha(t) \hat{\psi}_{\alpha'}^\dagger(t') | 0 \rangle \quad (1.526)$$

defined in section 1.2.3 [Eq. (1.191)]. $\hat{\psi}_\alpha(t)$ and $\hat{\psi}_\alpha^\dagger(t)$ are operators in the Heisenberg picture and the index α labels the one-body states. Using

$$\begin{aligned} \lim_{T \rightarrow \infty(1-i\eta)} e^{-i\hat{H}\frac{T}{2}} |\phi_0\rangle &= e^{-iE_0\frac{T}{2}} |0\rangle \langle 0 | \phi_0\rangle, \\ \lim_{T \rightarrow \infty(1-i\eta)} \langle \phi_0 | e^{-i\hat{H}\frac{T}{2}} &= e^{-iE_0\frac{T}{2}} \langle \phi_0 | 0\rangle \langle 0 |, \end{aligned} \quad (1.527)$$

we obtain

$$iG(\alpha t, \alpha' t') = \lim_{T \rightarrow \infty(1-i\eta)} \frac{\langle \phi_0 | e^{-i\hat{H}\frac{T}{2}} (T \hat{\psi}_\alpha(t) \hat{\psi}_{\alpha'}^\dagger(t')) e^{-i\hat{H}\frac{T}{2}} | \phi_0 \rangle}{\langle \phi_0 | e^{-i\hat{H}T} | \phi_0 \rangle}. \quad (1.528)$$

We show below that both $\langle \phi_0 | e^{-i\hat{H}T} | \phi_0 \rangle$ and the Green function (1.528) can be expressed as a coherent-state functional integral. We shall consider a contour in the complex t plane which is slightly tilted wrt the real axis and extends from $-T/2$ and $T/2$ (Fig. 1.16). A time $t = \tilde{t}(1 - i\eta)$ on this contour can be parameterized by a real variable \tilde{t} . In practice, we will distinguish between t and \tilde{t} only when necessary.

1.8.1 Fermions

In the case of fermions, the ground state is a Slater determinant,

$$|\phi_0\rangle = \prod_{\alpha=1}^N \hat{\psi}_\alpha^\dagger |\text{vac}\rangle, \quad (1.529)$$

⁵⁵The time-ordering operator T in (1.526) should not be confused with the time T appearing e.g. in (1.525).

with the N lowest one-particle states occupied. Here we assume the one-body states $|\alpha\rangle$ to be labeled in order in increasing eigenvalues ϵ_α . We require $|\phi_0\rangle$ to be non-degenerate, which implies that there is a finite energy gap $\epsilon_{N+1} - \epsilon_N$ between the last occupied state and the first unoccupied state. We shift the energies ϵ_α such that

$$\begin{cases} \epsilon_\alpha < 0 & \text{for } \alpha \leq N, \\ \epsilon_\alpha > 0 & \text{for } \alpha > N, \end{cases} \quad (1.530)$$

and define the operators

$$\hat{\chi}_\alpha^\dagger = \begin{cases} \hat{\psi}_\alpha^\dagger & (\alpha > N), \\ \hat{\psi}_\alpha & (\alpha \leq N), \end{cases} \quad \hat{\chi}_\alpha = \begin{cases} \hat{\psi}_\alpha & (\alpha > N), \\ \hat{\psi}_\alpha^\dagger & (\alpha \leq N). \end{cases} \quad (1.531)$$

$\hat{\chi}_\alpha^\dagger$ creates an elementary excitation wrt $|\phi_0\rangle$, i.e. a particle for $\alpha > N$ and a hole for $\alpha \leq N$. Since $\hat{\chi}_\alpha|\phi_0\rangle = 0$ for any α , $|\phi_0\rangle$ is the vacuum state wrt the excitations of the $\hat{\chi}$ operator. The Green function (1.526) is expressed as

$$G(\alpha t, \alpha' t') = \begin{cases} -i\langle 0|T\hat{\chi}_\alpha(t)\hat{\chi}_{\alpha'}^\dagger(t')|0\rangle & \text{if } \alpha > N, \\ i\langle 0|T\hat{\chi}_{\alpha'}(t')\hat{\chi}_\alpha^\dagger(t)|0\rangle & \text{if } \alpha \leq N. \end{cases} \quad (1.532)$$

Coherent-state functional integral

We can now construct coherent states by associating to $\hat{\chi}_\alpha$ and $\hat{\chi}_\alpha^\dagger$ a pair of complex conjugate Grassmann variables ψ_α and ψ_α^* (Sec. 1.3.3). Since $|\phi_0\rangle$ is the vacuum state wrt to the ψ field, it can be seen formally as the coherent state $|\psi\rangle$ with $\psi_\alpha = 0$. Dividing the time T into $M = \beta/\epsilon$ steps and inserting $M - 1$ the closure relation (1.203) or (1.240), one obtains

$$\begin{aligned} \langle \phi_0|e^{-i\hat{H}T}|\phi_0\rangle &= \int \prod_{k=1}^{M-1} d(\psi_k^*, \psi_k) e^{-\sum_{k=1}^{M-1} \sum_\alpha |\psi_{k,\alpha}|^2} \prod_{k=1}^M \langle \psi_k|e^{-i\epsilon\hat{H}}|\psi_{k-1}\rangle \\ &= \int \prod_{k=1}^{M-1} d(\psi_k^*, \psi_k) e^{-\sum_{k=1}^M [\sum_\alpha \psi_{k,\alpha}^* (\psi_{k,\alpha} - \psi_{k-1,\alpha}) + i\epsilon H(\psi_{k,\alpha}^*, \psi_{k,\alpha})]}, \end{aligned} \quad (1.533)$$

with $\psi_{0,\alpha} = \psi_{M,\alpha}^* = 0$. The integration measure $d(\psi_\alpha^*, \psi_\alpha)$ is defined by (1.248) and we assume the Hamiltonian $\hat{H} = H(\hat{\chi}_\alpha^\dagger, \hat{\chi}_\alpha)$ to be normal ordered. In the continuum-time limit ($M \rightarrow \infty$), we may write

$$\langle \phi_0|e^{-i\hat{H}T}|\phi_0\rangle = \int \mathcal{D}[\psi^*, \psi] e^{iS[\psi^*, \psi]} \quad (1.534)$$

with the action

$$S[\psi^*, \psi] = \int_{-T/2}^{T/2} dt \left[\sum_\alpha \psi_\alpha^*(t) i\partial_t \psi_\alpha(t) - H(\psi_\alpha^*(t), \psi_\alpha(t)) \right], \quad (1.535)$$

and the boundary conditions $\psi_\alpha(-T/2) = \psi_\alpha^*(T/2) = 0$. Except for the boundary conditions at $\pm T/2$, the real-time action (1.535) can be deduced from the Euclidean action (1.259) by a Wick rotation $\tau \rightarrow it$ and $-S_E \rightarrow iS$.

Similarly, we find

$$\langle \phi_0 | e^{-i\hat{H}\frac{T}{2}} (T\hat{\chi}_\alpha(t)\hat{\chi}_{\alpha'}^\dagger(t')) e^{-i\hat{H}\frac{T}{2}} | \phi_0 \rangle = \int \prod_{k=1}^{M-1} d(\psi_k^*, \psi_k) \psi_{k_1, \alpha} \psi_{k_2, \alpha'}^* e^{iS(\psi_k^*, \psi_k)}, \quad (1.536)$$

where the action $S(\psi_k^*, \psi_k)$ is defined by (1.533). $t_{k_1} = -T/2 + k_1\epsilon$ and $t_{k_2} = -T/2 + k_2\epsilon$ are the discrete times corresponding to t and t' , respectively. Equation (1.536) is analog to (1.264) and can be derived in the same way. In the continuum-time limit, we therefore obtain

$$\langle 0 | T \hat{\chi}_\alpha(t) \hat{\chi}_{\alpha'}^\dagger(t') | 0 \rangle = \lim_{T \rightarrow \infty(1-i\eta)} \frac{\int \mathcal{D}[\psi^*, \psi] \psi_\alpha(t) \psi_{\alpha'}^*(t') e^{iS[\psi^*, \psi]}}{\int \mathcal{D}[\psi^*, \psi] e^{iS[\psi^*, \psi]}} \quad (1.537)$$

with the boundary conditions $\psi_\alpha(-T/2) = \psi_\alpha^*(T/2) = 0$. The Green function $G(\alpha t, \alpha' t')$ can be deduced from (1.532) and (1.537).

Non-interacting fermions

Assuming that the non-interacting Hamiltonian is diagonal in the one-body state basis $\{|\alpha\rangle\}$,

$$\hat{H}_0 = \sum_{\alpha=1}^N \epsilon_\alpha \hat{\chi}_\alpha \hat{\chi}_\alpha^\dagger + \sum_{\alpha>N} \epsilon_\alpha \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha = \sum_{\alpha=1}^N \epsilon_\alpha (1 - \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha) + \sum_{\alpha>N} \epsilon_\alpha \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha, \quad (1.538)$$

which gives the action

$$\begin{aligned} iS_0 &= -iT \sum_{\alpha=1}^N \epsilon_\alpha - \sum_{k=1}^{M-1} \sum_{\alpha} \left[\psi_{k, \alpha}^* (\psi_{k, \alpha} - \psi_{k-1, \alpha}) + i \frac{T}{M} |\epsilon_\alpha| \psi_{k, \alpha}^* \psi_{k-1, \alpha} \right] \\ &\equiv -iT \sum_{\alpha=1}^N \epsilon_\alpha - \sum_{\alpha} \sum_{k, k'=1}^{M-1} \psi_{k, \alpha}^* S_{k, k'}^{(\alpha)} \psi_{k', \alpha}, \end{aligned} \quad (1.539)$$

where $S^{(\alpha)}$ is the $(M-1) \times (M-1)$ matrix

$$S^{(\alpha)} = \begin{pmatrix} 1 & 0 & \cdots & \cdots & 0 & 0 \\ -a & 1 & 0 & & & 0 \\ 0 & -a & 1 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & 1 & \ddots & \vdots \\ \vdots & & \ddots & -a & 1 & 0 \\ 0 & \cdots & \cdots & 0 & -a & 1 \end{pmatrix} \quad (1.540)$$

with $a = 1 - i \frac{T}{M} |\epsilon_\alpha|$. Since $\det S^{(\alpha)} = 1$, we find

$$\langle \phi_0 | e^{-i\hat{H}_0 T} | \phi_0 \rangle = e^{-iT \sum_{\alpha=1}^N \epsilon_\alpha} \prod_{\alpha} \det S^{(\alpha)} = e^{-iT \sum_{\alpha=1}^N \epsilon_\alpha} \quad (1.541)$$

so that the non-interacting ground state energy is $E_0^{(0)} = \sum_{\alpha=1}^N \epsilon_{\alpha}$ [Eq. (1.525)]. From the inverse matrix

$$S^{(\alpha)-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & \cdots & 0 \\ a & 1 & 0 & \ddots & & \vdots \\ a^2 & a & 1 & 0 & \ddots & \vdots \\ \vdots & \ddots & a & 1 & 0 & 0 \\ \vdots & & \ddots & a & 1 & 0 \\ a^{M-2} & \cdots & \cdots & a^2 & a & 1 \end{pmatrix}, \quad (1.542)$$

we deduce

$$\langle \phi_0 | T \hat{\chi}_{\alpha}(t) \hat{\chi}_{\alpha'}^{\dagger}(t') | \phi_0 \rangle = \lim_{\substack{M \rightarrow \infty \\ T \rightarrow \infty(1-i\eta)}} S_{k,k'}^{(\alpha)-1} = \lim_{\substack{M \rightarrow \infty \\ T \rightarrow \infty(1-i\eta)}} \begin{cases} 0 & \text{if } k < k', \\ a^{k-k'} & \text{if } k \geq k', \end{cases} \quad (1.543)$$

where $t_k = -T/2 + kT/M$ and $t_{k'} = -T/2 + k'T/M$ are the discrete times corresponding to t and t' , respectively. Making use of (1.532) and

$$\lim_{M \rightarrow \infty} a^{k-k'} = \lim_{M \rightarrow \infty} \left(1 - i \frac{T}{M} |\epsilon_{\alpha}| \right)^{(t_k - t_{k'}) \frac{M}{T}} = e^{-i|\epsilon_{\alpha}|(t-t')}, \quad (1.544)$$

we finally obtain

$$iG_0(\alpha, t) = e^{-i\epsilon_{\alpha}t} [(1 - n_{\alpha})\Theta(t) - n_{\alpha}\Theta(-t)], \quad (1.545)$$

where

$$n_{\alpha} = \begin{cases} 1 & \text{if } \alpha \leq N, \\ 0 & \text{if } \alpha > N, \end{cases} \quad (1.546)$$

is the occupation of the one-body state $|\alpha\rangle$ in the non-interacting ground state $|\phi_0\rangle$.

So far we have ignored the fact that the time $t = \tilde{t}(1 - i\eta)$ (\tilde{t} real) contains a small imaginary part (Fig. 1.16). A more correct expression of the Green function would then be

$$iG_0(\alpha, \tilde{t}) = e^{-i\epsilon_{\alpha}\tilde{t}(1-i\eta)} [(1 - n_{\alpha})\Theta(\tilde{t}) - n_{\alpha}\Theta(-\tilde{t})]. \quad (1.547)$$

In Fourier space, this yields

$$\begin{aligned} G_0(\alpha, \omega) &= \int_{-\infty}^{\infty} d\tilde{t} e^{i\omega\tilde{t}} G_0(\alpha, \tilde{t}) \\ &= \frac{1 - n_{\alpha}}{\omega - \epsilon_{\alpha}(1 - i\eta)} e^{i\tilde{t}[\omega - \epsilon_{\alpha}(1 - i\eta)]} \Big|_0^{\infty} - \frac{n_{\alpha}}{\omega - \epsilon_{\alpha}(1 - i\eta)} e^{i\tilde{t}[\omega - \epsilon_{\alpha}(1 - i\eta)]} \Big|_{-\infty}^0. \end{aligned} \quad (1.548)$$

Since $\epsilon_{\alpha} < 0$ for $n_{\alpha} = 1$ and $\epsilon_{\alpha} > 0$ for $n_{\alpha} = 0$, the infinitesimal $\eta = 0^+$ ensures the convergence of the time integral,

$$G_0(\alpha, \omega) = \frac{n_{\alpha}}{\omega - \epsilon_{\alpha} - i\eta} + \frac{1 - n_{\alpha}}{\omega - \epsilon_{\alpha} + i\eta}. \quad (1.549)$$

Perturbation theory

Perturbation theory is derived by expanding e^{iS} in powers of the interacting action

$$S_{\text{int}}[\psi^*, \psi] = - \int_{-T/2}^{T/2} dt H_{\text{int}}(\psi_\alpha^*(t), \psi_\alpha(t)) \quad (1.550)$$

For example, to obtain the ground state energy using (1.525), one uses

$$\begin{aligned} \langle \phi_0 | e^{-i\hat{H}T} | \phi_0 \rangle &= \int \mathcal{D}[\psi^*, \psi] e^{iS_0[\psi^*, \psi] + iS_{\text{int}}[\psi^*, \psi]} \\ &= \int \mathcal{D}[\psi^*, \psi] e^{iS_0[\psi^*, \psi]} \sum_{n=0}^{\infty} \frac{i^n}{n!} (S_{\text{int}}[\psi^*, \psi])^n. \end{aligned} \quad (1.551)$$

The average value

$$\langle (S_{\text{int}}[\psi^*, \psi])^n \rangle_0 = \frac{\int \mathcal{D}[\psi^*, \psi] (S_{\text{int}}[\psi^*, \psi])^n e^{iS_0[\psi^*, \psi]}}{\int \mathcal{D}[\psi^*, \psi] e^{iS_0[\psi^*, \psi]}} \quad (1.552)$$

can be evaluated using Wick's theorem and represented by Feynman diagrams. The diagrammatic rules follow straightforwardly from those of the finite-temperature formalism. The linked cluster theorem states that the ground state energy

$$\begin{aligned} E_0 &= \lim_{T \rightarrow \infty(1-i\eta)} \frac{i}{T} \ln \langle \phi_0 | e^{-i\hat{H}T} | \phi_0 \rangle \\ &= E_0^{(0)} + \lim_{T \rightarrow \infty(1-i\eta)} \frac{i}{T} \sum \text{connected graphs} \end{aligned} \quad (1.553)$$

is given by the sum of the connected diagrams. More generally, most results derived in sections 1.4-1.6 carry over to the zero-temperature formalism.

1.8.2 Bosons

The ground state of a non-interacting system of N bosons is a Bose-Einstein condensate,

$$|\phi_0(N)\rangle = \frac{1}{\sqrt{N!}} [\hat{\psi}^\dagger(\mathbf{k}=0)]^N |\text{vac}\rangle, \quad (1.554)$$

where all the particles occupy the $\mathbf{k}=0$ one-body state. For simplicity, we consider spin-zero bosons and assume the system to be translation invariant. Since

$$\begin{aligned} \hat{\psi}(\mathbf{k}=0) |\phi_0(N)\rangle &= \sqrt{N} |\phi_0(N-1)\rangle, \\ \hat{\psi}^\dagger(\mathbf{k}=0) |\phi_0(N)\rangle &= \sqrt{N+1} |\phi_0(N+1)\rangle, \end{aligned} \quad (1.555)$$

neither $\hat{\psi}(\mathbf{k}=0)$ nor $\hat{\psi}^\dagger(\mathbf{k}=0)$ annihilates the ground state $|\phi_0(N)\rangle$, and it is not possible to separate the operators between creation and annihilation parts as in the fermion case [Eq. (1.531)].

Let us consider the rescaled $\mathbf{k} = 0$ operators

$$\begin{aligned}\hat{\xi}_0 &= \frac{1}{\sqrt{V}} \hat{\psi}(\mathbf{k} = 0) = \frac{1}{V} \int d^d r \hat{\psi}(\mathbf{r}), \\ \hat{\xi}_0^\dagger &= \frac{1}{\sqrt{V}} \hat{\psi}^\dagger(\mathbf{k} = 0) = \frac{1}{V} \int d^d r \hat{\psi}^\dagger(\mathbf{r}).\end{aligned}\tag{1.556}$$

Their commutator

$$[\hat{\xi}_0, \hat{\xi}_0^\dagger] = \frac{1}{V}\tag{1.557}$$

vanishes in the thermodynamic limit, while they yield a finite factor when acting on $|\phi_0(N)\rangle$,

$$\begin{aligned}\hat{\xi}_0 |\phi_0(N)\rangle &= \left(\frac{N}{V}\right)^{1/2} |\phi_0(N-1)\rangle \simeq \left(\frac{N}{V}\right)^{1/2} |\phi_0(N)\rangle, \\ \hat{\xi}_0^\dagger |\phi_0(N)\rangle &= \left(\frac{N+1}{V}\right)^{1/2} |\phi_0(N+1)\rangle \simeq \left(\frac{N}{V}\right)^{1/2} |\phi_0(N)\rangle.\end{aligned}\tag{1.558}$$

They can therefore be replaced by c-numbers as long as we consider only states where a finite fraction of the particles occupies the $\mathbf{k} = 0$ one-body state. This leads us to rewrite the boson operator as

$$\begin{aligned}\hat{\psi}(\mathbf{r}) &= \xi_0 + \frac{1}{\sqrt{V}} \sum_{\mathbf{k} \neq 0} e^{i\mathbf{k} \cdot \mathbf{r}} \hat{\psi}(\mathbf{k}) \equiv \xi_0 + \hat{\chi}(\mathbf{r}), \\ \hat{\psi}^\dagger(\mathbf{r}) &= \xi_0^* + \frac{1}{\sqrt{V}} \sum_{\mathbf{k} \neq 0} e^{-i\mathbf{k} \cdot \mathbf{r}} \hat{\psi}^\dagger(\mathbf{k}) \equiv \xi_0^* + \hat{\chi}^\dagger(\mathbf{r}).\end{aligned}\tag{1.559}$$

Since $\hat{\chi}(\mathbf{r})$ annihilates the non-interacting ground state $|\phi_0(N)\rangle$, we can proceed as in the fermion case and write $\langle \phi_0(N) | e^{-iHT} | \phi_0(N) \rangle$ as a functional integral over a complex bosonic field with the action

$$S[\psi^*, \psi] = \int_{-T/2}^{T/2} dt \left[\int d^d r \psi^*(\mathbf{r}, t) i \partial_t \psi(\mathbf{r}, t) - H(\psi^*(\mathbf{r}, t), \psi(\mathbf{r}, t)) \right],\tag{1.560}$$

where $\psi(\mathbf{r}, -T/2) = \psi^*(\mathbf{r}, T/2) = 0$. Again, we see that the real-time action (1.560) can be deduced from the Euclidean action (1.259) by a Wick rotation $\tau = it$. As in section 1.7.2, the interaction vertices coming from the interacting Hamiltonian are of four different types depending on the number of condensate lines attached to them.

Considering $\hat{\xi}_0$ and $\hat{\xi}_0^\dagger$ as c-numbers breaks the (global) gauge invariance, i.e. the invariance of the Hamiltonian under the transformation $\hat{\psi}(\mathbf{r}) \rightarrow e^{i\Lambda} \hat{\psi}(\mathbf{r})$. As a result the total number of particles is not conserved, $[\hat{N}, \hat{H}] \neq 0$, and the canonical ensemble cannot be used. Instead, one should work in the grand canonical ensemble where the Hamiltonian is replaced by $\hat{H} - \mu \hat{N}$, with the chemical potential μ chosen such that $\langle 0 | \hat{N} | 0 \rangle = N$. In the interacting ground state, not all the particles are in the $\mathbf{k} = 0$ one-body state, and the average value

$$\langle 0 | \hat{\xi}_0^\dagger \hat{\xi}_0 | 0 \rangle = \frac{N_0}{V} = n_0\tag{1.561}$$

is less than the total density N/V . As long as the condensate density n_0 remains finite, the replacement of $\hat{\xi}_0$ and $\hat{\xi}_0^\dagger$ by c-numbers ξ_0 and ξ_0^* (with $|\xi_0| = \sqrt{n_0}$) is permissible. To determine the condensate density n_0 , we require that

$$\frac{\partial}{\partial n_0} \langle 0 | \hat{H} - \mu \hat{N} | 0 \rangle \Big|_\mu = 0, \quad (1.562)$$

which is an implicit equation for $n_0(\mu)$.

1.8.3 The zero-temperature limit

We have now two different ways to compute perturbatively the ground state energy or a correlation function. One can either use the $T = 0$ perturbation theory or consider the $T \rightarrow 0$ limit of the finite-temperature formalism discussed in sections 1.4-1.6. While one would naively expect these two approaches to give always the same result, this is in fact not the case. In the zero-temperature formalism, the interacting ground state $|0\rangle$ is obtained from (1.525) provided that $|0\rangle$ and $|\phi_0\rangle$ are not orthogonal. In some cases, $e^{-i\hat{H}T}|\phi_0\rangle$ is trapped in a given symmetry space selected by $|\phi_0\rangle$ and produces the lowest energy eigenstate in that space. In contrast, the finite-temperature theory obtains the state of the system from a statistical average (over a certain ensemble) which has access to all possible symmetries. In principle, it is always possible to use the zero-temperature theory, provided that one chooses a Hamiltonian \hat{H}_0 with a ground state $|\phi_0\rangle$ which has the right symmetries. In practice however, it is often preferable to use the (Euclidean) finite-temperature even when one is interested only in the $T = 0$ limit.

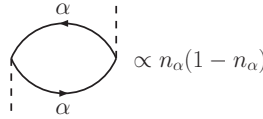
From a technical point of view, there are two differences between the zero- and finite-temperature formalisms:

1. In the finite-temperature formalism, the chemical potential μ should be adjusted so that $N = -\partial\Omega/\partial\mu$. In general, μ differs from the chemical potential μ_0 of the non-interacting system defined by $N = -\partial\Omega_0/\partial\mu_0$. Thus the correction

$$E_0 - E_0^{(0)} = \lim_{T \rightarrow 0} [\Omega - \Omega_0 + (\mu - \mu_0)N] \quad (1.563)$$

to the ground state energy is determined not only by $\Omega - \Omega_0$ (i.e. the vacuum fluctuation diagrams) but also by the variation $\mu - \mu_0$ of the chemical potential. In the zero-temperature theory, $E_0 - E_0^{(0)}$ is directly given by the perturbation expansion of $\langle \phi_0(N) | e^{-i\hat{H}T} | \phi_0(N) \rangle$, i.e. by the vacuum fluctuation diagrams [Eq. (1.553)].

2. The finite-temperature perturbation theory yields “anomalous” diagrams which include parts such as



where a particle and a hole propagate in the same one-body state α . Since the one-body state α is either empty ($n_\alpha = 0$) or occupied ($n_\alpha = 1$) in the zero-temperature non-interacting ground state, the anomalous diagrams

vanish at $T = 0$. On the contrary, $\lim_{T \rightarrow 0} n_\alpha(1 - n_\alpha)$ does not necessarily vanish in the finite-temperature formalism.⁵⁶

For the zero- and finite-temperature perturbation theories to agree, the differences (1) and (2) must cancel.

1.9 Quantization of the electromagnetic field

In this section, we discuss the functional integral describing charged particles coupled to the electromagnetic field. We start by briefly reviewing the Lagrangian and Hamiltonian formalism of classical electromagnetism. The difficulties due to the redundancy of degrees of freedom are resolved by using the Coulomb gauge. We then discuss the canonical quantization in the Coulomb gauge and express the partition function of the coupled system matter-field as a functional integral.

1.9.1 Lagrangian and Hamiltonian formalism

The standard Lagrangian of classical electrodynamics reads

$$L = L'_m + \frac{\epsilon_0}{2} \int d^3r \left\{ [\nabla\phi(\mathbf{r}, t) + \partial_t \mathbf{A}(\mathbf{r}, t)]^2 - c_l^2 [\nabla \times \mathbf{A}(\mathbf{r}, t)]^2 \right\} - \int d^3r [\phi(\mathbf{r}, t)\rho(\mathbf{r}, t) - \mathbf{J}(\mathbf{r}, t) \cdot \mathbf{A}(\mathbf{r}, t)] \quad (1.564)$$

(c_l denotes the velocity of light), where $L'_m = (m/2) \sum_i \dot{\mathbf{r}}_i^2$ is the Lagrangian of the matter in the absence of electromagnetic interactions with \mathbf{r}_i and $\dot{\mathbf{r}}_i$ the position and velocity of the i th particle. The electric and magnetic fields can be expressed as a function of the electromagnetic potentials,

$$\begin{aligned} \mathbf{E}(\mathbf{r}, t) &= -\nabla\phi(\mathbf{r}, t) - \partial_t \mathbf{A}(\mathbf{r}, t), \\ \mathbf{B}(\mathbf{r}, t) &= \nabla \times \mathbf{A}(\mathbf{r}, t). \end{aligned} \quad (1.565)$$

The field-matter coupling involves the charge and current densities

$$\begin{aligned} \rho(\mathbf{r}, t) &= e \sum_i \delta(\mathbf{r} - \mathbf{r}_i(t)), \\ \mathbf{J}(\mathbf{r}, t) &= e \sum_i \dot{\mathbf{r}}_i \delta(\mathbf{r} - \mathbf{r}_i(t)) \end{aligned} \quad (1.566)$$

(e denotes the charge of the particles). The Euler-Lagrange equations deduced from (1.564) reproduce Maxwell equations (Appendix 1.A).

It is tempting to quantize the theory in the usual way, i.e. by introducing the momenta \mathbf{p}_i of the particles and the canonical conjugates $(\Pi_0, \mathbf{\Pi})$ to the electromagnetic potential (ϕ, \mathbf{A}) , and assuming the usual commutation rules between conjugate variables. However, since $\dot{\phi} = \partial_t \phi$ does not appear in the Lagrangian, $\Pi_0 = 0$. One should therefore first eliminate the scalar potential by expressing it as a function of the other dynamical variables to obtain a reduced Lagrangian which is a function of

⁵⁶For example, $\beta n_F(\xi_\alpha)[1 - n_F(\xi_\alpha)] = -\frac{\partial n_F(\xi_\alpha)}{\partial \xi_\alpha} \rightarrow \delta(\xi_\alpha)$ for $T \rightarrow 0$.

the vector potential \mathbf{A} and its time derivative $\dot{\mathbf{A}}$, as well as the positions and velocities of the particles. Before quantizing, one should also get rid of the arbitrariness of \mathbf{A} which follows from gauge invariance. A gauge transformation

$$\begin{aligned}\mathbf{A}'(\mathbf{r}, t) &= \mathbf{A}(\mathbf{r}, t) + \nabla \Lambda(\mathbf{r}, t), \\ \phi'(\mathbf{r}, t) &= \phi(\mathbf{r}, t) - \partial_t \Lambda(\mathbf{r}, t)\end{aligned}\tag{1.567}$$

does not change the electromagnetic field and therefore leaves the Maxwell equations invariant. By choosing a particular gauge, we fix the longitudinal component \mathbf{A}_{\parallel} of the vector potential, which is otherwise arbitrary. Once this is done, we are left with four degrees of freedom of the field at each position in space, the two components of the transverse vector potential \mathbf{A}_{\perp} and their time derivatives. Since the longitudinal components \mathbf{E}_{\parallel} and \mathbf{B}_{\parallel} of the field are fixed by the Maxwell equations $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$ and $\nabla \cdot \mathbf{B} = 0$, they are not true dynamical variables and we indeed expect any description of the electromagnetic field to contain four independent variables.

Using $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$, we obtain $\nabla^2 \phi + \nabla \cdot \dot{\mathbf{A}}_{\parallel} = -\rho/\epsilon_0$, i.e.

$$\phi(\mathbf{k}, t) = \frac{1}{\mathbf{k}^2} \left[i\mathbf{k} \cdot \dot{\mathbf{A}}_{\parallel}(\mathbf{k}, t) + \frac{1}{\epsilon_0} \rho(\mathbf{k}, t) \right],\tag{1.568}$$

and the electric field is given by

$$\begin{aligned}\mathbf{E}_{\parallel}(\mathbf{k}, t) &= -i\mathbf{k} \frac{\rho(\mathbf{k}, t)}{\epsilon_0 \mathbf{k}^2}, \\ \mathbf{E}_{\perp}(\mathbf{k}, t) &= -\dot{\mathbf{A}}_{\perp}(\mathbf{k}, t).\end{aligned}\tag{1.569}$$

In the following, we shall work in the Coulomb gauge where \mathbf{A}_{\parallel} vanishes,

$$\nabla \cdot \mathbf{A}(\mathbf{r}, t) = 0 \quad (\text{Coulomb gauge}),\tag{1.570}$$

the Lagrangian being given by

$$\begin{aligned}L = L'_m + L_c + \int d^3r \left\{ \frac{\epsilon_0}{2} \left[(\partial_t \mathbf{A}_{\perp}(\mathbf{r}, t))^2 - c_l^2 (\nabla \times \mathbf{A}_{\perp}(\mathbf{r}, t))^2 \right] \right. \\ \left. + \mathbf{J}_{\perp}(\mathbf{r}, t) \cdot \mathbf{A}_{\perp}(\mathbf{r}, t) \right\},\end{aligned}\tag{1.571}$$

where⁵⁷

$$L_c = -\frac{1}{2} \sum_{\mathbf{k}} \frac{\rho(-\mathbf{k}, t) \rho(\mathbf{k}, t)}{\epsilon_0 \mathbf{k}^2} = -\frac{1}{2} \int d^3r d^3r' \frac{\rho(\mathbf{r}, t) \rho(\mathbf{r}', t)}{4\pi \epsilon_0 |\mathbf{r} - \mathbf{r}'|}\tag{1.572}$$

is (minus) the Coulomb energy of the charge distribution $\rho(\mathbf{r}, t)$.

Let us discuss in more detail the role of the longitudinal component of the vector potential. Equation (1.568) enables to rewrite the Lagrangian as

$$\begin{aligned}L = L'_m + L_c + \frac{\epsilon_0}{2} \sum_{\mathbf{k}} [\dot{\mathbf{A}}_{\perp}(-\mathbf{k}, t) \cdot \dot{\mathbf{A}}_{\perp}(\mathbf{k}, t) - c_l^2 \mathbf{A}_{\perp}(-\mathbf{k}, t) \cdot \mathbf{A}_{\perp}(\mathbf{k}, t)] \\ + \sum_{\mathbf{k}} [\mathbf{J}_{\perp}(-\mathbf{k}, t) \cdot \mathbf{A}_{\perp}(\mathbf{k}, t) + \mathbf{J}_{\parallel}(-\mathbf{k}, t) \cdot \mathbf{A}_{\parallel}(\mathbf{k}, t) - i\rho(-\mathbf{k}, t) \frac{\mathbf{k}}{\mathbf{k}^2} \cdot \dot{\mathbf{A}}_{\parallel}(\mathbf{k}, t)].\end{aligned}\tag{1.573}$$

⁵⁷The Fourier transformed variables are defined as $\rho(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \rho(\mathbf{k}, t)$, etc.

The Lagrange equation for \mathbf{A}_{\parallel} ,

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\mathbf{A}}_{\parallel}(\mathbf{k}, t)} = \frac{\partial L}{\partial \mathbf{A}_{\parallel}(\mathbf{k}, t)}, \quad (1.574)$$

gives

$$i \frac{\mathbf{k}}{k^2} \dot{\rho}(\mathbf{k}, t) = \mathbf{J}_{\parallel}(\mathbf{k}, t), \quad \text{i.e.} \quad \partial_t \rho(\mathbf{r}, t) + \nabla \cdot \mathbf{J}_{\parallel}(\mathbf{r}, t) = 0. \quad (1.575)$$

This is a continuity equation, not an equation of motion for \mathbf{A}_{\parallel} . Using (1.575), we find

$$\begin{aligned} \sum_{\mathbf{k}} \left[\mathbf{J}_{\parallel}(-\mathbf{k}, t) \cdot \mathbf{A}_{\parallel}(\mathbf{k}, t) - i \rho(-\mathbf{k}, t) \frac{\mathbf{k}}{k^2} \cdot \dot{\mathbf{A}}_{\parallel}(\mathbf{k}, t) \right] \\ = \sum_{\mathbf{k}} \frac{1}{k^2} [\mathbf{k} \cdot \mathbf{J}_{\parallel}(-\mathbf{k}, t) \mathbf{k} \cdot \mathbf{A}_{\parallel}(\mathbf{k}, t) - i \rho(-\mathbf{k}, t) \mathbf{k} \cdot \dot{\mathbf{A}}_{\parallel}(\mathbf{k}, t)] \\ = \sum_{\mathbf{k}} \frac{1}{k^2} [-\dot{\rho}(-\mathbf{k}, t) i \mathbf{k} \cdot \mathbf{A}_{\parallel}(\mathbf{k}, t) - \rho(-\mathbf{k}, t) i \mathbf{k} \cdot \dot{\mathbf{A}}_{\parallel}(\mathbf{k}, t)] \\ = -i \frac{d}{dt} \sum_{\mathbf{k}} \frac{1}{k^2} \rho(-\mathbf{k}, t) \mathbf{k} \cdot \mathbf{A}_{\parallel}(\mathbf{k}, t), \end{aligned} \quad (1.576)$$

and the Lagrangian becomes

$$\begin{aligned} L = L'_m + L_c + \frac{\epsilon_0}{2} \sum_{\mathbf{k}} [\dot{\mathbf{A}}_{\perp}(-\mathbf{k}, t) \cdot \dot{\mathbf{A}}_{\perp}(\mathbf{k}, t) - c_i^2 \mathbf{A}_{\perp}(-\mathbf{k}, t) \cdot \mathbf{A}_{\perp}(\mathbf{k}, t)] \\ + \sum_{\mathbf{k}} \mathbf{J}_{\perp}(-\mathbf{k}, t) \cdot \mathbf{A}_{\perp}(\mathbf{k}, t) - i \frac{d}{dt} \sum_{\mathbf{k}} \frac{1}{k^2} \rho(-\mathbf{k}, t) \mathbf{k} \cdot \mathbf{A}_{\parallel}(\mathbf{k}, t). \end{aligned} \quad (1.577)$$

The last term being a total derivative, it does not affect the equations of motion and can therefore be removed from the Lagrangian which then becomes independent of \mathbf{A}_{\parallel} . Thus the longitudinal component of the vector potential does not affect the dynamics of the system and is not a true dynamical variable. Of course, the possibility to arbitrarily choose \mathbf{A}_{\parallel} is nothing but a consequence of gauge invariance.

The Hamiltonian is obtained by introducing the momenta of the particles,

$$\mathbf{p}_i = \frac{\partial L}{\partial \dot{\mathbf{r}}_i} = m \dot{\mathbf{r}}_i + e \mathbf{A}_{\perp}(\mathbf{r}_i, t), \quad (1.578)$$

and the momentum conjugate to \mathbf{A}_{\perp} ,

$$\mathbf{\Pi}_{\perp}(\mathbf{r}, t) = \frac{\delta L}{\delta \dot{\mathbf{A}}_{\perp}(\mathbf{r}, t)}. \quad (1.579)$$

Since $\mathbf{A}_{\perp}(\mathbf{r}, t)$ is transverse, we cannot vary its components independently. We should therefore obtain $\mathbf{\Pi}_{\perp}$ in reciprocal space, using

$$\begin{aligned} \frac{\epsilon_0}{2} \int d^3r \dot{\mathbf{A}}_{\perp}(\mathbf{r}, t)^2 &= \frac{\epsilon_0}{2} \sum_{\mathbf{k}} \dot{\mathbf{A}}_{\perp}(-\mathbf{k}, t) \cdot \dot{\mathbf{A}}_{\perp}(\mathbf{k}, t) \\ &= \frac{\epsilon_0}{2} \sum_{\substack{\mathbf{k} \\ \epsilon = \epsilon_1, \epsilon_2}} \dot{A}_{\perp \epsilon}(-\mathbf{k}, t) \dot{A}_{\perp \epsilon}(\mathbf{k}, t), \end{aligned} \quad (1.580)$$

where $A_{\perp\epsilon_1}$ and $A_{\perp\epsilon_2}$ denote the two independent components of \mathbf{A}_{\perp} ,

$$\mathbf{A}_{\perp}(\mathbf{k}, t) = A_{\perp\epsilon_1}(\mathbf{k}, t)\epsilon_1 + A_{\perp\epsilon_2}(\mathbf{k}, t)\epsilon_2, \quad (1.581)$$

with $\epsilon_1, \epsilon_2, \mathbf{k}$ mutually orthogonal and $\epsilon_1^2 = \epsilon_2^2 = 1$. The conjugate momentum is then given by

$$\Pi_{\perp\epsilon}(\mathbf{k}, t) = \frac{\partial L}{\partial \dot{A}_{\perp\epsilon}(-\mathbf{k}, t)} = \epsilon_0 \dot{A}_{\perp\epsilon}(\mathbf{k}, t) \quad (1.582)$$

(see equation (1.671) in Appendix 1.A), so that

$$\mathbf{\Pi}_{\perp}(\mathbf{r}, t) = \epsilon_0 \dot{\mathbf{A}}_{\perp}(\mathbf{r}, t). \quad (1.583)$$

$\mathbf{\Pi}_{\perp}$ is transverse: $\nabla \cdot \mathbf{\Pi}_{\perp}(\mathbf{r}, t) = 0$. In the Coulomb gauge, the Hamiltonian is therefore defined by

$$\begin{aligned} H &= \sum_i \mathbf{p}_i(t) \cdot \dot{\mathbf{r}}_i(t) + \int d^3r \mathbf{\Pi}_{\perp}(\mathbf{r}, t) \cdot \dot{\mathbf{A}}_{\perp}(\mathbf{r}, t) - L, \\ &= \sum_i \frac{[\mathbf{p}_i(t) - e\mathbf{A}_{\perp}(\mathbf{r}_i, t)]^2}{2m} + H_c \\ &\quad + \frac{1}{2\epsilon_0} \int d^3r \left[\mathbf{\Pi}_{\perp}(\mathbf{r}, t)^2 + \epsilon_0^2 c_l^2 (\nabla \times \mathbf{A}_{\perp}(\mathbf{r}, t))^2 \right], \end{aligned} \quad (1.584)$$

where $H_c = -L_c$ is the Coulomb energy. The electromagnetic field is now given by

$$\begin{aligned} \mathbf{E}_{\parallel}(\mathbf{k}, t) &= -ik \frac{\rho(\mathbf{k}, t)}{\epsilon_0 \mathbf{k}^2}, & \mathbf{E}_{\parallel}(\mathbf{r}, t) &= \int d^3r' \frac{\rho(\mathbf{r}', t)(\mathbf{r} - \mathbf{r}')}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|^3}, \\ \mathbf{E}_{\perp}(\mathbf{k}, t) &= -\frac{1}{\epsilon_0} \mathbf{\Pi}_{\perp}(\mathbf{k}, t), & \text{i.e.} \quad \mathbf{E}_{\perp}(\mathbf{r}, t) &= -\frac{1}{\epsilon_0} \mathbf{\Pi}_{\perp}(\mathbf{r}, t), \\ \mathbf{B}(\mathbf{k}, t) &= i\mathbf{k} \times \mathbf{A}_{\perp}(\mathbf{k}, t), & \mathbf{B}(\mathbf{r}, t) &= \nabla \times \mathbf{A}_{\perp}(\mathbf{r}, t). \end{aligned} \quad (1.585)$$

The Hamiltonian of the particles can be written as

$$H = H'_m + H_c - \int d^3r \mathbf{j}(\mathbf{r}, t) \cdot \mathbf{A}_{\perp}(\mathbf{r}, t) + \frac{e}{2m} \int d^3r \rho(\mathbf{r}, t) \mathbf{A}_{\perp}^2(\mathbf{r}, t), \quad (1.586)$$

where

$$\mathbf{j}(\mathbf{r}, t) = \frac{e}{m} \sum_i \mathbf{p}_i \delta(\mathbf{r} - \mathbf{r}_i) \quad (1.587)$$

is the paramagnetic part of the current

$$\mathbf{J}(\mathbf{r}, t) = e \sum_i \dot{\mathbf{r}}_i \delta(\mathbf{r} - \mathbf{r}_i) = \frac{e}{m} \sum_i [\mathbf{p}_i - e\mathbf{A}_{\perp}(\mathbf{r}_i, t)] \delta(\mathbf{r} - \mathbf{r}_i). \quad (1.588)$$

$H'_m = \sum_i \mathbf{p}_i^2/2m$ is the Hamiltonian of the matter in the absence of electromagnetic interactions.

1.9.2 Canonical quantization in the Coulomb gauge

We are now in a position to quantize the theory by promoting the variables $(\mathbf{r}_i, \mathbf{p}_i)$ and $(\mathbf{A}_\perp, \mathbf{\Pi}_\perp)$ to operators. The position and momentum operators $\hat{\mathbf{r}}_i$ and $\hat{\mathbf{p}}_i$ satisfy the usual commutations relations (Appendix 1.B). As for the electromagnetic field, there are two independent dynamical variables $A_{\perp\epsilon_1}$ and $A_{\perp\epsilon_2}$, and their conjugate momenta $\Pi_{\perp\epsilon_1}$ and $\Pi_{\perp\epsilon_2}$, for each wave vector \mathbf{k} . The reality of $\mathbf{A}_\perp(\mathbf{r}, t)$ and $\mathbf{\Pi}_\perp(\mathbf{r}, t)$ implies $A_{\perp\epsilon}^*(\mathbf{k}, t) = A_{\perp\epsilon}(-\mathbf{k}, t)$ and $\Pi_{\perp\epsilon}^*(\mathbf{k}, t) = \Pi_{\perp\epsilon}(-\mathbf{k}, t)$. The corresponding operators satisfy

$$\begin{aligned} [\hat{A}_{\perp\epsilon}(\mathbf{k}), \hat{A}_{\perp\epsilon'}(\mathbf{k}')] &= [\hat{\Pi}_{\perp\epsilon}(\mathbf{k}), \hat{\Pi}_{\perp\epsilon'}(\mathbf{k}')] = 0, \\ [\hat{A}_{\perp\epsilon}(\mathbf{k}), \hat{\Pi}_{\perp\epsilon'}^\dagger(\mathbf{k}')] &= i\delta_{\epsilon,\epsilon'}\delta_{\mathbf{k},\mathbf{k}'}, \end{aligned} \quad (1.589)$$

where $\hat{\Pi}_{\perp\epsilon}^\dagger(\mathbf{k}) = \hat{\Pi}_{\perp\epsilon}(-\mathbf{k})$ and $\hat{A}_{\perp\epsilon}^\dagger(\mathbf{k}) = \hat{A}_{\perp\epsilon}(-\mathbf{k})$. Note that we consider here the Schrödinger picture where the operators do not depend on time (Appendix 1.B). The quantum Hamiltonian \hat{H} is obtained from (1.584) by replacing the classical variables by the corresponding operators. Using

$$\begin{aligned} \hat{A}_{\perp\mu}(\mathbf{k}) &= \sum_{\epsilon} \hat{A}_{\perp\epsilon}(\mathbf{k})\epsilon_{\mu}, \\ \hat{\Pi}_{\perp\mu}(\mathbf{k}) &= \sum_{\epsilon} \hat{\Pi}_{\perp\epsilon}(\mathbf{k})\epsilon_{\mu} \end{aligned} \quad (1.590)$$

($\mu = x, y, z$), we obtain⁵⁸

$$[\hat{A}_{\perp\mu}(\mathbf{k}), \hat{\Pi}_{\perp\mu'}^\dagger(\mathbf{k}')] = i\delta_{\mathbf{k},\mathbf{k}'} \sum_{\epsilon} \epsilon_{\mu}\epsilon_{\mu'} = i\delta_{\mathbf{k},\mathbf{k}'} (\delta_{\mu,\mu'} - k_{\mu}k_{\mu'}/\mathbf{k}^2). \quad (1.591)$$

In direct space, the commutation relations (1.589) become

$$\begin{aligned} [\hat{A}_{\perp\mu}(\mathbf{r}), \hat{A}_{\perp\mu'}(\mathbf{r}')] &= [\hat{\Pi}_{\perp\mu}(\mathbf{r}), \hat{\Pi}_{\perp\mu'}(\mathbf{r}')] = 0, \\ [\hat{A}_{\perp\mu}(\mathbf{r}), \hat{\Pi}_{\perp\mu'}(\mathbf{r}')] &= i\delta_{\mu,\mu'}^\perp(\mathbf{r} - \mathbf{r}'). \end{aligned} \quad (1.592)$$

The “transverse delta function”

$$\delta_{\mu,\mu'}^\perp(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \left(\delta_{\mu,\mu'} - \frac{k_{\mu}k_{\mu'}}{\mathbf{k}^2} \right) = \delta_{\mu,\mu'}\delta(\mathbf{r}) - \frac{\partial}{\partial r_{\mu}} \frac{\partial}{\partial r_{\mu'}} \frac{1}{4\pi|\mathbf{r}|} \quad (1.593)$$

appearing in (1.592) (in place of $\delta_{\mu,\mu'}\delta(\mathbf{r} - \mathbf{r}')$) reflects the fact that the three components of $\hat{\mathbf{A}}_\perp(\mathbf{r})$ and $\hat{\mathbf{\Pi}}_\perp(\mathbf{r})$ are not independent but constrained by the transversality conditions $\nabla \cdot \hat{\mathbf{A}}_\perp(\mathbf{r}) = \nabla \cdot \hat{\mathbf{\Pi}}_\perp(\mathbf{r}) = 0$.

Second-quantization and photons

Let us consider the Hamiltonian of the free field (no coupling to the matter)

$$\hat{H}_{\text{em}} = \frac{1}{2\epsilon_0} \sum_{\mathbf{k}, \epsilon} [\hat{\Pi}_{\perp\epsilon}^\dagger(\mathbf{k})\hat{\Pi}_{\perp\epsilon}(\mathbf{k}) + \epsilon_0^2 c_l^2 \mathbf{k}^2 \hat{A}_{\perp\epsilon}^\dagger(\mathbf{k})\hat{A}_{\perp\epsilon}(\mathbf{k})]. \quad (1.594)$$

⁵⁸Since $(\mathbf{k}, \epsilon_1, \epsilon_2)$ forms a basis in reciprocal space, $\epsilon_{1\mu}\epsilon_{1\mu'} + \epsilon_{2\mu}\epsilon_{2\mu'} + k_{\mu}k_{\mu'}/\mathbf{k}^2 = \delta_{\mu,\mu'}$.

Given the commutation relations (1.589) between $\hat{A}_{\perp\epsilon}$ and $\hat{\Pi}_{\perp\epsilon}$, this Hamiltonian describes a sum of independent harmonic oscillators, one for each mode (\mathbf{k}, ϵ) . It can be diagonalized by introducing the ladder operators

$$\begin{aligned}\hat{a}_\epsilon(\mathbf{k}) &= \sqrt{\frac{\epsilon_0\omega_{\mathbf{k}}}{2}} \left[\hat{A}_{\perp\epsilon}(\mathbf{k}) + \frac{i}{\epsilon_0\omega_{\mathbf{k}}} \hat{\Pi}_{\perp\epsilon}(\mathbf{k}) \right], \\ \hat{a}_\epsilon^\dagger(\mathbf{k}) &= \sqrt{\frac{\epsilon_0\omega_{\mathbf{k}}}{2}} \left[\hat{A}_{\perp\epsilon}^\dagger(\mathbf{k}) - \frac{i}{\epsilon_0\omega_{\mathbf{k}}} \hat{\Pi}_{\perp\epsilon}^\dagger(\mathbf{k}) \right],\end{aligned}\tag{1.595}$$

with $\omega_{\mathbf{k}} = c_l|\mathbf{k}|$. \hat{a} and \hat{a}^\dagger satisfy the commutation relations

$$\begin{aligned}[\hat{a}_\epsilon(\mathbf{k}), \hat{a}_{\epsilon'}(\mathbf{k}')] &= [\hat{a}_\epsilon^\dagger(\mathbf{k}), \hat{a}_{\epsilon'}^\dagger(\mathbf{k}')] = 0, \\ [\hat{a}_\epsilon(\mathbf{k}), \hat{a}_{\epsilon'}^\dagger(\mathbf{k}')] &= \delta_{\epsilon,\epsilon'}\delta_{\mathbf{k},\mathbf{k}'},\end{aligned}\tag{1.596}$$

and \hat{H}_{em} takes the form

$$\hat{H}_{\text{em}} = \sum_{\mathbf{k}, \epsilon} \omega_{\mathbf{k}} \left(\hat{a}_\epsilon^\dagger(\mathbf{k}) \hat{a}_\epsilon(\mathbf{k}) + \frac{1}{2} \right).\tag{1.597}$$

The Hamiltonian of the free field is similar to the one obtained for the quantum harmonic string in section 1.1.2. The elementary excitations of the quantized field (photons) are created and annihilated by the operators \hat{a}^\dagger and \hat{a} . The eigenstates of \hat{H}_{em} can be written as

$$\begin{aligned}|n_1 \cdots n_i \cdots\rangle &= \prod_i \frac{(\hat{a}_i^\dagger)^{n_i}}{\sqrt{n_i!}} |\text{vac}\rangle, \\ \hat{H}_{\text{em}} |n_1 \cdots n_i \cdots\rangle &= \sum_j \omega_j \left(n_j + \frac{1}{2} \right) |n_1 \cdots n_i \cdots\rangle,\end{aligned}\tag{1.598}$$

where n_i denotes the number photons in the mode $i \equiv (\mathbf{k}_i, \epsilon_i)$ and $|\text{vac}\rangle$ the (normalized) vacuum state: $\hat{a}_i |\text{vac}\rangle = 0$. From (1.585) and (1.595), we can express the transverse field in terms of the photon operators,

$$\begin{aligned}\hat{\mathbf{E}}_{\perp}(\mathbf{r}) &= \frac{i}{\sqrt{V}} \sum_{\mathbf{k}, \epsilon} \sqrt{\frac{\omega_{\mathbf{k}}}{2\epsilon_0}} \left[\hat{a}_\epsilon(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} - \hat{a}_\epsilon^\dagger(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}} \right] \boldsymbol{\epsilon}, \\ \hat{\mathbf{B}}(\mathbf{r}) &= \frac{i}{\sqrt{V}} \sum_{\mathbf{k}, \epsilon} \frac{1}{\sqrt{2\epsilon_0\omega_{\mathbf{k}}}} \left[\hat{a}_\epsilon(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} - \hat{a}_\epsilon^\dagger(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}} \right] \mathbf{k} \times \boldsymbol{\epsilon}.\end{aligned}\tag{1.599}$$

Coherent states. As with any bosonic operators, we can define the (normalized) coherent state

$$|z\rangle = \exp \left\{ - \sum_i \left(\frac{|z_i|^2}{2} - z_i \hat{a}_i^\dagger \right) \right\} |\text{vac}\rangle,\tag{1.600}$$

where z_i is a c-number. One easily finds⁵⁹

$$\begin{aligned}\langle z | \hat{A}_i | z \rangle &= \sqrt{\frac{2}{\epsilon_0\omega_i}} \Re(z_i), & \langle z | \hat{A}_i^2 | z \rangle &= \frac{1}{2\epsilon_0\omega_i} [4\Re(z_i)^2 + 1], \\ \langle z | \hat{\Pi}_i | z \rangle &= \sqrt{2\epsilon_0\omega_i} \Im(z_i), & \langle z | \hat{\Pi}_i^2 | z \rangle &= \frac{\epsilon_0\omega_i}{2} [4\Im(z_i)^2 + 1],\end{aligned}\tag{1.601}$$

⁵⁹These relations can be deduced from (1.214) and (1.215) by the correspondence $\hat{p} \rightarrow \hat{\Pi}_i$, $\hat{x} \rightarrow \hat{A}_i$, $m \rightarrow \epsilon_0$ and $\omega \rightarrow \omega_i$.

and therefore

$$\Delta A_i^2 = \frac{1}{2\epsilon_0\omega_i}, \quad (\Delta \Pi_i)^2 = \frac{\epsilon_0\omega_i}{2}. \quad (1.602)$$

The coherent state minimizes the uncertainty relation $\Delta A_i \Delta \Pi_i \geq \hbar/2$ (we have restored Planck's constant), and is the quantum state which is closest to the classical field. Since the coherent state evolves in time as

$$e^{-i\hat{H}t}|z\rangle = e^{-\frac{i}{2}\sum_i \omega_i t}|z(t)\rangle \quad (1.603)$$

(see Eq. (1.217)) with $z_i(t) = z_i e^{-i\omega_i t}$, the mean value of the transverse field reads

$$\begin{aligned} \langle z(t)|\hat{\mathbf{E}}_\perp(\mathbf{r})|z(t)\rangle &= \frac{i}{\sqrt{V}} \sum_{\mathbf{k}, \epsilon} \sqrt{\frac{\omega_{\mathbf{k}}}{2\epsilon_0}} \left[z_\epsilon(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} - \text{c.c.} \right] \boldsymbol{\epsilon}, \\ \langle z(t)|\hat{\mathbf{B}}(\mathbf{r})|z(t)\rangle &= \frac{i}{\sqrt{V}} \sum_{\mathbf{k}, \epsilon} \frac{1}{\sqrt{2\epsilon_0\omega_{\mathbf{k}}}} \left[z_\epsilon(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} - \text{c.c.} \right] \mathbf{k} \times \boldsymbol{\epsilon}. \end{aligned} \quad (1.604)$$

One easily verifies that these mean values are solutions of the Maxwell equations. By virtue of (1.602), the fluctuations

$$\langle z(t)|\hat{\mathbf{E}}_\perp^2(\mathbf{r})|z(t)\rangle - \langle z(t)|\hat{\mathbf{E}}_\perp(\mathbf{r})|z(t)\rangle^2 \quad (1.605)$$

and

$$\langle z(t)|\hat{\mathbf{B}}^2(\mathbf{r})|z(t)\rangle - \langle z(t)|\hat{\mathbf{B}}(\mathbf{r})|z(t)\rangle^2 \quad (1.606)$$

are the smallest ones compatible with the Heisenberg uncertainty relations.

1.9.3 Functional integral in the Coulomb gauge

We are now in a position to write the partition function $Z = \text{Tr } e^{-\beta \hat{H}}$ as a functional integral. In the free field case, the Hamiltonian (1.594) reduces to a sum of independent harmonic oscillators. Following the general method introduced in section 1.1.1, and in particular the derivation of the functional integral of the quantum harmonic string in section 1.1, one finds

$$Z_{\text{em}} = \int \mathcal{D}[\mathbf{A}_\perp] e^{-S_{\text{em}}[\mathbf{A}_\perp]}, \quad (1.607)$$

with the boundary condition $\mathbf{A}_\perp(\mathbf{r}, \beta) = \mathbf{A}_\perp(\mathbf{r}, 0)$ and the Euclidean action

$$\begin{aligned} S_{\text{em}}[\mathbf{A}_\perp] &= \int_0^\beta d\tau \sum_{\mathbf{k}, \epsilon} \frac{\epsilon_0}{2} \left[|\partial_\tau A_{\perp\epsilon}(\mathbf{k}, \tau)|^2 + c_l^2 \mathbf{k}^2 |A_{\perp\epsilon}(\mathbf{k}, \tau)|^2 \right] \\ &= \int_0^\beta d\tau \int d^3r \frac{\epsilon_0}{2} \left[(\partial_\tau \mathbf{A}_\perp(x))^2 + c_l^2 (\nabla \times \mathbf{A}_\perp(x))^2 \right] \end{aligned} \quad (1.608)$$

($x = (\mathbf{r}, \tau)$). The measure in the functional integral is defined by

$$\mathcal{D}[\mathbf{A}_\perp] = \prod_{\mathbf{k}, \epsilon, \tau} dA_{\perp\epsilon}^*(\mathbf{k}, \tau) dA_{\perp\epsilon}(\mathbf{k}, \tau) = \mathcal{D}[\mathbf{A}] \prod_{\mathbf{r}, \tau} \delta(\nabla \cdot \mathbf{A}(\mathbf{r}, \tau)) \quad (1.609)$$

(up to an irrelevant multiplicative constant), where the prime means that the product over \mathbf{k} is restricted to half the reciprocal space in order to take into account the

constraint $A_{\perp\epsilon}^*(\mathbf{k}) = A_{\perp\epsilon}(-\mathbf{k})$. The discretization of the space (necessary to properly define the integration measure) introduces an irrelevant multiplicative constant in the continuum limit.

When the coupling to the matter is introduced, the Hamiltonian is given by

$$\hat{H} = \hat{H}'_m + \hat{H}_c - \int d^3r \hat{\mathbf{j}}(\mathbf{r}, t) \cdot \hat{\mathbf{A}}_{\perp}(\mathbf{r}, t) + \frac{e}{2m} \int d^3r \hat{\rho}(\mathbf{r}, t) \hat{\mathbf{A}}_{\perp}^2(\mathbf{r}, t) + \hat{H}_{\text{em}} \quad (1.610)$$

(see equation (1.586)), where

$$\hat{H}_c = \frac{1}{2} \int d^3r d^3r' \frac{\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')}{4\pi\epsilon_0|\mathbf{r} - \mathbf{r}'|}. \quad (1.611)$$

The degrees of freedom of the particles can be described by field operators (Sec. 1.2.2). The charge and current density operators are then defined by

$$\begin{aligned} \hat{\rho}(\mathbf{r}) &= e \sum_{\sigma} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}), \\ \hat{\mathbf{J}}(\mathbf{r}) &= -\frac{ie}{2m} \sum_{\sigma} [\hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \nabla \hat{\psi}_{\sigma}(\mathbf{r}) - \text{h.c.}] - \frac{e}{m} \hat{\rho}(\mathbf{r}) \hat{\mathbf{A}}_{\perp}(\mathbf{r}) \\ &= \hat{\mathbf{j}}(\mathbf{r}) - \frac{e}{m} \hat{\rho}(\mathbf{r}) \hat{\mathbf{A}}_{\perp}(\mathbf{r}), \end{aligned} \quad (1.612)$$

for spin- σ particles (Sec. 1.2.2). $\hat{\mathbf{j}}$ is the paramagnetic part of the current and $\hat{H}'_m = \hat{H}_m - \hat{H}_c$ the Hamiltonian of the particles in the absence of electromagnetic interactions. Proceeding as in section 1.4, we derive from (1.610) the coherent-state functional integral

$$Z = \int \mathcal{D}[\psi^*, \psi, \mathbf{A}_{\perp}] e^{-S[\psi^*, \psi, \mathbf{A}_{\perp}]} \quad (1.613)$$

with the action

$$\begin{aligned} S[\psi^*, \psi, \mathbf{A}_{\perp}] &= S_{\text{em}}[\mathbf{A}_{\perp}] + S_m[\psi^*, \psi] \\ &+ \int_0^{\beta} d\tau \int d^3r \left[\frac{e}{2m} \rho(x) \mathbf{A}_{\perp}^2(x) - \hat{\mathbf{j}}(x) \cdot \mathbf{A}_{\perp}(x) \right], \end{aligned} \quad (1.614)$$

and the boundary conditions $\mathbf{A}_{\perp}(\mathbf{r}, \beta) = \mathbf{A}_{\perp}(\mathbf{r}, 0)$ and $\psi_{\sigma}^{(*)}(\mathbf{r}, \beta) = \zeta \psi_{\sigma}^{(*)}(\mathbf{r}, 0)$.

It is now possible to reintroduce the scalar potential by rewriting the Coulomb interaction as a functional integral over an auxiliary real bosonic field $\phi(x)$,⁶⁰

$$\begin{aligned} &\exp \left\{ -\frac{1}{2} \sum_k \frac{\rho(-k)\rho(k)}{\epsilon_0 \mathbf{k}^2} \right\} \\ &= \int \mathcal{D}[\phi] \exp \left\{ -\frac{1}{2} \sum_k [\epsilon_0 \mathbf{k}^2 \phi(-k)\phi(k) + 2i\phi(-k)\rho(k)] \right\} \\ &= \int \mathcal{D}[\phi] \exp \left\{ -\frac{1}{2} \int_0^{\beta} d\tau \int d^3r [\epsilon_0 (\nabla \phi(x))^2 + 2i\phi(x)\rho(x)] \right\} \end{aligned} \quad (1.615)$$

⁶⁰The transformation (1.615) is known as a Hubbard-Stratonovich transformation. It will be encountered many times in the following chapters (see, e.g., Sec. 5.2.3).

(again we neglect an irrelevant multiplicative term), where we use the notation $k = (\mathbf{k}, i\omega_n)$ with ω_n a bosonic Matsubara frequency. Equation (1.615) is obtained using the basic results of Gaussian integration derived in Appendix 1.E. The action becomes

$$S[\psi^*, \psi, \phi, \mathbf{A}_\perp] = S_{\text{em}}[\phi, \mathbf{A}_\perp] + S'_m[\psi^*, \psi] + \int_0^\beta d\tau \int d^3r \left[\frac{e}{2m} \rho(x) \mathbf{A}_\perp^2(x) + i\phi(x) \rho(x) - \mathbf{j}(x) \cdot \mathbf{A}_\perp(x) \right], \quad (1.616)$$

with the action of the electromagnetic potentials given by

$$S_{\text{em}}[\phi, \mathbf{A}_\perp] = \int_0^\beta d\tau \int d^3r \frac{\epsilon_0}{2} \left[(\nabla \phi(x))^2 + (\partial_\tau \mathbf{A}_\perp(x))^2 + c_l^2 (\nabla \times \mathbf{A}_\perp(x))^2 \right]. \quad (1.617)$$

$S'_m = S_m - S_c$ denotes the action of the particles with no electromagnetic interaction. According to (1.616), the field $i\phi(x)$ plays the role of the scalar potential, since it couples to the particle density. The factor i cannot be eliminated by a redefinition of the ϕ field, $i\phi \rightarrow \phi$, since this would change the sign of $(\nabla \phi)^2$ in S_{em} and makes the functional integral ill-defined. Thus, in the Euclidean formalism, the mean values of the electric and magnetic fields are

$$\begin{aligned} \langle \mathbf{E}(x) \rangle &= -\nabla \langle i\phi(x) \rangle - i\partial_\tau \langle \mathbf{A}_\perp(x) \rangle, \\ \langle \mathbf{B}(x) \rangle &= \nabla \times \langle \mathbf{A}_\perp(x) \rangle, \end{aligned} \quad (1.618)$$

or, in Fourier space,

$$\begin{aligned} \langle \mathbf{E}(k) \rangle &= \mathbf{k} \langle \phi(k) \rangle - \omega_n \langle \mathbf{A}_\perp(k) \rangle, \\ \langle \mathbf{B}(k) \rangle &= i\mathbf{k} \times \langle \mathbf{A}_\perp(k) \rangle. \end{aligned} \quad (1.619)$$

According to (1.585), the mean value of the longitudinal electric field is given by

$$\langle \mathbf{E}_\parallel(k) \rangle = -i\mathbf{k} \frac{\langle \rho(k) \rangle}{\epsilon_0 \mathbf{k}^2}. \quad (1.620)$$

The mean particle density can be calculated from

$$\langle \rho(k) \rangle = \left. \frac{\partial \ln Z[h]}{\partial h(-k)} \right|_{h=0}, \quad (1.621)$$

where $Z[h]$ is the partition function obtained by adding to the action the source term $-\sum_k h(-k)\rho(k)$. After the Hubbard-Stratonovich transformation (1.615), the action reads

$$\begin{aligned} S &= \frac{1}{2} \sum_k [\epsilon_0 \mathbf{k}^2 \phi(-k) \phi(k) + 2i\phi(-k) \rho(k) - 2h(-k) \rho(k)] + \dots \\ &= \frac{1}{2} \sum_k [\epsilon_0 \mathbf{k}^2 (\phi(-k) - ih(-k)) (\phi(k) - ih(k)) + 2i\phi(-k) \rho(k)] \dots \end{aligned} \quad (1.622)$$

(we do not write the part of the action which is independent of h). The second line of (1.622) is obtained by shifting the field $\phi \rightarrow \phi - ih$ in the functional integral. From (1.621) and (1.622), we then deduce

$$\begin{aligned} \langle \rho(k) \rangle &= \epsilon_0 \mathbf{k}^2 \langle i\phi(k) \rangle, \\ \langle \mathbf{E}_\parallel(k) \rangle &= \mathbf{k} \langle \phi(k) \rangle, \end{aligned} \quad (1.623)$$

in agreement with (1.619).

More generally, one can define the propagators of the electromagnetic potentials,

$$\begin{aligned} D_{00}(k) &= \langle \phi(k) \phi(-k) \rangle, \\ D_{0\mu}(k) &= \langle \phi(k) A_\mu(-k) \rangle, \\ D_{\mu\nu}(k) &= \langle A_\mu(k) A_\nu(-k) \rangle = \frac{k_\mu k_\nu}{\mathbf{k}^2} D_{\parallel}(k) + \left(\delta_{\mu,\nu} - \frac{k_\mu k_\nu}{\mathbf{k}^2} \right) D_{\perp}(k) \end{aligned} \quad (1.624)$$

($\mu = x, y, z$), where $D_{\parallel}(k)$ and $D_{\perp}(k)$ are functions of ($|\mathbf{k}|, i\omega_n$). In (1.624), we have taken advantage of the homogeneity and isotropy of the system to write the propagator $D_{\mu\nu}$ in terms of its longitudinal and transverse parts. In the absence of coupling to the particles, one finds

$$\begin{aligned} D_{00}^{(0)}(k) &= \langle \phi(k) \phi(-k) \rangle = \frac{1}{\epsilon_0 \mathbf{k}^2}, \\ D_{\perp}^{(0)}(k) &= \frac{1}{\epsilon_0 (\omega_n^2 + c_l^2 \mathbf{k}^2)}. \end{aligned} \quad (1.625)$$

In the Coulomb gauge, the propagator of the vector potential is transverse: $D_{\parallel}^{(0)}(k) = D_{0\mu}^{(0)}(k) = 0$. $D_{00}^{(0)}(k)$ is the Fourier transform of the Coulomb interaction, whereas $D_{\perp}^{(0)}(k)$ is the propagator of the (transverse) electromagnetic field in free space. We shall see in section 3.4 that the propagators D_{00} and D_{\perp} contain important informations about the collective excitations of the particles, besides describing the propagation of the electromagnetic field in the matter.

In the Coulomb gauge, the electric field is split into a Coulomb field and a transverse field. Although the Coulomb interaction is instantaneous [Eq. (1.611)], the interaction between two charged particles takes place with a retardation due to the propagation of the field with velocity c_l . This retardation results from an exact compensation of the instantaneous contributions of the Coulomb and transverse fields [16]. In non-relativistic systems, the separation between an instantaneous Coulomb field and a transverse field is very natural since the magnetic interactions mediated by the vector potential are negligible when the characteristic velocity of the particles is small wrt the velocity of light. To see this, let us integrate out the vector potential in (1.614). If we approximate $\rho(x)$ in the diamagnetic term $\rho(x) \mathbf{A}_{\perp}^2(x)$ by its mean value en , we are left with a simple Gaussian functional integral (Appendix 1.E.4) which gives a contribution⁶¹

$$-\frac{1}{2\epsilon_0} \sum_{\mathbf{k}} \frac{\mathbf{j}_{\perp}(-\mathbf{k}) \cdot \mathbf{j}_{\perp}(\mathbf{k})}{\omega_n^2 + c_l^2 \mathbf{k}^2 + \omega_p^2} \quad (1.626)$$

to the action of the particles. \mathbf{j}_{\perp} is the transverse part of the paramagnetic current and $\omega_p = (ne^2/\epsilon_0 m)^{1/2}$ is called the plasma frequency for reasons given in chapter 3. For particles with characteristic velocity v , $j_{\perp} \sim v\rho$ so that the magnetic interaction (1.626) is of order v^2/c_l^2 wrt to the Coulomb interaction $\rho(k)\rho(-k)/\epsilon_0 \mathbf{k}^2$. If $v \ll c_l$, the magnetic interaction can be omitted, which amounts to neglecting the retardation effects in the electromagnetic interaction between particles. When studying systems

⁶¹The functional integral should be done in Fourier space where the transverse vector potential is defined by its two independent components $A_{\perp\epsilon_1}(\mathbf{k}, \tau)$ and $A_{\perp\epsilon_2}(\mathbf{k}, \tau)$.

of charged particles, we will therefore in general consider the action $S_m = S'_m + S_c$ including the Coulomb interaction but not the coupling to the vector potential. Only when considering the response to an external transverse field (i.e. induced by a current distribution external to the system) or the propagation of the electromagnetic field in the matter should we include the transverse vector potential in the action (see e.g. Sec. 3.4.2).

1.10 Spin systems

1.A Review of classical mechanics⁶²

In the following sections, we review the Lagrangian and Hamiltonian formalisms for both a finite number and a continuum of degrees of freedom. In particular we discuss symmetries of their consequences.

1.A.1 Lagrangian formalism

Let us consider a system with n degrees of freedom described by n generalized coordinates q_1, \dots, q_n . The latter can be represented by a point in a n -dimensional configuration space. The trajectory of the system is determined by the time dependence of the coordinates. The coordinates q_i and the velocities $\dot{q}_i = \partial_t q_i$ form the dynamical variables of the system. The accelerations \ddot{q}_i can be expressed at any time as a function of these variables. The resulting equations of motion are then second-order differential equations in time.

In the Lagrangian approach, the dynamics of the system is determined by the Lagrangian $L(q_i, \dot{q}_i, t)$, a function of the dynamical variables which can also explicitly depend on time. The principle of least action stipulates that the trajectory of the system between times t_1 and t_2 , with initial and final coordinates assumed to be known, corresponds to an extremum of the action

$$S = \int_{t_1}^{t_2} dt L(q_i, \dot{q}_i, t). \quad (1.627)$$

For an arbitrary variation δq_i of the coordinate q_i , the variation of the action is

$$\begin{aligned} \delta S &= \int_{t_1}^{t_2} dt \sum_i \left[\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right] \\ &= \int_{t_1}^{t_2} dt \sum_i \left[\frac{\partial L}{\partial q_i} \delta q_i - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) \delta q_i \right] + \sum_i \frac{\partial L}{\partial \dot{q}_i} \delta q_i \Big|_{t_1}^{t_2}, \end{aligned} \quad (1.628)$$

where we have integrated by parts. The last term in (1.628) vanishes since $\delta q_i(t_1) = \delta q_i(t_2) = 0$ (the initial and final coordinates $q_i(t_1)$ and $q_i(t_2)$ are fixed), and we deduce the Euler-Lagrange equations

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0. \quad (1.629)$$

⁶²A thorough discussion of classical mechanics can be found in Refs. [20, 21].

The resolution of these n second-order differential equations requires the knowledge of $2n$ parameters: $q_i(t_1)$ and $q_i(t_2)$. The Lagrangian is not unique. In particular, adding to the Lagrangian a total time derivative,

$$L(q_i, \dot{q}_i, t) \rightarrow L(q_i, \dot{q}_i, t) + \frac{d}{dt}F(q_i, t) \quad (1.630)$$

($F(q_i, t)$ is an arbitrary function) modifies the action only by the surface term $F(q_i(t_2), t_2) - F(q_i(t_1), t_1)$ and therefore does not affect the equations of motion ($q_i(t_1)$ and $q_i(t_2)$ being fixed). For the transformed Lagrangian to be a function of the dynamical variables q_i and \dot{q}_i , the function $F(q_i, t)$ should not depend on the velocities.

Symmetries and invariance

Suppose we describe the system by two sets of coordinates, $\{q_i\}$ and $\{q'_i\}$, corresponding to Lagrangians $L(q_i, \dot{q}_i, t)$ and $L'(q'_i, \dot{q}'_i, t)$, respectively. The transformation $q_i \rightarrow q'_i$ is called a symmetry transformation.⁶³ Since both sets $\{q_i\}$ and $\{q'_i\}$ refer to the same system, we must have $L(q_i, \dot{q}_i, t) = L'(q'_i, \dot{q}'_i, t)$ (up to a total time derivative). The equations of motion for the new set of coordinates read

$$\frac{d}{dt} \frac{\partial L'}{\partial \dot{q}'_i} = \frac{\partial L'}{\partial q'_i} \quad (1.631)$$

and follow from the principle of least action applied to the action $S'[q'] = \int dt L'(q'_i, \dot{q}'_i, t)$. In general, L and L' are different functions.⁶⁴ If, however, the action $S'[q']$ and $S[q]$ coincide – i.e. if $L'(q'_i, \dot{q}'_i, t)$ and $L(q'_i, \dot{q}'_i, t)$ differ only by a total derivative – then the equation of motion of q'_i [Eq. (1.631)] is identical to that of q_i [Eq. (1.629)]; the system is invariant in the symmetry transformation $q_i \rightarrow q'_i$.

Let us now consider an infinitesimal (continuous) transformation $q_i \rightarrow q_i + \epsilon f_i$ ($\epsilon \rightarrow 0$) which leaves the system invariant. To order ϵ , the variation of the Lagrangian can be written as

$$\delta L = \epsilon \sum_i \left(\frac{\partial L}{\partial q_i} f_i + \frac{\partial L}{\partial \dot{q}_i} \dot{f}_i \right) = \epsilon \frac{d}{dt} F(q_i, t), \quad (1.632)$$

with $F(q_i, t)$ some function, i.e.

$$\sum_i \left[\frac{\partial L}{\partial q_i} f_i + \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} f_i \right) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) f_i \right] = \frac{d}{dt} F(q_i, t). \quad (1.633)$$

If q_i satisfies the equation of motion (1.629), equation (1.633) implies that

$$\frac{d}{dt} \sum_i \left(\frac{\partial L}{\partial \dot{q}_i} f_i - F(q_i, t) \right) = 0. \quad (1.634)$$

Thus, to any transformation which leaves the action invariant, there corresponds a constant of motion (Noether's theorem).

⁶³This is the so-called passive point of view where two observers, \mathcal{O} (coordinates $\{q_i\}$) and \mathcal{O}' (coordinates $\{q'_i\}$), look at the same system. Alternatively, one can adopt the active point of view where a symmetry transformation is defined with a single observer \mathcal{O} and two systems \mathcal{S} and \mathcal{S}' .

⁶⁴It is crucial here to distinguish L and L' . In general, however, we shall follow the usual convention to denote a given dynamical variable (such as the Lagrangian or the Hamiltonian) by the same symbol in all coordinate systems.

Let us illustrate Noether's theorem with a few examples. We consider a three-dimensional system.

For a system which is translation invariant $L(\mathbf{q}_i + \boldsymbol{\epsilon}, \dot{\mathbf{q}}_i, t) = L(\mathbf{q}_i, \dot{\mathbf{q}}_i, t)$, we can apply (1.634) with $F = 0$ and $f_{i\mu} = \delta_{\mu,x}$ if $\boldsymbol{\epsilon}$ is parallel to the x axis ($f_{i\mu} = \delta_{\mu,y}$ if $\boldsymbol{\epsilon}$ is parallel to the y axis, etc.). One then finds that the total momentum of the system, defined as

$$\mathbf{P} = \sum_i \mathbf{p}_i = \sum_i \frac{\partial L}{\partial \dot{\mathbf{q}}_i}, \quad (1.635)$$

is conserved. \mathbf{p}_i denotes the momentum of the i th particle.

The Lagrangian of a rotation invariant system is unchanged by the transformation $\mathbf{q}_i \rightarrow \mathbf{q}_i + \theta \mathbf{n} \times \mathbf{q}_i$, i.e. $q_{i\mu} \rightarrow q_{i\mu} + \theta \sum_{\nu,\delta} \epsilon_{\mu\nu\delta} n_\nu q_{i\delta}$ (rotation of angle θ about the axis \mathbf{n}). $\epsilon_{\mu\nu\delta}$ denotes the antisymmetric tensor. One then finds that the quantity

$$\sum_{i,\mu,\nu,\delta} \frac{\partial L}{\partial \dot{q}_{i\mu}} \epsilon_{\mu\nu\delta} n_\nu q_{i\delta} = \sum_{i,\mu,\nu,\delta} n_\nu \epsilon_{\nu\delta\mu} q_{i\delta} \frac{\partial L}{\partial \dot{q}_{i\mu}} = \sum_i \mathbf{n} \cdot \left(\mathbf{q}_i \times \frac{\partial L}{\partial \dot{\mathbf{q}}_i} \right) \quad (1.636)$$

is conserved. Since (1.636) holds for any unit vector \mathbf{n} , we conclude that the total angular momentum

$$\mathbf{J} = \sum_i \mathbf{q}_i \times \frac{\partial L}{\partial \dot{\mathbf{q}}_i} = \sum_i \mathbf{q}_i \times \mathbf{p}_i \quad (1.637)$$

is a constant of motion.

If the Lagrangian $L(\mathbf{q}_i, \dot{\mathbf{q}}_i)$ does not depend explicitly on time,

$$L(\mathbf{q}_i(t + \epsilon), \dot{\mathbf{q}}_i(t + \epsilon)) = L(\mathbf{q}_i + \epsilon \dot{\mathbf{q}}_i, \dot{\mathbf{q}}_i + \epsilon \ddot{\mathbf{q}}_i) = L + \epsilon \frac{dL}{dt} \quad (1.638)$$

to first order in ϵ . From (1.634) with $\mathbf{f}_i = \dot{\mathbf{q}}_i$ and $F = L$, we deduce that the Hamiltonian of the system

$$H = \sum_i \frac{\partial L}{\partial \dot{\mathbf{q}}_i} \cdot \dot{\mathbf{q}}_i - L = \sum_i \mathbf{p}_i \cdot \dot{\mathbf{q}}_i - L \quad (1.639)$$

(which is usually identified to the total energy) is conserved.

Let us finally consider a Galilean transformation $\mathbf{q}_i \rightarrow \mathbf{q}_i + \mathbf{v}t$ ($\mathbf{f}_i = \mathbf{v}t$) for a Lagrangian of the form

$$L = \sum_i \frac{1}{2} m \dot{\mathbf{q}}_i^2 - V, \quad (1.640)$$

where V depends only on the differences $\mathbf{q}_i - \mathbf{q}_j$. To $\mathcal{O}(\mathbf{v})$, the Lagrangian changes by

$$\delta L = \sum_i \left(\frac{\partial L}{\partial \mathbf{q}_i} \cdot \mathbf{v}t + \frac{\partial L}{\partial \dot{\mathbf{q}}_i} \cdot \mathbf{v} \right) = \sum_i m \dot{\mathbf{q}}_i \cdot \mathbf{v} = \mathbf{v} \cdot \frac{d}{dt} M \mathbf{R}, \quad (1.641)$$

where \mathbf{R} is the position of the center of mass and M is the total mass. We conclude that

$$\sum_i \frac{\partial L}{\partial \dot{\mathbf{q}}_i} t - M \mathbf{R} = \mathbf{P}t - M \mathbf{R} \quad (1.642)$$

is conserved. Since the total momentum \mathbf{P} is conserved for a translation invariant system, we deduce that the center of mass moves with a constant velocity,

$$M \frac{d\mathbf{R}}{dt} = \mathbf{P}. \quad (1.643)$$

1.A.2 Hamiltonian formalism

In the Hamiltonian approach, the state of the system is specified by n generalized coordinates q_i and n conjugate momenta p_i defined by

$$p_i = \frac{\partial L}{\partial \dot{q}_i}. \quad (1.644)$$

Coordinates and momenta can be represented by a point in a $2n$ -dimensional phase space. The Hamiltonian $H(p_i, q_i, t)$, which is a function of coordinates and momenta, is defined as the Legendre transform of the Lagrangian,

$$H(p_i, q_i, t) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i, t). \quad (1.645)$$

Using the Euler-Lagrange equations (1.629), one obtains Hamilton's equations of motion,

$$\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i}, \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i}. \end{aligned} \quad (1.646)$$

The dynamics of the system is described by $2n$ first-order differential equations.

The Poisson bracket of 2 functions $F(p_i, q_i, t)$ and $G(p_i, q_i, t)$ is defined by

$$[F, G] = \sum_i \left(\frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial G}{\partial q_i} \frac{\partial F}{\partial p_i} \right). \quad (1.647)$$

Hamilton's equations of motion can be rewritten as

$$\begin{aligned} \dot{q}_i &= [q_i, H], \\ \dot{p}_i &= [p_i, H]. \end{aligned} \quad (1.648)$$

The time evolution of an arbitrary function $F(p_i, q_i, t)$,

$$\begin{aligned} \frac{dF}{dt} &= \frac{\partial F}{\partial t} + \sum_i \left(\frac{\partial F}{\partial p_i} \dot{p}_i + \frac{\partial F}{\partial q_i} \dot{q}_i \right) \\ &= \frac{\partial F}{\partial t} + \sum_i \left(-\frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i} + \frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} \right) \\ &= \frac{\partial F}{\partial t} + [F, H], \end{aligned} \quad (1.649)$$

can also be expressed by means of its Poisson bracket with the Hamiltonian.

It is possible to describe the system in terms of new coordinates and momenta,

$$\begin{aligned} Q_i &\equiv Q_i(p_j, q_j, t), \\ P_i &\equiv P_i(p_j, q_j, t). \end{aligned} \quad (1.650)$$

The transformation $(q_i, p_i) \rightarrow (Q_i, P_i)$ is canonical if P_i and Q_i are canonically conjugate, i.e. if they satisfy

$$[Q_i, Q_j] = [P_i, P_j] = 0 \quad \text{and} \quad [Q_i, P_j] = \delta_{i,j}. \quad (1.651)$$

In this case, the Poisson bracket (1.647) of 2 functions F and G keeps the same form

$$[F, G] = \sum_i \left(\frac{\partial F}{\partial Q_i} \frac{\partial G}{\partial P_i} - \frac{\partial G}{\partial Q_i} \frac{\partial F}{\partial P_i} \right). \quad (1.652)$$

When the transformation (1.650) does not depend explicitly on time, Hamilton's equations of motion (1.648) are invariant, i.e. $\dot{Q}_i = [Q_i, H]$ and $\dot{P}_i = [P_i, H]$, where the Poisson bracket is calculated with the new coordinates Q_i and P_i .

Symmetries and invariance

For any function $G(p_i, q_i, t)$, we can define the infinitesimal (canonical) continuous transformation ($\epsilon \rightarrow 0$)

$$\begin{aligned} q_i &\rightarrow q_i - \epsilon [G, q_i] = q_i + \epsilon \frac{\partial G}{\partial p_i}, \\ p_i &\rightarrow p_i - \epsilon [G, p_i] = p_i - \epsilon \frac{\partial G}{\partial q_i}. \end{aligned} \quad (1.653)$$

G is called the generator of the transformation.⁶⁵ For a given transformation, the generator is unique, apart from an arbitrary additive function of t , independent of p_i and q_i . If the transformation (1.653) does not involve the time explicitly, G can be chosen time independent.

The system is invariant in the transformation if the equations of motion are preserved. If G is time independent, this implies that the Hamiltonian is unchanged (see the remark after (1.652)), i.e.

$$\delta H = \epsilon \sum_i \left(-\frac{\partial H}{\partial p_i} \frac{\partial G}{\partial q_i} + \frac{\partial H}{\partial q_i} \frac{\partial G}{\partial p_i} \right) = \epsilon [H, G] = 0. \quad (1.654)$$

to order ϵ . Since $\partial G / \partial t = 0$, equations (1.649) and (1.654) imply

$$\frac{dG}{dt} = 0. \quad (1.655)$$

The generator of the transformation is a constant of motion. When G has an explicit dependence on t , the Hamiltonian cannot be invariant in the transformation (1.653), since the energy of a system does depend on the choice of the (moving) reference frame. Nevertheless, the condition for the equations of motion to be unchanged is still given by (1.655). For the first of equations (1.646) to be unchanged, we need⁶⁶

$$\delta \dot{q}_i = \delta \frac{\partial H}{\partial p_i}, \quad \text{i.e.} \quad \frac{d}{dt} \frac{\partial G}{\partial p_i} = - \left[G, \frac{\partial H}{\partial p_i} \right]. \quad (1.656)$$

⁶⁵There is a close analogy between symmetries in the (classical) Hamiltonian formalism and symmetries in quantum mechanics. In particular, to the canonical transformation generated by $G(p_i, q_i, t)$ corresponds, in quantum mechanics, a unitary transformation generated by $G(\hat{p}_i, \hat{q}_i, t)$ (Sec. 2.1).

⁶⁶We use the fact that any function $F(p_i, q_i, t)$ changes by $\delta F = \sum_i \left(\frac{\partial F}{\partial q_i} \delta q_i + \frac{\partial F}{\partial p_i} \delta p_i \right) = -\epsilon [G, F]$ in the transformation (1.653).

Using (1.649) for the time evolution of $\partial G/\partial p_i$ and G , one finds that (1.656) is equivalent to

$$\frac{\partial}{\partial p_i} \frac{dG}{dt} = 0. \quad (1.657)$$

Similarly, from the invariance of the second of equations (1.646), one deduces

$$\frac{\partial}{\partial q_i} \frac{dG}{dt} = 0. \quad (1.658)$$

It follows that dG/dt must be a function of t alone. But since we can always add to G any function of t without affecting the transformation it generates, we can choose it such that $dG/dt = 0$.

It is straightforward to verify that the constants of motion obtained from the Lagrangian formalism (Sec. 1.A.1) are the generators of the corresponding symmetry transformations. The total momentum $\mathbf{P} = \sum_i \mathbf{p}_i$ satisfies

$$\begin{aligned} \mathbf{q}_i - [\mathbf{P} \cdot \delta \mathbf{a}, \mathbf{q}_i] &= \mathbf{q}_i + \delta \mathbf{a}, \\ \mathbf{p}_i - [\mathbf{P} \cdot \delta \mathbf{a}, \mathbf{p}_i] &= \mathbf{p}_i, \end{aligned} \quad (1.659)$$

and is therefore the generator of translations. Similarly, one finds that the total angular momentum $\mathbf{J} = \sum_i \mathbf{q}_i \times \mathbf{p}_i$ is the generator of rotations,

$$\begin{aligned} \mathbf{q}_i - [\mathbf{J} \cdot \delta \mathbf{a}, \mathbf{q}_i] &= \mathbf{q}_i + \delta \mathbf{a} \times \mathbf{q}_i, \\ \mathbf{p}_i - [\mathbf{J} \cdot \delta \mathbf{a}, \mathbf{p}_i] &= \mathbf{p}_i + \delta \mathbf{a} \times \mathbf{p}_i \end{aligned} \quad (1.660)$$

($\delta \mathbf{a} = \delta \theta \mathbf{n}$ for a rotation of angle $\delta \theta$ about the \mathbf{n} axis), and the Hamiltonian the generator of time translations [Eq. (1.648)]. The generator of a Galilean transformation is given by $\mathbf{P}t - M\mathbf{R}$,

$$\begin{aligned} \mathbf{q}_i - [(\mathbf{P}t - M\mathbf{R}) \cdot \delta \mathbf{v}, \mathbf{q}_i] &= \mathbf{q}_i + \delta \mathbf{v}t, \\ \mathbf{p}_i - [(\mathbf{P}t - M\mathbf{R}) \cdot \delta \mathbf{v}, \mathbf{p}_i] &= \mathbf{p}_i + m\delta \mathbf{v}. \end{aligned} \quad (1.661)$$

1.A.3 Classical field theory

The Lagrangian and Hamiltonian formalisms also apply to systems with a continuum of degrees of freedom described by a field $\psi_j(\mathbf{r}, t)$ which depends on a continuous variable \mathbf{r} (which is generally the position in space) and a discrete index j . $\psi_j(\mathbf{r}, t)$ is usually assumed to be real.⁶⁷ The Lagrangian is a functional of the dynamical variables $\psi_j(\mathbf{r}, t)$ and $\dot{\psi}_j(\mathbf{r}, t) = \partial_t \psi_j(\mathbf{r}, t)$,⁶⁸ which can be written as

$$L[\psi(t), \dot{\psi}(t)] = \int d^d r \mathcal{L}(\psi_j, \dot{\psi}_j, \nabla \psi_j), \quad (1.662)$$

where \mathcal{L} is called the Lagrangian density. For simplicity we assume that \mathcal{L} has no explicit dependence on \mathbf{r} and t . The notation $L[\psi(t), \dot{\psi}(t)]$ emphasizes that the Lagrangian is a functional of $\psi_j(\mathbf{r}, t)$ and $\dot{\psi}_j(\mathbf{r}, t)$ at a given time t . It should be noticed

⁶⁷If the theory is naturally expressed in terms of a complex field ψ and its complex conjugate ψ^* , we write $\psi = \frac{1}{\sqrt{2}}(\psi_1 + i\psi_2)$ and $\psi^* = \frac{1}{\sqrt{2}}(\psi_1 - i\psi_2)$ where ψ_1 and ψ_2 are two real fields.

⁶⁸Functionals are defined and discussed in Appendix 1.D.

that $\nabla\psi_j(\mathbf{r}, t)$ is not an independent dynamical variable but a mere function of the field $\psi_j(\mathbf{r}, t)$ at different positions \mathbf{r} . Although the Lagrangian (1.662) describes a large number of physical systems, the Lagrangian density \mathcal{L} may depend on spatial derivatives to all orders.

To obtain the Euler-Lagrange equations of motion, we require the action⁶⁹

$$S[\psi] = \int_{t_1}^{t_2} dt L[\psi(t), \dot{\psi}(t)] = \int_{t_1}^{t_2} dt \int d^d r \mathcal{L}(\psi_j, \dot{\psi}_j, \nabla\psi_j) \quad (1.663)$$

to be stationary under infinitesimal variations $\delta\psi_j(\mathbf{r}, t)$ with the condition $\delta\psi_j(\mathbf{r}, t_1) = \delta\psi_j(\mathbf{r}, t_2) = 0$. Applying the rules of functional derivatives (Appendix 1.D), one finds⁷⁰

$$\begin{aligned} 0 &= \frac{\delta S}{\delta\psi_j(\mathbf{r}, t)} = \frac{\delta L}{\delta\psi_j(\mathbf{r}, t)} - \frac{d}{dt} \frac{\delta L}{\delta\dot{\psi}_j(\mathbf{r}, t)} \\ &= \frac{\partial \mathcal{L}}{\partial\psi_j(\mathbf{r}, t)} - \nabla \cdot \frac{\partial \mathcal{L}}{\partial(\nabla\psi_j(\mathbf{r}, t))} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial\dot{\psi}_j(\mathbf{r}, t)} \end{aligned} \quad (1.664)$$

under the assumption that the field vanishes at infinity ($|\mathbf{r}| \rightarrow \infty$) or satisfies periodic boundary conditions. Without changing the equations of motion, we can add to the Lagrangian density a total time or space derivative,⁷¹

$$\mathcal{L} \rightarrow \mathcal{L} + \frac{d}{dt} \mathcal{F}_0(\psi_j) + \nabla \cdot \vec{\mathcal{F}}(\psi_j). \quad (1.665)$$

The space integral of $\nabla \cdot \vec{\mathcal{F}}$ gives a surface integral at infinity which vanishes. The transformed Lagrangian then differs from the original one by a total time derivative which does not affect the equations of motion.

The conjugate momentum and the Hamiltonian are defined by

$$\begin{aligned} \Pi_j(\mathbf{r}, t) &= \frac{\delta L}{\delta\dot{\psi}_j(\mathbf{r}, t)} = \frac{\partial \mathcal{L}}{\partial\dot{\psi}_j(\mathbf{r}, t)}, \\ H[\Pi(t), \psi(t)] &= \int d^d r \sum_j \Pi_j(\mathbf{r}, t) \dot{\psi}_j(\mathbf{r}, t) - L[\psi(t), \dot{\psi}(t)] \\ &= \int d^d r \mathcal{H}(\Pi_j, \psi_j, \nabla\psi_j), \end{aligned} \quad (1.666)$$

where \mathcal{H} is the Hamiltonian density. From (1.664) and (1.666), we obtain Hamilton's equations of motion

$$\begin{aligned} \dot{\psi}_j(\mathbf{r}, t) &= \frac{\delta H}{\delta\Pi_j(\mathbf{r}, t)} = \frac{\partial \mathcal{H}}{\partial\Pi_j(\mathbf{r}, t)}, \\ \dot{\Pi}_j(\mathbf{r}, t) &= -\frac{\delta H}{\delta\psi_j(\mathbf{r}, t)} = -\frac{\partial \mathcal{H}}{\partial\psi_j(\mathbf{r}, t)} + \nabla \cdot \frac{\partial \mathcal{H}}{\partial(\nabla\psi_j(\mathbf{r}, t))}. \end{aligned} \quad (1.667)$$

⁶⁹The knowledge of $\psi_j(\mathbf{r}, t)$ over the time interval $[t_1, t_2]$ fixes the value of $\dot{\psi}_j(\mathbf{r}, t)$ over the same time interval. The action $S[\psi]$ is therefore a functional of $\psi_j(\mathbf{r}, t)$, whereas the Lagrangian $L[\psi(t), \dot{\psi}(t)]$ at time t is a functional of both $\psi_j(\mathbf{r}, t)$ and $\dot{\psi}_j(\mathbf{r}, t)$.

⁷⁰Equation (1.664) is a direct consequence of the equation (1.817) in Appendix 1.D.

⁷¹In the general case, the functions \mathcal{F}_0 and $\vec{\mathcal{F}}$ can depend explicitly on \mathbf{r} and t .

It is often convenient to work with the Fourier transformed variables

$$\begin{aligned}\psi_j(\mathbf{k}, t) &= \frac{1}{\sqrt{V}} \int d^d r e^{-i\mathbf{k}\cdot\mathbf{r}} \psi_j(\mathbf{r}, t), \\ \Pi_j(\mathbf{k}, t) &= \frac{1}{\sqrt{V}} \int d^d r e^{-i\mathbf{k}\cdot\mathbf{r}} \Pi_j(\mathbf{r}, t),\end{aligned}\tag{1.668}$$

where $\psi_j(-\mathbf{k}, t) = \psi_j^*(\mathbf{k}, t)$ and $\Pi_j(-\mathbf{k}, t) = \Pi_j^*(\mathbf{k}, t)$ for real fields $\psi_j(\mathbf{r}, t)$ and $\Pi_j(\mathbf{r}, t)$. For periodic boundary conditions, $k_x = \frac{2\pi}{L_x} n_x$ (n_x integer) with L_x the system size in the x direction, and similar relations for k_y , etc. One then has⁷²

$$\begin{aligned}\Pi_j(\mathbf{k}, t) &= \frac{1}{\sqrt{V}} \int d^d r e^{-i\mathbf{k}\cdot\mathbf{r}} \frac{\delta L}{\delta \dot{\psi}_j(\mathbf{r}, t)} \\ &= \frac{1}{\sqrt{V}} \int d^d r e^{-i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{k}'} \frac{\partial L}{\partial \dot{\psi}_j(\mathbf{k}', t)} \frac{\delta \dot{\psi}_j(\mathbf{k}', t)}{\delta \dot{\psi}_j(\mathbf{r}, t)}.\end{aligned}\tag{1.669}$$

Since

$$\frac{\delta \dot{\psi}_j(\mathbf{k}', t)}{\delta \dot{\psi}_j(\mathbf{r}, t)} = \frac{e^{-i\mathbf{k}'\cdot\mathbf{r}}}{\sqrt{V}},\tag{1.670}$$

we finally obtain

$$\begin{aligned}\Pi_j(\mathbf{k}, t) &= \frac{1}{V} \sum_{\mathbf{k}'} \int d^d r e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}} \frac{\partial L}{\partial \dot{\psi}_j(\mathbf{k}', t)} \\ &= \sum_{\mathbf{k}'} \delta_{\mathbf{k}+\mathbf{k}', 0} \frac{\partial L}{\partial \dot{\psi}_j(\mathbf{k}', t)} \\ &= \frac{\partial L}{\partial \dot{\psi}_j(-\mathbf{k}, t)}.\end{aligned}\tag{1.671}$$

Symmetries and Noether's theorem

Suppose we describe the system with two fields, $\psi_j(x)$ and $\psi'_j(x)$, corresponding to Lagrangian densities $\mathcal{L}(\psi_j(x), \partial_\mu \psi_j(x))$ and $\mathcal{L}'(\psi'_j(x), \partial_\mu \psi'_j(x))$, respectively.⁷³ Here $\mu = 0, x, \dots$, $\partial_0 = \partial_t$ and $\psi_j(x) = \psi_j(\mathbf{r}, t)$. The transformation $\psi_j(x) \rightarrow \psi'_j(x)$ can arise from a genuine transformation of the field (such as a rotation for a N -component vector field $\boldsymbol{\psi} = (\psi_1, \dots, \psi_N)$) or a mere transformation of the space-time coordinates (such as a space translation $\psi_j(\mathbf{r}, t) \rightarrow \psi_j(\mathbf{r} + \mathbf{a}, t)$).⁷⁴ Since both fields refer to the same system, we must have $\mathcal{L}(\psi_j, \partial_\mu \psi_j) = \mathcal{L}'(\psi'_j, \partial_\mu \psi'_j)$ (up to a total time or space derivative), i.e. $S'[\psi'] = S[\psi]$. If $\mathcal{L}'(\psi'_j, \partial_\mu \psi'_j)$ and $\mathcal{L}(\psi'_j, \partial_\mu \psi'_j)$ differ only by a total time or space derivative, i.e. $S'[\psi'] = S[\psi']$, then the equation of motion of $\psi'_j(x)$ is identical to that of $\psi_j(x)$ and the system is invariant in the transformation $\psi_j(x) \rightarrow \psi_j(x')$.

⁷²Note that as long as the system volume V is kept finite, \mathbf{k} is not a continuous variable and $\partial L / \partial \dot{\psi}_j(\mathbf{k}, t)$ is a usual derivative (not a functional derivative).

⁷³See footnote 63 page 124.

⁷⁴Alternatively, the symmetry transformation can be defined by a change of space-time coordinates $x \rightarrow x'$ together with a change of the field, i.e. $\psi_j(x) \rightarrow \psi'_j(x')$. The transformed action satisfies $S'[\psi'_j] = \int d^{d+1}x' \mathcal{L}'(\psi'_j(x'), \partial_{\mu'} \psi'_j(x')) = \int d^{d+1}x \mathcal{L}(\psi_j(x), \partial_\mu \psi_j(x))$ and the condition for invariance reads $S'[\psi'] = S[\psi']$. In the text, we adopt the point of view that the transformation $x \rightarrow x'$ is included in the transformation of the field $\psi_j(x) \rightarrow \psi'_j(x)$.

To derive Noether's theorem, we express the fact that the change

$$\delta S = \int d^{d+1}x \{ \mathcal{L}(\psi'_j(x), \partial_\mu \psi'_j(x)) - \mathcal{L}(\psi_j(x), \partial_\mu \psi_j(x)) \} = 0 \quad (1.672)$$

in the action $S[\psi]$ vanishes if the system is invariant in the transformation $\psi_j(x) \rightarrow \psi'_j(x)$ (this follows from the two conditions $S'[\psi'] = S[\psi]$ and $S'[\psi'] = S[\psi']$). Let us consider an infinitesimal (continuous) transformation,

$$\psi_j(x) \rightarrow \psi_j(x) + i\epsilon F_j(x) \quad (\epsilon \rightarrow 0), \quad (1.673)$$

which satisfies (1.672). The Lagrangian density \mathcal{L} is invariant up to a total derivative

$$\mathcal{L}(\psi_j, \partial_\mu \psi_j) \rightarrow \mathcal{L}(\psi_j, \partial_\mu \psi_j) + \epsilon \sum_\mu \partial_\mu \mathcal{F}_\mu(\psi_j), \quad (1.674)$$

where $\mu = 0, x, \dots$. Equations (1.673) and (1.674) imply

$$\sum_j \left[\frac{\partial \mathcal{L}}{\partial \psi_j(x)} i F_j(x) + \sum_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu \psi_j(x))} i \partial_\mu F_j(x) \right] = \sum_\mu \partial_\mu \mathcal{F}_\mu, \quad (1.675)$$

i.e.

$$\begin{aligned} \sum_j \left[\frac{\partial \mathcal{L}}{\partial \psi_j(x)} i F_j(x) + \sum_\mu \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\mu \psi_j(x))} i \partial_\mu F_j(x) \right) \right. \\ \left. - \sum_\mu \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\mu \psi_j(x))} \right) i F_j(x) \right] = \sum_\mu \partial_\mu \mathcal{F}_\mu. \end{aligned} \quad (1.676)$$

If we assume that the field $\psi_j(x)$ satisfies the classical equations of motion (1.664), equation (1.676) becomes

$$\sum_{j,\mu} \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\mu \psi_j(x))} i F_j(x) \right) = \sum_\mu \partial_\mu \mathcal{F}_\mu. \quad (1.677)$$

We deduce the existence of a conserved (divergenceless) current $(j_0(x), \mathbf{j}(x))$,

$$\begin{aligned} \sum_\mu \partial_\mu j_\mu(x) &= 0, \\ j_\mu(x) &= -i \sum_j \frac{\partial \mathcal{L}}{\partial (\partial_\mu \psi_j(x))} F_j(x) + \mathcal{F}_\mu(x). \end{aligned} \quad (1.678)$$

The continuity equation implies the existence of a conserved (time-independent) charge,

$$Q = \int d^d r j_0(x), \quad \frac{dQ}{dt} = 0. \quad (1.679)$$

In classical field theory, Noether's theorem states that for any continuous transformation which leaves the action invariant, there is a density $j_0(x)$ and a current $\mathbf{j}(x)$ which satisfy the continuity equation $\partial_t j_0(x) + \nabla \cdot \mathbf{j}(x) = 0$.

For a Lagrangian density $\mathcal{L}(\psi_j, \nabla\psi_j, \dot{\psi}_j)$ which does not depend explicitly on time, an infinitesimal time translation $\psi_j(x) \rightarrow \psi_j(x) - \epsilon\dot{\psi}_j(x)$ gives $F_j(x) = i\dot{\psi}_j(x)$ and $\mathcal{F}_\mu = -\delta_{\mu,0}\mathcal{L}$. The density

$$j_0(x) = \sum_j \Pi_j(x) \dot{\psi}_j(x) - \mathcal{L} \quad (1.680)$$

is the Hamiltonian density and the conserved charge

$$\int d^d r j_0(x) = H \quad (1.681)$$

is the Hamiltonian. Similarly, for a space translation $\psi_j(x) \rightarrow \psi_j(x) + \epsilon\partial_\mu\psi_j(x)$ along the μ axis, $F_j(x) = -i\partial_\mu\psi_j(x)$ and $\mathcal{F}_\nu = \delta_{\nu,\mu}\mathcal{L}$. This gives

$$\mathbf{j}_0(x) = -\sum_j \Pi_j(x) \nabla\psi_j(x) \quad (1.682)$$

(we use the fact that the axis μ is arbitrary) and the conserved charged

$$\int d^d r \mathbf{j}_0(x) = -\int d^d r \sum_j \Pi_j(x) \nabla\psi_j(x) = \mathbf{P} \quad (1.683)$$

is naturally interpreted as the momentum carried by the field. Finally, for a space rotation about an arbitrary axis \mathbf{n} , $\psi_j(x) \rightarrow \psi_j(x) + \epsilon(\mathbf{n} \times \mathbf{r}) \cdot \nabla\psi_j(x)$ (we consider a three-dimensional system), we obtain

$$j_0(x) = -\sum_j \Pi_j(x) (\mathbf{n} \times \mathbf{r}) \cdot \nabla\psi_j(x) = -\sum_j \Pi_j(x) \mathbf{n} \cdot (\mathbf{r} \times \nabla)\psi_j(x), \quad (1.684)$$

which leads to the conservation of the angular momentum

$$\mathbf{J} = -\int d^3 r \sum_j \Pi_j(x) (\mathbf{r} \times \nabla)\psi_j(x). \quad (1.685)$$

Classical electromagnetism

Classical electromagnetism follows from the Lagrangian

$$\begin{aligned} L = \frac{m}{2} \sum_i \dot{\mathbf{r}}_i^2 + \frac{\epsilon_0}{2} \int d^3 r \left\{ [\nabla\phi(\mathbf{r}, t) + \partial_t \mathbf{A}(\mathbf{r}, t)]^2 - c_l^2 [\nabla \times \mathbf{A}(\mathbf{r}, t)]^2 \right\} \\ - \int d^3 r [\phi(\mathbf{r}, t) \rho(\mathbf{r}, t) - \mathbf{J}(\mathbf{r}, t) \cdot \mathbf{A}(\mathbf{r}, t)] \end{aligned} \quad (1.686)$$

(c_l denotes the velocity of light). L is a function of the positions \mathbf{r}_i and velocities $\dot{\mathbf{r}}_i$ of the particles and a functional of the electromagnetic potentials $\phi(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$. The electric and magnetic fields can be expressed as $\mathbf{E} = -\nabla\phi - \partial_t \mathbf{A}$ and $\mathbf{B} = \nabla \times \mathbf{A}$. The matter-field coupling involves the charge and current densities, $\rho(\mathbf{r}, t) = e \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$ and $\mathbf{J}(\mathbf{r}, t) = e \sum_i \dot{\mathbf{r}}_i \delta(\mathbf{r} - \mathbf{r}_i)$, where e is the charge of the particles. Using⁷⁵

$$\begin{aligned} \frac{\partial L}{\partial \dot{\mathbf{r}}_i} &= m\dot{\mathbf{r}}_i + e\mathbf{A}(\mathbf{r}_i, t), \\ \frac{\partial L}{\partial \mathbf{r}_i} &= -e\nabla\phi(\mathbf{r}_i, t) + e(\dot{\mathbf{r}}_i \cdot \nabla)\mathbf{A}(\mathbf{r}_i, t) + e\dot{\mathbf{r}}_i \times (\nabla \times \mathbf{A}(\mathbf{r}_i, t)), \end{aligned} \quad (1.687)$$

⁷⁵We have used the vector identity $\nabla(\mathbf{A} \cdot \mathbf{B}) = (\mathbf{A} \cdot \nabla)\mathbf{B} + (\mathbf{B} \cdot \nabla)\mathbf{A} + \mathbf{A} \times (\nabla \times \mathbf{B}) + \mathbf{B} \times (\nabla \times \mathbf{A})$ to obtain the second of equations (1.687).

we find that the Euler-Lagrange equation

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\mathbf{r}}_i} = \frac{\partial L}{\partial \mathbf{r}_i} \quad (1.688)$$

reproduces the Newton-Lorentz equation

$$m\ddot{\mathbf{r}}_i = e\mathbf{E}(\mathbf{r}_i, t) + e\dot{\mathbf{r}}_i \times \mathbf{B}(\mathbf{r}_i, t). \quad (1.689)$$

Similarly, from

$$\begin{aligned} \frac{\delta L}{\delta \dot{\phi}(\mathbf{r}, t)} &= 0, \\ \frac{\delta L}{\delta \phi(\mathbf{r}, t)} &= -\epsilon_0[\nabla^2 \phi(\mathbf{r}, t) + \nabla \cdot \mathbf{A}(\mathbf{r}, t)] - \rho(\mathbf{r}, t), \end{aligned} \quad (1.690)$$

and

$$\begin{aligned} \frac{\delta L}{\delta \dot{\mathbf{A}}(\mathbf{r}, t)} &= \epsilon_0[\nabla \phi(\mathbf{r}, t) + \dot{\mathbf{A}}(\mathbf{r}, t)], \\ \frac{\delta L}{\delta \mathbf{A}(\mathbf{r}, t)} &= -\epsilon_0 c_t^2 \nabla \times (\nabla \times \mathbf{A}(\mathbf{r}, t)) + \mathbf{J}(\mathbf{r}, t), \end{aligned} \quad (1.691)$$

as well as the Euler-Lagrange equations

$$\begin{aligned} \frac{d}{dt} \frac{\delta L}{\delta \dot{\phi}(\mathbf{r}, t)} &= \frac{\delta L}{\delta \phi(\mathbf{r}, t)}, \\ \frac{d}{dt} \frac{\delta L}{\delta \dot{\mathbf{A}}(\mathbf{r}, t)} &= \frac{\delta L}{\delta \mathbf{A}(\mathbf{r}, t)}, \end{aligned} \quad (1.692)$$

we deduce the Maxwell equations

$$\begin{aligned} \nabla \cdot \mathbf{E}(\mathbf{r}, t) &= \frac{\rho(\mathbf{r}, t)}{\epsilon_0}, \\ \nabla \times \mathbf{B}(\mathbf{r}, t) &= \mu_0 \mathbf{J}(\mathbf{r}, t) + \frac{1}{c_t^2} \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t}. \end{aligned} \quad (1.693)$$

1.B Review of quantum mechanics⁷⁶

In this section, we review elementary aspects of quantum mechanics and introduce the concept of quantum fields which is discussed at length in section 1.2.

1.B.1 The postulates of quantum mechanics

State space

To any physical system, we associate a Hilbert space \mathcal{H} called the state space. A Hilbert space is a vector space with a inner product (or scalar product).⁷⁷ In Dirac's

⁷⁶See, for instance, Refs. [22, 23, 24, 25].

⁷⁷For a vector space to be a Hilbert space, it must also be complete: if a sequence of vectors is Cauchy, then it converges to some limit in the space.

notation a vector Ψ is represented by a ket $|\Psi\rangle$. Physical states are represented by rays in the Hilbert space. A ray is a set of normalized vectors which differ only by a phase factor. Thus $|\Psi\rangle$ and $|\Psi'\rangle$ belong to the same ray if $|\Psi'\rangle = e^{i\alpha}|\Psi\rangle$ (α real). To each ket $|\Psi\rangle$, one can associate a bra $\langle\Psi|$ which is an element of the dual space \mathcal{H}^* and such that the action of $\langle\Psi|$ on $|\Phi\rangle$ yields the scalar product $\langle\Psi|\Phi\rangle$ between $|\Psi\rangle$ and $|\Phi\rangle$.⁷⁸

We can define coordinates in the state space by choosing a complete orthonormal basis, i.e. a set $\{|n\rangle\}$ of vectors satisfying

$$\langle n|m\rangle = \delta_{n,m} \quad (1.694)$$

and the closure relation

$$\sum_n |n\rangle\langle n| = 1, \quad (1.695)$$

where the symbol “1” in the rhs denotes the identity operator acting in \mathcal{H} .

Observables

To any measurable quantity A we associate an Hermitean operator \hat{A} whose normalized eigenvectors $|n\rangle$ form an orthonormal basis of the Hilbert space \mathcal{H} .⁷⁹ Such an operator is called an observable. In a given basis $\{|n\rangle\}$, \hat{A} is defined by its matrix elements $\langle n|\hat{A}|m\rangle$.

The only possible result of the measurement of the physical quantity A is one of the eigenvalues a_n of the operator \hat{A} with probability $\mathcal{P}(a_n) = |\langle n|\Psi\rangle|^2$ (we assume $\langle\Psi|\Psi\rangle = 1$). The expectation value of the observable \hat{A} is therefore

$$\langle\hat{A}\rangle = \sum_n \mathcal{P}(a_n) a_n = \sum_n \langle\Psi|n\rangle a_n \langle n|\Psi\rangle = \langle\Psi|\hat{A}|\Psi\rangle \quad (1.696)$$

and its statistical fluctuations (of quantum origin) are given by the variance

$$\Delta A^2 = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2 = \langle\Psi|(\hat{A} - \langle\hat{A}\rangle)^2|\Psi\rangle. \quad (1.697)$$

If the eigenvalue a_n is measured then the state of the system after the measurement is the corresponding eigenstate $|n\rangle$ of the observable \hat{A} (collapse of the state vector).

Coordinate and momentum representations

For a spinless particle moving in a d -dimensional space, a convenient basis is given by the eigenstates $|\mathbf{r}\rangle$ of the position operator $\hat{\mathbf{r}}$: $\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle$. These states are not normalizable and therefore not physical states. They satisfy

$$\langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r} - \mathbf{r}') \quad \text{and} \quad \int d^d r |\mathbf{r}\rangle\langle\mathbf{r}| = 1. \quad (1.698)$$

Any state can be expanded on this basis as

$$|\Psi\rangle = \int d^d r \Psi(\mathbf{r})|\mathbf{r}\rangle, \quad (1.699)$$

⁷⁸The dual space \mathcal{H}^* is defined as the set of all linear functionals on \mathcal{H} .

⁷⁹An operator \hat{A} is Hermitean if it is equal to its adjoint \hat{A}^\dagger , where \hat{A}^\dagger is defined by $\langle\Psi|\hat{A}^\dagger|\Phi\rangle = \langle\Phi|\hat{A}|\Psi\rangle^*$. To the ket $\hat{A}|\Psi\rangle$ corresponds the bra $\langle\Psi|\hat{A}^\dagger$.

where $\Psi(\mathbf{r}) = \langle \mathbf{r} | \Psi \rangle$ is the wavefunction in the coordinate representation. If the state is normalized,

$$\langle \Psi | \Psi \rangle = \int d^d r |\Psi(\mathbf{r})|^2 = 1, \quad (1.700)$$

$|\Psi(\mathbf{r})|^2$ gives the probability density for the particle to be at point \mathbf{r} .

Another useful basis is given by the eigenstates $|\mathbf{p}\rangle$ of the momentum operator $\hat{\mathbf{p}}$: $\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle$. They satisfy

$$|\mathbf{p}\rangle = \int d^d r \langle \mathbf{r} | \mathbf{p} \rangle |\mathbf{r}\rangle = \frac{1}{\sqrt{V}} \int d^d r e^{i\mathbf{p}\cdot\mathbf{r}} |\mathbf{r}\rangle, \quad (1.701)$$

or the inverse relation

$$|\mathbf{r}\rangle = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{r}} |\mathbf{p}\rangle \quad (1.702)$$

($V = L^d$ is the volume of the system), as well as the closure relation

$$\sum_{\mathbf{p}} |\mathbf{p}\rangle \langle \mathbf{p}| = 1. \quad (1.703)$$

The wavefunction in the \mathbf{p} representation is the Fourier transform of $\Psi(\mathbf{r})$,

$$\Psi(\mathbf{p}) = \langle \mathbf{p} | \Psi \rangle = \frac{1}{\sqrt{V}} \int d^d r e^{-i\mathbf{p}\cdot\mathbf{r}} \Psi(\mathbf{r}). \quad (1.704)$$

For periodic boundary conditions, $\Psi(\mathbf{r} + L\hat{\mathbf{x}}) = \Psi(\mathbf{r} + L\hat{\mathbf{y}}) = \dots = \Psi(\mathbf{r})$,⁸⁰ \mathbf{p} is a discrete variable which takes quantized value

$$p_\mu = \frac{2\pi}{L} n_\mu, \quad n_\mu \in Z \quad (\mu = x, y, \dots). \quad (1.705)$$

When the volume of the system tends to infinity, \mathbf{p} becomes a continuous variable and

$$\lim_{V \rightarrow \infty} \frac{1}{V} \sum_{\mathbf{p}} = \int \frac{d^d p}{(2\pi)^d}. \quad (1.706)$$

Canonical quantization

In the Hamiltonian formalism of classical mechanics, the system is described by N coordinates $q_i(t)$ and N conjugate momenta $p_i(t)$. In the quantum formalism, these variables become operators $\hat{q}_i(t), \hat{p}_i(t)$ acting in the state space \mathcal{H} . For any physical quantity $A(p_i, q_i, t)$ of the classical theory one then obtains an observable $\hat{A}(t) \equiv A(\hat{p}_i(t), \hat{q}_i(t), t)$ (Heisenberg's correspondence principle). When this correspondence rule yields products of the non-commuting operators \hat{p}_i and \hat{q}_i , the order of the operators should be determined by additional conditions such as the Hermiticity of the observable $\hat{A}(t)$.

⁸⁰ $\hat{\mathbf{x}}$ denotes the unit vector in the x direction, etc.

Moreover the Poisson bracket $[A, B]$ is replaced by the commutator of the two corresponding operators,

$$[A, B] \equiv \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right) \rightarrow \frac{1}{i\hbar} (\hat{A}\hat{B} - \hat{B}\hat{A}) \equiv \frac{1}{i\hbar} [\hat{A}, \hat{B}]. \quad (1.707)$$

The factor i ensures that the rhs in (1.707) is Hermitean is both \hat{A} and \hat{B} are, and the factor \hbar preserves the units of the Poisson bracket. Equations (1.651) yield the equal-time commutation relations

$$\begin{aligned} [\hat{q}_i(t), \hat{q}_j(t)] &= [\hat{p}_i(t), \hat{p}_j(t)] = 0, \\ [\hat{q}_i(t), \hat{p}_j(t)] &= i\hbar \delta_{i,j}. \end{aligned} \quad (1.708)$$

The time evolution of these operators is deduced from (1.648),

$$\begin{aligned} \frac{d}{dt} \hat{q}_i(t) &= \frac{1}{i\hbar} [\hat{q}_i(t), \hat{H}(t)], \\ \frac{d}{dt} \hat{p}_i(t) &= \frac{1}{i\hbar} [\hat{p}_i(t), \hat{H}(t)], \end{aligned} \quad (1.709)$$

where $\hat{H}(t) \equiv H(\hat{p}_i(t), \hat{q}_i(t), t)$ is the quantum Hamiltonian. For an observable $\hat{A}(t) \equiv A(\hat{p}_i(t), \hat{q}_i(t), t)$, equation (1.649) yields

$$\frac{d\hat{A}(t)}{dt} = \frac{\partial \hat{A}(t)}{\partial t} + \frac{1}{i\hbar} [\hat{A}(t), \hat{H}(t)], \quad (1.710)$$

where $\partial \hat{A}/\partial t$ comes from the explicit time dependence of the operator $\hat{A}(t)$. From (1.710), we deduce that the time evolution of the expectation value $\langle \hat{A}(t) \rangle = \langle \Psi | \hat{A}(t) | \Psi \rangle$ of an observable is given by

$$\frac{d\langle \hat{A}(t) \rangle}{dt} = \left\langle \frac{\partial \hat{A}(t)}{\partial t} \right\rangle + \frac{1}{i\hbar} \langle [\hat{A}(t), \hat{H}(t)] \rangle \quad (1.711)$$

(Ehrenfest's equation). An observable which commutes with the Hamiltonian \hat{H} and does not depend on time explicitly is a constant of motion.

So far we have discussed the Heisenberg picture of quantum mechanics where the state vector $|\Psi_H\rangle$ is time independent while the dynamics of the system is given by the time evolution of the observables $\hat{A}_H(t)$ [Eq. (1.710)]. Alternatively one can choose the Schrödinger picture where the state vector $|\Psi_S(t)\rangle$ is time dependent while the operators $\hat{A}_S(t)$ are not (except for a possible explicit time dependence). Both descriptions are related by a unitary transformation,

$$\begin{aligned} \hat{A}_H(t) &= \hat{U}^\dagger(t, t_0) \hat{A}_S(t) \hat{U}(t, t_0), \\ |\Psi_H\rangle &= \hat{U}^\dagger(t, t_0) |\Psi_S(t)\rangle \end{aligned} \quad (1.712)$$

$(\hat{U}^\dagger(t, t_0) \hat{U}(t, t_0) = \hat{U}(t, t_0) \hat{U}^\dagger(t, t_0) = 1)$, which preserves the value of any matrix element

$$\langle \Psi_H | \hat{A}_H(t) | \Phi_H \rangle = \langle \Psi_H | \hat{U}^\dagger(t, t_0) \hat{A}_S(t) \hat{U}(t, t_0) | \Phi_H \rangle = \langle \Psi_S(t) | \hat{A}_S(t) | \Phi_S(t) \rangle. \quad (1.713)$$

t_0 is some arbitrary fixed time. If the two descriptions coincide at t_0 then $\hat{U}(t_0, t_0) = 1$ and the equation

$$|\Psi_S(t)\rangle = \hat{U}(t, t_0)|\Psi_H\rangle = \hat{U}(t, t_0)|\Psi_S(t_0)\rangle \quad (1.714)$$

shows that $\hat{U}(t, t_0)$ is the time evolution operator in the Schrödinger picture. The unitary operator $\hat{U}(t, t_0)$ is further defined by its time evolution equation

$$i\hbar \frac{d}{dt} \hat{U}(t, t_0) = \hat{H}_S(t) \hat{U}(t, t_0), \quad (1.715)$$

where $\hat{H}_S(t)$ is the Hamiltonian in the Schrödinger picture. Equation (1.715) implies that the state vector $|\Psi_S(t)\rangle$ obeys the Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi_S(t)\rangle = \hat{H}_S(t) |\Psi_S(t)\rangle. \quad (1.716)$$

From (1.712) and (1.715), one deduces

$$\frac{d}{dt} \hat{q}_{iH}(t) = \frac{1}{i\hbar} [\hat{q}_{iH}(t), \hat{H}_H(t)] + \hat{U}^\dagger(t, t_0) \frac{d\hat{q}_{iS}(t)}{dt} \hat{U}(t, t_0) \quad (1.717)$$

and a similar equation for $\hat{p}_{iH}(t)$. Comparing with (1.709), we conclude that the operators \hat{q}_{iS} and \hat{p}_{iS} are time independent in the Schrödinger picture. It follows that the time dependence of an observable $\hat{A}_S(t) \equiv A(\hat{p}_{iS}, \hat{q}_{iS}, t)$ in the Schrödinger picture can only be explicit. For an arbitrary observable, equations (1.712) and (1.715) imply

$$\begin{aligned} \frac{d}{dt} \hat{A}_H(t) &= \frac{1}{i\hbar} [\hat{A}_H(t), \hat{H}_H(t)] + \hat{U}^\dagger(t, t_0) \frac{\partial \hat{A}_S(t)}{\partial t} \hat{U}(t, t_0) \\ &= \frac{1}{i\hbar} [\hat{A}_H(t), \hat{H}_H(t)] + \frac{\partial \hat{A}_H(t)}{\partial t} \end{aligned} \quad (1.718)$$

in agreement with the Heisenberg equation of motion (1.710). When the Hamiltonian $\hat{H}_S(t) \equiv \hat{H}$ in the Schrödinger picture is time independent, the time evolution operator takes the form

$$\hat{U}(t, t_0) = \hat{U}(t - t_0) = \exp\left(-\frac{i}{\hbar} \hat{H}(t - t_0)\right) \quad (1.719)$$

and the Hamiltonian $\hat{H}_H(t) = \hat{H}$ in the Heisenberg picture is also time independent.

1.B.2 Quantum fields

To quantize a classical field theory defined by its Hamiltonian density $\mathcal{H}(\Pi_j, \psi_j, \nabla\psi_j)$ (Sec. 1.A.2), we promote the field $\psi_j(\mathbf{r}, t)$ and its conjugate variable $\Pi_j(\mathbf{r}, t)$ to operators acting in the state space \mathcal{H} and satisfying the equal-time commutation relations

$$\begin{aligned} [\hat{\psi}_j(\mathbf{r}, t), \hat{\psi}_{j'}(\mathbf{r}', t)] &= [\hat{\Pi}_j(\mathbf{r}, t), \hat{\Pi}_{j'}(\mathbf{r}', t)] = 0, \\ [\hat{\psi}_j(\mathbf{r}, t), \hat{\Pi}_{j'}(\mathbf{r}', t)] &= i\hbar \delta_{j,j'} \delta(\mathbf{r} - \mathbf{r}'). \end{aligned} \quad (1.720)$$

In the Heisenberg picture, the quantum fields $\hat{\psi}_j(\mathbf{r}, t)$ and $\hat{\Pi}_j(\mathbf{r}, t)$ are time dependent while the state of the system is described by a time independent ket $|\Psi\rangle$. Alternatively one can use the Schrödinger picture as explained in the preceding section.

In section 1.9 we use this procedure to quantize the classical electromagnetic field.⁸¹ A similar approach can be used to quantize a system of particles.⁸² Let us first consider a single particle. Its wavefunction satisfies the Schrödinger equation (1.716),

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \hat{H}\Psi(\mathbf{r}, t). \quad (1.721)$$

We can see (1.721) as a wave equation for the matter, analogous to Maxwell's equations for electromagnetic waves, where $\Psi(\mathbf{r}, t)$ is considered as a classical field (the Schrödinger field) rather than the wavefunction of a single particle. Equation (1.721) derives from a Lagrangian. The canonical quantization procedure leads to Hermitean conjugate quantum fields $\hat{\psi}(\mathbf{r}, t)$ and $\hat{\psi}^\dagger(\mathbf{r}, t)$ whose quantized excitations correspond to the particles of the system. While the standard commutation relations

$$\begin{aligned} [\hat{\psi}(\mathbf{r}, t), \hat{\psi}(\mathbf{r}', t)] &= [\hat{\psi}^\dagger(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', t)] = 0, \\ [\hat{\psi}(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', t)] &= \delta(\mathbf{r} - \mathbf{r}') \end{aligned} \quad (1.722)$$

can be used for bosons, they would violate the Pauli principle for fermions. In this case, it is necessary to use anticommutators instead of commutators in (1.722). This quantization procedure is often (improperly) called “second quantization” as it seems to be based on a quantization of the Schrödinger equation, which is itself a quantum equation of motion. In fact, $\psi(\mathbf{r}, t)$ should be seen as a classical field (not the wave function of a quantum particle) which is quantized only once.

While the introduction of a classical field is a necessary step to quantize relativistic particles [7], a different quantization procedure, which does not rely on a classical field, can be used for non-relativistic particles. In this approach, one first constructs the Hilbert space (Fock space) of the many-particle system and then directly define the quantum fields $\hat{\psi}(\mathbf{r}, t)$ and $\hat{\psi}^\dagger(\mathbf{r}, t)$ by their action on the many-body states. This is the route followed in section 1.2.

1.C Review of statistical physics⁸³

In this section, we review the basis of quantum statistical physics.

1.C.1 Macrostates – Density operators

In quantum mechanics, the system is described by a normalized vector $|\Psi\rangle$ of the Hilbert space. Such a state, where the system is completely known or ideally prepared (*via* the control of a complete set of commuting observables), is called a microstate or a pure state. In statistical physics, one is interested in macroscopic systems with a very large number of degrees of freedom. These systems are never ideally prepared or completely known and are usually described by the specification of a small number of macroscopic variables. On the microscopic scale, a partially known or incompletely prepared system is described by a macrostate (or statistical mixture), i.e. by the set

⁸¹An elementary example, the quantization of the classical harmonic string, is also discussed in section 1.1.2.

⁸²For a detailed discussion, see Refs. [22] (chapter XIII) and [16] (chapter II and exercise $D_{II.8}$).

⁸³This section closely follows chapters 2-5 of Ref. [26].

of possible microstates $|\Psi_\lambda\rangle$ and the corresponding probabilities q_λ . In this statistical description, a “system” denotes an element of a statistical ensemble of systems, all prepared under the same conditions.

Density operator

All the information about the macrostate is contained in the density operator

$$\hat{\rho} = \sum_{\lambda} |\Psi_\lambda\rangle q_\lambda \langle\Psi_\lambda|, \quad (1.723)$$

where the probabilities q_λ are positive and normalized: $\sum_{\lambda} q_\lambda = 1$. For instance, the expectation value of an observable \hat{A} is given by

$$\langle\hat{A}\rangle = \sum_{\lambda} q_\lambda \langle\Psi_\lambda|\hat{A}|\Psi_\lambda\rangle = \text{Tr}(\hat{\rho}\hat{A}). \quad (1.724)$$

The random character of the measurement has now two origins, the probabilities q_λ on the one hand and the quantum nature of the microstates $|\Psi_\lambda\rangle$ on the other hand.

Two different statistical mixtures, $\{|\Psi_\lambda\rangle, q_\lambda\}$ and $\{|\Psi'_\mu\rangle, q'_\mu\}$, can lead to the same density operator and therefore the same physical reality. Thus the only meaningful representation of macrostates is given by density operators. A microstate $|\Psi\rangle$ corresponds to the density operator $\hat{\rho} = |\Psi\rangle\langle\Psi|$. Note that all state vector $|\Psi\rangle$ belonging to the same ray (i.e. differing only by a phase factor) yield the same density operator.

The definition (1.723) gives the following properties:

1. $\hat{\rho}$ is Hermitean: $\hat{\rho}^\dagger = \hat{\rho}$.
2. $\hat{\rho}$ has unit trace: $\text{Tr}(\hat{\rho}) = 1$.
3. $\hat{\rho}$ is non-negative: $\langle\Psi|\hat{\rho}|\Psi\rangle \geq 0, \quad \forall |\Psi\rangle \in \mathcal{H}$.

Conversely, any operator $\hat{\rho}$ satisfying these properties can be written in the basis of its eigenstates,

$$\hat{\rho} = \sum_m |m\rangle p_m \langle m|. \quad (1.725)$$

It follows from the properties (2) and (3) that $p_m \geq 0$ and $\sum_m p_m = 1$, which allows us to regard p_m as the probability of the microstate $|m\rangle$.

Time evolution of the density operator

In the Schrödinger picture, the time evolution of the density operator is directly obtained from the Schrödinger equation satisfied by the states $|m\rangle$ [Eq. (1.725)],

$$i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}] \quad (1.726)$$

(Liouville-von Neumann's equation). The evolution of the expectation value of an observable follows from (1.726),

$$\frac{d}{dt} \text{Tr}(\hat{\rho}\hat{A}) = \frac{1}{i\hbar} \text{Tr}([\hat{H}, \hat{\rho}]\hat{A}) + \text{Tr}\left(\hat{\rho} \frac{\partial \hat{A}}{\partial t}\right) = \frac{1}{i\hbar} \langle[\hat{A}, \hat{H}]\rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle, \quad (1.727)$$

in agreement with Ehrenfest's equation (1.711). In the Heisenberg picture, the states $|m\rangle$ are time independent and $d\hat{\rho}/dt = 0$.

In statistical physics, one is often interested in a subsystem of the whole system. Knowing the density operator $\hat{\rho}$ of the system, it is possible to define a reduced density operator for the subsystem. Let us assume for instance that the system contains two subsystems a and b . The Hilbert space $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$ is then the tensor product of the Hilbert spaces of the subsystems. Let $\{|k_a, l_b\rangle\} = \{|k_a\rangle \otimes |l_b\rangle\}$ be a basis of \mathcal{H} . For an observable $\hat{A}_a \otimes 1_b$ acting only in \mathcal{H}_a , one has

$$\begin{aligned} \langle \hat{A}_a \rangle &= \text{Tr}[\hat{\rho}(\hat{A}_a \otimes 1_b)] \\ &= \sum_{k_a, l_b, k'_a, l'_b} \langle k_a, l_b | \hat{\rho} | k'_a, l'_b \rangle \langle k'_a, l'_b | \hat{A}_a \otimes 1_b | k_a, l_b \rangle \\ &= \sum_{k_a, l_b, k'_a} \langle k_a, l_b | \hat{\rho} | k'_a, l_b \rangle \langle k'_a | \hat{A}_a | k_a \rangle \\ &= \text{Tr}(\hat{\rho}_a \hat{A}_a), \end{aligned} \tag{1.728}$$

where

$$\hat{\rho}_a = \text{Tr}_b(\hat{\rho}) \tag{1.729}$$

is the density operator in the subsystem a . The definition of a density operator for a subsystem is particularly natural in the functional integral formalism where it relies on a partial integration of the degrees of freedom.

1.C.2 Statistical entropy – Boltzmann-Gibbs distribution

The knowledge of the system based on the density operator is incomplete. The missing information can be estimated by the statistical entropy

$$S = -k_B \sum_{m=1}^M p_m \ln p_m = -k_B \text{Tr}(\hat{\rho} \ln \hat{\rho}), \tag{1.730}$$

where the p_m 's are the probabilities of the states $|m\rangle$ that diagonalize the density operator. The factor k_B is *a priori* arbitrary. By choosing the Boltzmann constant, we ensure that the statistical entropy coincides with the thermodynamic entropy (see below). From the definition (1.730), we deduce the following properties:

1. S is a symmetric function of p_1, \dots, p_M .
2. S is non-negative and vanishes when the system is in a pure state (one probability equals one and all others vanish): $S(1, 0, \dots, 0) = 0$.
3. For M fixed, S is maximum when all probabilities are equal to $1/M$:

$$S\left(\frac{1}{M}, \dots, \frac{1}{M}\right) = k_B \ln M. \tag{1.731}$$

4. If we divide the microstates $\{|\Psi_m\rangle\}$ into two groups of states, $A = \{|\Psi_1\rangle|\cdots|\Psi_N\rangle\}$ and $B = \{|\Psi_{N+1}\rangle|\cdots|\Psi_M\rangle\}$, then the entropy satisfies the following additivity property,

$$S = S(q_A, q_B) + q_A S\left(\frac{p_1}{q_A}, \dots, \frac{p_N}{q_A}\right) + q_B S\left(\frac{p_{N+1}}{q_B}, \dots, \frac{p_M}{q_B}\right), \quad (1.732)$$

where

$$q_A = \sum_{m=1}^N p_m \quad \text{and} \quad q_B = \sum_{m=N+1}^M p_m. \quad (1.733)$$

The first term in (1.732) corresponds to the missing information due to the choice between the sets of states A and B . The second term comes from the missing information once we know that the system is in a microstate of the set A (hence the factor q_A). p_m/p_N is the conditional probability giving the probability to find the system in the microstate $|\Psi_m\rangle$ knowing that $|\Psi_m\rangle$ belongs to the set A . The last term of (1.732) has a similar interpretation with the role of the sets A and B interchanged.

While these properties are a consequence of the definition (1.730), one can proceed the other way round and show that the expression (1.730) of the statistical entropy follows from the above properties, the most important one being the additivity postulate (1.732).

The maximum statistical entropy principle

When some information about the system is known exactly (e.g. the energy and the volume of the system or the number of particles in a fluid), it is taken into account through the definition of the Hilbert space. If no other information is available, it is natural to use a statistical ensemble where the probabilities of the W possible microstates are equal. In macroscopic equilibrium, the macrostate is then defined by the density operator

$$\hat{\rho} = \sum_{m=1}^W |m\rangle \frac{1}{W} \langle m| \quad (1.734)$$

and the entropy is given by

$$S = k_B \ln W. \quad (1.735)$$

In many cases, however, the macrostate is characterized by the knowledge of the expectation values $\langle \hat{A}_i \rangle$ of some observables \hat{A}_i such as the Hamiltonian \hat{H} or the total number \hat{N} of particles (while other properties such as the volume may be known exactly). This happens for instance when the system is put into contact with a large system with which it can exchange energy or particles. This large system plays the role of a reservoir which fixes the mean value of the energy $\langle \hat{H} \rangle$ or the mean total number of particles $\langle \hat{N} \rangle$ in the system we are interested in. The density operator must then satisfy the constraints

$$\langle \hat{A}_i \rangle = \text{Tr}(\hat{\rho} \hat{A}_i). \quad (1.736)$$

The maximum statistical entropy principle states that the density operator $\hat{\rho}$ describing the system in macroscopic equilibrium is the one which maximizes the entropy while being compatible with the known information about the system. Any other choice would mean that we assumed possessing information which is actually not available and consequently would lead to biased predictions.

Boltzmann-Gibbs distribution

We are thus led to maximize the entropy $S = -k_B \text{Tr}(\hat{\rho} \ln \hat{\rho})$ with the constraints $\text{Tr}(\hat{\rho}) = 1$ and (1.736), and the fact that $\hat{\rho}$ must be Hermitean and non-negative. This can be done by introducing Lagrange multipliers λ_0, λ_i and requiring

$$-\text{Tr}(\hat{\rho} \ln \hat{\rho}) - \sum_i \lambda_i \text{Tr}(\hat{\rho} \hat{A}_i) - \lambda_0 \text{Tr}(\hat{\rho}) \quad (1.737)$$

to be stationary. When $\hat{\rho}$ changes by $\delta \hat{\rho}$, (1.737) changes by

$$-\text{Tr} \left[\delta \hat{\rho} \left(\ln \hat{\rho} + 1 + \sum_i \lambda_i \hat{A}_i + \lambda_0 \right) \right], \quad (1.738)$$

so that the stationary condition gives

$$\hat{\rho} = \exp \left(-1 - \lambda_0 - \sum_i \lambda_i \hat{A}_i \right). \quad (1.739)$$

The density operator $\hat{\rho}$ is Hermitean, since the observables \hat{A}_i are, and non-negative. Since $\text{Tr}(\hat{\rho}) = 1$, we can eliminate the Lagrange multiplier λ_0 . Defining the partition function

$$Z = e^{1+\lambda_0} = \text{Tr} e^{-\sum_i \lambda_i \hat{A}_i}, \quad (1.740)$$

we can rewrite the density operator as

$$\hat{\rho} = \frac{1}{Z} e^{-\sum_i \lambda_i \hat{A}_i}. \quad (1.741)$$

This expression, which corresponds to the Boltzmann-Gibbs distribution, gives the general form of the density operator in thermodynamic equilibrium when the averages of the constants of motion $\langle \hat{A}_i \rangle$ are given. To complete our derivation, we must show that equation (1.741) corresponds to a maximum of the statistical entropy (and not to a minimum). Write the entropy as

$$S(\hat{\rho}) = -k_B \langle \ln \hat{\rho} \rangle = k_B \ln Z + k_B \sum_i \lambda_i \langle \hat{A}_i \rangle \quad (1.742)$$

and use the fact that two non-negative operators \hat{X} and \hat{Y} satisfy the inequality

$$\text{Tr}(\hat{X} \ln \hat{Y}) - \text{Tr}(\hat{X} \ln \hat{X}) \leq \text{Tr}(\hat{Y}) - \text{Tr}(\hat{X}). \quad (1.743)$$

For $\hat{X} = \hat{\rho}'$ an arbitrary density operator and $\hat{Y} = \hat{\rho}$, this gives

$$\text{Tr}(\hat{\rho}' \ln \hat{\rho}) - \text{Tr}(\hat{\rho}' \ln \hat{\rho}') \leq 0, \quad (1.744)$$

and therefore

$$\begin{aligned}
 S(\hat{\rho}') &\leq -k_B \text{Tr}(\hat{\rho}' \ln \hat{\rho}) \\
 &\leq k_B \ln Z + k_B \sum_i \lambda_i \text{Tr}(\hat{\rho}' \hat{A}_i) \\
 &\leq S(\hat{\rho}),
 \end{aligned} \tag{1.745}$$

where we have used $\text{Tr}(\hat{\rho}' \hat{A}_i) = \text{Tr}(\hat{\rho} \hat{A}_i) = \langle \hat{A}_i \rangle$ to obtain the last inequality. Thus the Boltzmann-Gibbs distribution provides a statistical entropy which is larger than that of any density operator satisfying the same constraints.

To determine the Lagrange multipliers λ_i as a function of the expectation values $\langle \hat{A}_i \rangle$, we use

$$\langle \hat{A}_i \rangle = \frac{1}{Z} \text{Tr}(e^{-\sum_j \lambda_j \hat{A}_j} \hat{A}_i) = -\frac{\partial \ln Z}{\partial \lambda_i}. \tag{1.746}$$

In practice, we take the Lagrange multipliers λ_i as the parameters characterizing the equilibrium state rather than the expectation values $\langle \hat{A}_i \rangle$. (We discuss below their physical meaning when \hat{A}_i corresponds to the Hamiltonian or the total number of particles.) The correlations and the statistical fluctuations of the constants of motion \hat{A}_i can also be obtained from the derivatives of the partition function $Z(\lambda_i)$,

$$\langle \hat{A}_i \hat{A}_j \rangle - \langle \hat{A}_i \rangle \langle \hat{A}_j \rangle = \frac{\partial^2 \ln Z}{\partial \lambda_i \partial \lambda_j}. \tag{1.747}$$

Using (1.742) and (1.746), we can write the entropy as

$$S = k_B \ln Z - k_B \sum_i \lambda_i \frac{\partial \ln Z}{\partial \lambda_i}. \tag{1.748}$$

If the parameters λ_i characterizing the equilibrium change by an infinitesimal amount $d\lambda_i$,

$$d \ln Z = - \sum_i \langle \hat{A}_i \rangle d\lambda_i \tag{1.749}$$

and, using (1.748),

$$dS = k_B d \ln Z - k_B \sum_i \left(d\lambda_i \frac{\partial \ln Z}{\partial \lambda_i} - \lambda_i d\langle \hat{A}_i \rangle \right) = k_B \sum_i \lambda_i d\langle \hat{A}_i \rangle. \tag{1.750}$$

While Z is a function of λ_i , the natural variables for the entropy are the expectation values $\langle \hat{A}_i \rangle$, and

$$\frac{\partial S}{\partial \langle \hat{A}_i \rangle} = k_B \lambda_i. \tag{1.751}$$

Equations (1.746, 1.748, 1.751) show that $k_B \ln Z(\lambda_i)$ and $S(\langle \hat{A}_i \rangle)$ are related by a Legendre transform.

1.C.3 Statistical ensembles

In this section, we discuss the three most common statistical ensembles for a quantum fluid. The main results are summarized in table 1.3.

Microcanonical ensemble

In the microcanonical ensemble, the number of particles N and the volume V of the system are known exactly, while the energy is assumed to be between E and $E + \Delta E$. ΔE is a small energy interval as compared to the accuracy to which E is known, but large wrt the typical energy level spacing. The density operator and the entropy are then given by (1.734) and (1.735) where $W = \mathcal{D}(E)\Delta E$ is the number of possible microstates, with

$$\mathcal{D}(E) = \text{Tr}(E - \hat{H}) \quad (1.752)$$

the density of states of the system. Note that the dependence of $\hat{\rho}$ and S on E, V, N is not explicit but comes from that of W . The conjugate variables to E, N and V

$$\left. \frac{\partial S}{\partial E} \right|_{N,V} = \frac{1}{T}, \quad \left. \frac{\partial S}{\partial N} \right|_{E,V} = -\frac{\mu}{T}, \quad \left. \frac{\partial S}{\partial V} \right|_{E,N} = \frac{P}{T}, \quad (1.753)$$

are related to the temperature T , the chemical potential μ and the pressure P . These relations yield the usual thermodynamic definition of μ and P ,

$$\mu = \left. \frac{\partial E}{\partial N} \right|_{S,V} = -\frac{\left. \frac{\partial S}{\partial N} \right|_{E,V}}{\left. \frac{\partial S}{\partial E} \right|_{N,V}}, \quad P = -\left. \frac{\partial E}{\partial V} \right|_{S,N} = \frac{\left. \frac{\partial S}{\partial V} \right|_{E,N}}{\left. \frac{\partial S}{\partial E} \right|_{N,V}}. \quad (1.754)$$

Canonical ensemble

In the canonical ensemble, the number of particles and the volume are known exactly but the energy $E = \langle \hat{H} \rangle$ is known only on average. The corresponding Lagrange multiplier is denoted by β , and is related to the thermodynamic absolute temperature T by $\beta = 1/k_B T$ (see the discussion on statistical and thermodynamic entropies page 149). The density operator is given by

$$\hat{\rho} = \frac{1}{Z_C} e^{-\beta \hat{H}}, \quad (1.755)$$

where

$$Z_C(\beta, N, V) = \text{Tr} e^{-\beta \hat{H}} \quad (1.756)$$

is the canonical partition function. The entropy reads

$$S(E, N, V) = k_B \ln Z_C + k_B \beta E \quad (1.757)$$

and satisfies

$$\left. \frac{\partial S}{\partial E} \right|_{N,V} = k_B \beta \quad (1.758)$$

(see equations (1.742) and (1.751)). In the canonical ensemble, it is traditional to use as thermodynamic potential the Helmholtz free energy

$$F(T, N, V) = E - TS = -\frac{1}{\beta} \ln Z_C(\beta, N, V) \quad (1.759)$$

defined as the Legendre transform of the energy. Its differential reads

$$dF = -SdT + \mu dN - PdV, \quad (1.760)$$

where

$$S = -\frac{\partial F}{\partial T}\bigg|_{N,V}, \quad \mu = \frac{\partial E}{\partial N}\bigg|_{S,V} = \frac{\partial F}{\partial N}\bigg|_{T,V}, \quad P = -\frac{\partial E}{\partial V}\bigg|_{S,N} = -\frac{\partial F}{\partial V}\bigg|_{T,N}. \quad (1.761)$$

Grand canonical ensemble

In the grand canonical ensemble, both the energy $E = \langle \hat{H} \rangle$ and the number of particles $N = \langle \hat{N} \rangle$ are known on average. When the number of particles is not fixed, one must use a Hilbert space (the Fock space) which is constructed from the direct sum of the N -particle spaces (Sec. 1.2.1). The density operator

$$\hat{\rho} = \frac{1}{Z_G} e^{-\beta \hat{H} + \alpha \hat{N}} \quad (1.762)$$

is expressed in terms of the two Lagrange multipliers β and $-\alpha$, the grand canonical partition function being defined by

$$Z_G(\beta, \alpha, V) = \text{Tr} e^{-\beta \hat{H} + \alpha \hat{N}}. \quad (1.763)$$

The equilibrium entropy is given by

$$S(E, N, V) = k_B \ln Z_G + k_B \beta E - k_B \alpha N \quad (1.764)$$

and satisfies

$$\frac{\partial S}{\partial E}\bigg|_{N,V} = k_B \beta, \quad \frac{\partial S}{\partial N}\bigg|_{E,V} = -k_B \alpha. \quad (1.765)$$

From these equations, we can relate the chemical potential

$$\mu = \frac{\partial E}{\partial N}\bigg|_{S,V} = -\frac{\frac{\partial S}{\partial N}\big|_{E,V}}{\frac{\partial S}{\partial E}\big|_{N,V}} = \frac{\alpha}{\beta} \quad (1.766)$$

to the Lagrange multipliers, so that $\alpha = \beta\mu = \mu/k_B T$. In the grand canonical ensemble it is traditional to use as thermodynamic potential the grand potential

$$\Omega(T, \mu, V) = E - TS - \mu N = -\frac{1}{\beta} \ln Z_G(\beta, \alpha, V) \quad (1.767)$$

defined as a double Legendre transform of the energy. Its differential reads

$$d\Omega = -SdT - Nd\mu - PdV, \quad (1.768)$$

where

$$S = -\frac{\partial \Omega}{\partial T}\bigg|_{\mu,V}, \quad N = -\frac{\partial \Omega}{\partial \mu}\bigg|_{T,V}, \quad P = -\frac{\partial \Omega}{\partial V}\bigg|_{T,\mu}. \quad (1.769)$$

| Ensemble | Microcanonical | Canonical | Grand canonical |
|----------------------------|--|---|--|
| Variables | E, N, V | T, N, V | T, μ, V |
| Partition function | W | $Z_C = \text{Tr} e^{-\beta \hat{H}}$ | $Z_G = \text{Tr} e^{-\beta(\hat{H} - \mu \hat{N})}$ |
| Density operator | $\hat{\rho} = \sum_m m\rangle \frac{1}{W} \langle m $ | $\hat{\rho} = \frac{1}{Z_C} e^{-\beta \hat{H}}$ | $\hat{\rho} = \frac{1}{Z_G} e^{-\beta(\hat{H} - \mu \hat{N})}$ |
| Thermodynamic potential | Entropy $S(E, N, V) = k_B \ln W$ | Helmholtz free energy $F(T, N, V) = -\frac{1}{\beta} \ln Z_C = E - TS$ | Grand potential $\Omega(T, \mu, V) = -\frac{1}{\beta} \ln Z_G = E - TS - \mu N$ |
| | $dS = \frac{1}{T}(dE - \mu dN + PdV)$ | $dF = -SdT + \mu dN - PdV$ | $d\Omega = -SdT - Nd\mu - PdV$ |

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Table 1.3: Table of thermodynamic potentials.

Thermodynamic limit – Equivalence between ensembles

In the thermodynamic limit, the size of the system becomes very large wrt the typical microscopic scales and can be considered to be infinite. Extensive variables are proportional to the volume. For instance, the entropy reads

$$S(E, N, V) = V s \left(\frac{E}{V}, \frac{N}{V} \right), \quad (1.770)$$

where s reaches a finite limit for $V \rightarrow \infty$ with $E/V, N/V$ or α, β constant.

Let us consider a system in equilibrium in the canonical ensemble. The density operator $\hat{\rho}$ can be written in terms of the eigenstates $\{|m\rangle, \epsilon_m\}$ of the Hamiltonian,

$$\hat{\rho} = \sum_m |m\rangle p_m \langle m|, \quad (1.771)$$

where

$$p_m = \frac{e^{-\beta \epsilon_m}}{Z_C} \quad (1.772)$$

is the probability for the system to be in the microstate $|m\rangle$. Thus the system has a probability $p(E)dE$ to have an energy in the interval $[E, E + dE]$,

$$p(E) = \frac{e^{-\beta E}}{Z_C} \mathcal{D}(E), \quad (1.773)$$

where $\mathcal{D}(E)$ is the density of states [Eq. (1.752)]. $\mathcal{D}(E)$ is related to the microcanonical entropy $S(E)$ via $S(E) = k_B \ln \mathcal{D}(E) \Delta E$, where ΔE is the energy uncertainty in the microcanonical ensemble. This enables us to rewrite $p(E)$ as

$$p(E) = \frac{e^{-\beta E + k_B^{-1} S(E)}}{Z_C \Delta E} \propto e^{-\beta E + k_B^{-1} S(E)}. \quad (1.774)$$

In the thermodynamic limit, $V \rightarrow \infty$, we thus obtain

$$p(E) \propto \exp \left\{ -V \left[\beta \frac{E}{V} - \frac{S(E)}{k_B V} \right] \right\}, \quad (1.775)$$

with both S/V and E/V taking a finite limit (independent of V) when $V \rightarrow \infty$. $p(E)$ is then strongly peaked about the most probable value \bar{E} and can be approximated by a Gaussian probability distribution⁸⁴

$$p(E) \propto \exp \left\{ -\frac{1}{2k_B} \frac{\partial^2 S}{\partial E^2} \bigg|_{\bar{E}} (E - \bar{E})^2 \right\}. \quad (1.776)$$

\bar{E} is defined by

$$\frac{1}{k_B} \frac{\partial S}{\partial E} \bigg|_{\bar{E}} - \beta = 0 \quad (1.777)$$

and therefore corresponds to the energy of the system in the microcanonical ensemble (recall that $S(E)$ is the entropy in the microcanonical ensemble) [Eq. (1.753)]. The

⁸⁴See section 1.7.1 for a mathematical justification of this approximation.

statistical fluctuations of the energy in the canonical ensemble are characterized by the variance

$$\Delta E^2 = \langle E^2 \rangle - \bar{E}^2 \sim \left(\frac{\partial^2 S}{\partial E^2} \Big|_{\bar{E}} \right)^{-1}. \quad (1.778)$$

Since $S \propto V$ and $E \propto V$, we deduce $\partial^2 S / \partial E^2 \propto 1/V$ and $\Delta E \propto \sqrt{V}$. In the thermodynamic limit, the relative fluctuations

$$\frac{\Delta E}{\bar{E}} \propto \frac{1}{\sqrt{V}} \quad (1.779)$$

of the energy become negligible and the microcanonical and canonical descriptions are equivalent.

Let us now consider a fluid in the grand canonical ensemble,

$$\hat{\rho} = \frac{1}{Z_G} e^{-\beta(\hat{H} - \mu \hat{N})} = \frac{1}{Z_G} \sum_m |m\rangle e^{-\beta(\epsilon_m - \mu N_m)} \langle m|, \quad (1.780)$$

where we have used the basis $\{|m\rangle\}$ which diagonalizes the Hamiltonian \hat{H} and the particle number operator \hat{N} . The probability to have N particles in the system is

$$p(N) = \frac{1}{Z_G} \sum_{\substack{m \\ (N_m = N)}} e^{-\beta(\epsilon_m - \mu N_m)} = e^{\beta \mu N} \frac{Z_C}{Z_G} = \frac{1}{Z_G} e^{-\beta(F - \mu N)}, \quad (1.781)$$

where $Z_C(\beta, N, V)$ is the canonical partition function and $F(T, N, V) = -\frac{1}{\beta} \ln Z_C$ is the Helmholtz free energy. In the thermodynamic limit, N is large and can be considered as a continuous variable. Moreover, since F/N takes a finite limit when $N \rightarrow \infty$, we can factorize out a factor N in the argument of the exponential in (1.781), and approximate $p(N)$ by the Gaussian distribution function⁸⁴

$$p(N) \propto \exp \left\{ -\beta \frac{\partial^2 F}{\partial N^2} \Big|_{\bar{N}} (N - \bar{N})^2 \right\}, \quad (1.782)$$

where the most probable value \bar{N} is defined by

$$\mu - \frac{\partial F}{\partial N} \Big|_{\bar{N}} = 0. \quad (1.783)$$

\bar{N} is therefore such that the canonical chemical potential $\partial F / \partial N$ [Eq. (1.761)] coincides with the grand canonical potential μ . The statistical fluctuations of N are given by

$$\Delta N^2 \sim \left(\beta \frac{\partial^2 F}{\partial N^2} \Big|_{\bar{N}} \right)^{-1} \propto \bar{N}, \quad (1.784)$$

so that the relative fluctuations

$$\frac{\Delta N}{\bar{N}} \propto \frac{1}{\sqrt{\bar{N}}} \quad (1.785)$$

become negligible when $\bar{N} \rightarrow \infty$. The canonical and grand canonical descriptions are equivalent in the thermodynamic limit.

Statistical entropy vs thermodynamic entropy. For an isolated system, the Liouville-von Neumann equation (1.726) ensures that the energy is conserved,

$$\frac{dE}{dt} = \frac{1}{i\hbar} \langle [\hat{H}, \hat{H}] \rangle = 0. \quad (1.786)$$

If the system is not isolated, its energy will vary by an amount

$$dE = \text{Tr}(d\hat{\rho}\hat{H}) + \text{Tr}(\hat{\rho}d\hat{H}) \quad (1.787)$$

in an infinitesimal transformation where the Hamiltonian and the density operator vary by $d\hat{H}$ and $d\hat{\rho}$, respectively. When $\hat{\rho}$ commutes with the Hamiltonian, it can be written as

$$\hat{\rho} = \sum_m |m\rangle p_m \langle m| \quad (1.788)$$

in the eigenbasis $\{|m\rangle, \epsilon_m\}$ of the eigenstates of \hat{H} , where p_m is the probability of the microstate $|m\rangle$. The energy of the equilibrium state is then $E = \sum_m p_m \epsilon_m$ and its variation (1.787) reads

$$dE = \sum_m (dp_m \epsilon_m + p_m d\epsilon_m). \quad (1.789)$$

The quantity

$$\delta W = \sum_m p_m d\epsilon_m = \text{Tr}(\hat{\rho}d\hat{H}) \quad (1.790)$$

corresponds to the work received by the system in the infinitesimal transformation. On the other hand, the energy variation

$$\delta Q = \sum_m dp_m \epsilon_m = \text{Tr}(d\hat{\rho}\hat{H}) \quad (1.791)$$

due to the change in the probabilities p_m is the heat transferred to the system.

Let us consider a system in equilibrium in the canonical ensemble. In a quasi-static transformation, the system remains in equilibrium and its statistical entropy changes by⁸⁵

$$\begin{aligned} dS &= -k_B \text{Tr}(d\hat{\rho} \ln \hat{\rho}) \\ &= k_B \text{Tr}[d\hat{\rho}(\ln Z + \beta \hat{H})] \\ &= k_B \beta \text{Tr}(d\hat{\rho} \hat{H}) \\ &= k_B \beta \delta Q. \end{aligned} \quad (1.792)$$

This result must be identified with Clausius' equation $\delta Q = T dS_{\text{th}}$ where S_{th} is the thermodynamic entropy at equilibrium. If we choose $k_B \beta = 1/T$ (with T the thermodynamic absolute temperature), then $dS = dS_{\text{th}}$, which implies that the statistical entropy S coincides with the thermodynamic entropy up to an additive constant [26].

1.C.4 The classical limit

In the Hamiltonian formalism, a classical microstate is represented by a point $\{q_i, p_i\}$ in phase space. A classical macrostate is characterized by the probability law for the classical microstates,

$$\rho_N(q_1, p_1, \dots, q_N, p_N) d\tau_N, \quad (1.793)$$

⁸⁵Since the density operator satisfies $\text{Tr}(\hat{\rho}) = 1$, $\text{Tr}(d\hat{\rho}) = 0$.

where ρ_N is the phase density (or density in phase) and $d\tau_N$ the volume element in phase space. ρ_N is real, positive and normalized. A classical observable A then becomes a random variable and its mean value is given by

$$\langle A \rangle = \int d\tau_N \rho_N(q_1, p_1, \dots, q_N, p_N) A(q_1, p_1, \dots, q_N, p_N). \quad (1.794)$$

The normalization of $d\tau_N$ does not matter, since ρ_N is normalized. However, when one derives (1.794) as a limiting case of quantum statistical physics, one finds

$$d\tau_N = \frac{1}{N!} \prod_{i=1}^N \frac{d^3 q_i d^3 p_i}{h^3} \quad (1.795)$$

for a three-dimensional fluid of N particles. The factor h^{-3N} makes $d\tau_N$ dimensionless, while the factor $1/N!$ is associated with the indistinguishability of the particles. This suggests that even in classical mechanics, two points in phase space which differ from one another by a permutation of the indices of the particles represent the same physical microstate.⁸⁶

The time evolution of the quantum density operator was derived from the Schrödinger equation and the conservation of the probability q_λ of the microstate $|\psi_\lambda\rangle$. Similarly, the probability $\rho_N d\tau_N$ is conserved along the classical trajectory defined by Hamilton's equations of motion (1.646). Moreover, the volume of a region in phase space remains constant when one follows the region during the temporal evolution (Liouville's theorem).⁸⁷ It follows that both $d\tau_N$ and ρ_N are conserved along the classical trajectories. From

$$\rho_N(q_i + \dot{q}_i dt, p_i + \dot{p}_i dt, t + dt) = \rho_N(q_i, p_i, t) \quad (dt \rightarrow 0), \quad (1.796)$$

we then deduce

$$\frac{\partial \rho_N}{\partial t} + \sum_i \left(\frac{\partial \rho_N}{\partial q_i} \dot{q}_i + \frac{\partial \rho_N}{\partial p_i} \dot{p}_i \right) = 0, \quad (1.797)$$

i.e.

$$\frac{\partial \rho_N}{\partial t} = [H, \rho_N] \quad (1.798)$$

(Liouville's equation), where $[,]$ denotes the Poisson bracket.

The classical statistical entropy is defined as

$$S = -k_B \sum_N \int d\tau_N \rho_N \ln \rho_N, \quad (1.799)$$

which can be shown to be the classical limit of (1.730). If the number of particles in the system is well defined, the sum over N in (1.799) is absent. The phase density

⁸⁶For arbitrary conjugate variables (q_i, p_i) , $N!$ is replaced by a factor \mathcal{S} equal to the number of configurations in phase space which describe the same situation if we take into account the indistinguishability of the particles.

⁸⁷Liouville's theorem follows from the fact that the infinitesimal transformation $q_i \rightarrow q_i + \dot{q}_i dt$, $p_i \rightarrow p_i + \dot{p}_i dt$ has a unit Jacobian, which is a direct consequence of Hamilton's equations of motion (1.646).

of the system in equilibrium is obtained from the maximum entropy principle. This leads to the classical Boltzmann-Gibbs distribution

$$\rho_N = \frac{1}{Z} e^{-\sum_i \lambda_i A_i}, \quad (1.800)$$

where the partition function is defined by

$$Z = \sum_N \int d\tau_N e^{-\sum_i \lambda_i A_i}. \quad (1.801)$$

The observables A_i in (1.800) and (1.801) correspond to the (known) constants of motion and the λ_i 's are Lagrange multipliers introduced to enforce the constraints $\langle A_i \rangle = \text{const.}$ For example, the classical canonical ensemble has a phase density

$$\rho_N = \frac{1}{Z_C} e^{-\beta H_N} \quad (1.802)$$

with a partition function

$$Z_C(\beta, N, V) = \int d\tau_N e^{-\beta H_N}, \quad (1.803)$$

while the classical grand canonical ensemble is defined by

$$\begin{aligned} \rho_N &= \frac{1}{Z_G} e^{-\beta H_N + \alpha N}, \\ Z_G(\beta, \alpha, V) &= \sum_N \int d\tau_N e^{-\beta H_N + \alpha N} = \sum_N e^{\alpha N} Z_C(\beta, N, V). \end{aligned} \quad (1.804)$$

1.C.5 Non-interacting quantum gases

In this section, we consider a system of non-interacting quantum particles (bosons or fermions) in equilibrium in the grand canonical ensemble. We denote by $\{|\alpha\rangle, \epsilon_\alpha\}$ an orthonormal basis of one-body states which diagonalizes the one-particle Hamiltonian. The many-particle Hilbert space \mathcal{H} (Fock space) is obtained from the direct sum $\oplus_{N=0}^{\infty} \mathcal{H}_N$ of the N -particle Hilbert spaces \mathcal{H}_N . An orthonormal basis in the Fock space is formed by the states⁸⁸

$$|n_{\alpha_1} \cdots n_{\alpha_i} \cdots\rangle \quad (1.805)$$

obtained by putting n_{α_i} particles in the one-body state $|\alpha_i\rangle$ and symmetrizing or antisymmetrizing the many-body states according to the quantum statistics of the particles. These states are eigenstates of the Hamiltonian and the total number of particles operator,

$$\begin{aligned} \hat{H}|n_{\alpha_1} \cdots n_{\alpha_i} \cdots\rangle &= \sum_j n_{\alpha_j} \epsilon_{\alpha_j} |n_{\alpha_1} \cdots n_{\alpha_i} \cdots\rangle, \\ \hat{N}|n_{\alpha_1} \cdots n_{\alpha_i} \cdots\rangle &= \sum_j n_{\alpha_j} |n_{\alpha_1} \cdots n_{\alpha_i} \cdots\rangle. \end{aligned} \quad (1.806)$$

⁸⁸See section 1.2.1 for more detail.

While for bosons there is no restriction on the occupation numbers n_α , for fermions they are constrained by the Pauli principle and can take only the values 0 or 1. Using the basis $\{|n_{\alpha_1} \cdots n_{\alpha_i} \cdots\rangle\}$, we easily calculate the grand canonical partition function,

$$Z = \text{Tr} e^{-\beta(\tilde{N} - \mu\tilde{N})} = \sum_{\{n_\alpha\}} e^{-\beta \sum_\alpha n_\alpha \xi_\alpha}, \quad (1.807)$$

where $\xi_\alpha = \epsilon_\alpha - \mu$. From (1.807), we obtain

$$Z = \sum_{n_{\alpha_1}, n_{\alpha_2}, \dots} e^{-\beta n_{\alpha_1} \xi_{\alpha_1}} e^{-\beta n_{\alpha_2} \xi_{\alpha_2}} \dots = \prod_\alpha \sum_{n_\alpha} e^{-\beta n_\alpha \xi_\alpha} = \prod_\alpha (1 - \zeta e^{-\beta \xi_\alpha})^{-\zeta}, \quad (1.808)$$

where $\zeta = 1$ for bosons and $\zeta = -1$ for fermions. We deduce that the grand potential reads

$$\Omega = \frac{\zeta}{\beta} \sum_\alpha \ln(1 - \zeta e^{-\beta \xi_\alpha}). \quad (1.809)$$

The mean number of particles is given by

$$N = - \left. \frac{\partial \Omega}{\partial \mu} \right|_T = \sum_\alpha \frac{1}{e^{\beta \xi_\alpha} - \zeta} \equiv \sum_\alpha n_\zeta(\xi_\alpha), \quad (1.810)$$

where $n_+(\xi_\alpha) = n_B(\xi_\alpha)$ (Bose-Einstein distribution function) and $n_-(\xi_\alpha) = n_F(\xi_\alpha)$ (Fermi-Dirac distribution function). From the grand potential, one can also deduce the mean energy

$$E = \left. \frac{\partial \beta \Omega}{\partial \beta} \right|_\mu + \mu N = \sum_\alpha \epsilon_\alpha n_\zeta(\xi_\alpha) \quad (1.811)$$

and the entropy

$$\begin{aligned} S = - \left. \frac{\partial \Omega}{\partial T} \right|_\mu &= \frac{1}{T} \sum_\alpha \left[\xi_\alpha n_\zeta(\xi_\alpha) - \frac{\zeta}{\beta} \ln(1 - \zeta e^{-\beta \xi_\alpha}) \right] \\ &= -k_B \sum_\alpha \left\{ n_\zeta(\xi_\alpha) \ln n_\zeta(\xi_\alpha) - \zeta [1 + \zeta n_\zeta(\xi_\alpha)] \ln [1 + \zeta n_\zeta(\xi_\alpha)] \right\}. \end{aligned} \quad (1.812)$$

1.D Functionals and functional derivatives

A functional is a function that maps functions to numbers. Its argument is conventionally written in square brackets rather than parentheses. The derivative of a functional $F[\phi]$ is defined in such a way that if one discretizes⁸⁹ the function $\phi(\mathbf{x})$ (\mathbf{x} denotes a d -dimensional variable), one recovers the standard rules for derivation of ordinary functions. We then impose

$$\frac{\delta \phi(\mathbf{x})}{\delta \phi(\mathbf{y})} = \delta(\mathbf{x} - \mathbf{y}), \quad (1.813)$$

⁸⁹The continuous variable \mathbf{x} then becomes a discrete variable defined on a d -dimensional lattice with lattice spacing a . The continuous formulation is recovered when a tends to zero. For example, for a one-dimensional variable, $x \rightarrow x_i = ia$ and $\phi(x) \rightarrow \phi(x_i) \equiv \phi_i$, with i integer.

which is the analog of $\partial\phi_i/\partial\phi_j = \delta_{i,j}$, and the standard rules

$$\begin{aligned}\frac{\delta}{\delta\phi(\mathbf{x})} (F_1[\phi] + F_2[\phi]) &= \frac{\delta F_1[\phi]}{\delta\phi(\mathbf{x})} + \frac{\delta F_2[\phi]}{\delta\phi(\mathbf{x})}, \\ \frac{\delta}{\delta\phi(\mathbf{x})} F_1[\phi] F_2[\phi] &= \frac{\delta F_1[\phi]}{\delta\phi(\mathbf{x})} F_2[\phi] + F_1[\phi] \frac{\delta F_2[\phi]}{\delta\phi(\mathbf{x})}, \\ \frac{\delta}{\delta\phi(\mathbf{x})} f(\phi(\mathbf{y})) &= f'(\phi(\mathbf{y})) \frac{\delta\phi(\mathbf{y})}{\delta\phi(\mathbf{x})} = f'(\phi(\mathbf{y})) \delta(\mathbf{x} - \mathbf{y}).\end{aligned}\tag{1.814}$$

Equation (1.813) also implies

$$\frac{\delta}{\delta\phi(\mathbf{x})} \nabla\phi(\mathbf{y}) = \nabla \frac{\delta\phi(\mathbf{y})}{\delta\phi(\mathbf{x})} = \nabla\delta(\mathbf{x} - \mathbf{y}).\tag{1.815}$$

For a functional $F[\phi]$ that can be expressed as an integral of a function of $\phi(\mathbf{x})$ and $\nabla\phi(\mathbf{x})$,

$$F[\phi] = \int d^d x f(\phi(\mathbf{x}), \nabla\phi(\mathbf{x})),\tag{1.816}$$

one then finds

$$\begin{aligned}\frac{\delta F[\phi]}{\delta\phi(\mathbf{x})} &= \int d^d y \left(\frac{\partial f}{\partial\phi(\mathbf{y})} \frac{\delta\phi(\mathbf{y})}{\delta\phi(\mathbf{x})} + \frac{\partial f}{\partial(\nabla\phi(\mathbf{y}))} \cdot \frac{\delta(\nabla\phi(\mathbf{y}))}{\delta\phi(\mathbf{x})} \right) \\ &= \int d^d y \left(\frac{\partial f}{\partial\phi(\mathbf{y})} \delta(\mathbf{x} - \mathbf{y}) + \frac{\partial f}{\partial(\nabla\phi(\mathbf{y}))} \cdot \nabla\delta(\mathbf{x} - \mathbf{y}) \right) \\ &= \frac{\partial f}{\partial\phi(\mathbf{x})} - \nabla \cdot \frac{\partial f}{\partial(\nabla\phi(\mathbf{x}))},\end{aligned}\tag{1.817}$$

where the last result is obtained by integrating the second term by parts assuming that the field $\phi(\mathbf{x})$ vanishes or at the boundaries of its domain of definition or satisfies periodic boundary conditions.

The functional $F[\phi]$ and its functional derivative can be expanded as

$$\begin{aligned}F[\phi] &= F[0] + \sum_{n=1}^{\infty} \frac{1}{n!} \int d^d x_1 \cdots d^d x_n F^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n) \phi(\mathbf{x}_1) \cdots \phi(\mathbf{x}_n), \\ \frac{\delta F[\phi]}{\delta\phi(\mathbf{x})} &= F^{(1)}(\mathbf{x}) + \sum_{n=2}^{\infty} \frac{1}{(n-1)!} \int d^d x_1 \cdots d^d x_{n-1} F^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{x}) \\ &\quad \times \phi(\mathbf{x}_1) \cdots \phi(\mathbf{x}_{n-1}),\end{aligned}\tag{1.818}$$

where the function $F^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n)$ is symmetric under the exchange $\mathbf{x}_i \leftrightarrow \mathbf{x}_j$. We

deduce

$$\begin{aligned}
F[\phi + u] &= F[0] + \sum_{n=1}^{\infty} \frac{1}{n!} \int d^d x_1 \cdots d^d x_n F^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n) \\
&\quad \times (\phi(\mathbf{x}_1) + u(\mathbf{x}_1)) \cdots (\phi(\mathbf{x}_n) + u(\mathbf{x}_n)) \\
&= F[\phi] + \int d^d x F^{(1)}(x) u(x) + \sum_{n=2}^{\infty} \frac{1}{(n-1)!} \int d^d x_1 \cdots d^d x_{n-1} F^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{x}) \\
&\quad \times \phi(\mathbf{x}_1) \cdots \phi(\mathbf{x}_{n-1}) u(\mathbf{x}) + \mathcal{O}(u^2) \\
&= F[\phi] + \int d^d x \frac{\delta F[\phi]}{\delta \phi(\mathbf{x})} u(\mathbf{x}) + \mathcal{O}(u^2). \tag{1.819}
\end{aligned}$$

More generally, one finds

$$F[\phi + u] = F[\phi] + \sum_{n=1}^{\infty} \frac{1}{n!} \int d^d x_1 \cdots d^d x_n \frac{\delta^{(n)} F[\phi]}{\delta \phi(\mathbf{x}_1) \cdots \delta \phi(\mathbf{x}_n)} u(\mathbf{x}_1) \cdots u(\mathbf{x}_n). \tag{1.820}$$

Grassmann variables

Similar rules can be defined for a functional $F[\psi^*, \psi]$ of a Grassmannian function $\psi(\mathbf{x})$ and its complex conjugate $\psi^*(\mathbf{x})$, provided the anticommuting properties of $\psi(\mathbf{x})$ and $\psi^*(\mathbf{x})$ are properly taken into account. For instance,

$$\begin{aligned}
\frac{\delta}{\delta \psi(\mathbf{x})} \int d^d y \psi^*(\mathbf{y}) \psi(\mathbf{y}) &= -\psi^*(\mathbf{x}), \\
\frac{\delta}{\delta \psi^*(\mathbf{x})} \int d^d y \psi^*(\mathbf{y}) \psi(\mathbf{y}) &= \psi(\mathbf{x}).
\end{aligned} \tag{1.821}$$

In particular, one has

$$\begin{aligned}
F[\psi^* + u^*, \psi + u] &= F[\psi^*, \psi] \\
&\quad + \int d^d x \left(u^*(\mathbf{x}) \frac{\delta F[\psi^*, \psi]}{\delta \psi^*(\mathbf{x})} + u(\mathbf{x}) \frac{\delta F[\psi^*, \psi]}{\delta \psi(\mathbf{x})} \right) + \mathcal{O}(u^2), \tag{1.822}
\end{aligned}$$

where the Grassmann numbers $u^*(\mathbf{x})$ and $u(\mathbf{x})$ should appear on the left of the functional derivatives in agreement with the chain rule for derivation with anticommuting variables [Eq. (1.226)].

1.E Gaussian integrals and Wick's theorem

1.E.1 Real variables

We consider the multi-dimensional integral

$$\begin{aligned}
Z(J) &= \int_{-\infty}^{\infty} dx_1 \cdots dx_n e^{-\frac{1}{2} \sum_{i,j} x_i A_{ij} x_j + \sum_i J_i x_i} \\
&= \int_{-\infty}^{\infty} dx_1 \cdots dx_n e^{-\frac{1}{2} x^T A x + J^T x}, \tag{1.823}
\end{aligned}$$

where x denotes the column vector $(x_1, \dots, x_n)^T$. The n -dimensional real matrix A is assumed to be symmetric and positive definite. It can be diagonalized by an orthogonal transformation: $A = O^T D O$, with O an orthogonal matrix ($O^T O = O O^T = 1$) and D a diagonal matrix with non-negative elements ($D_{ii} > 0$). With the change of variables $y = O(x - A^{-1}J)$ (Jacobian $|\det O| = 1$), we obtain

$$-\frac{1}{2}x^T A x + J^T x = -\frac{1}{2}y^T D y + \frac{1}{2}J^T A^{-1} J \quad (1.824)$$

and $Z(J)$ reduces to a product of Gaussian integrals,⁹⁰

$$\begin{aligned} Z(J) &= e^{\frac{1}{2}J^T A^{-1} J} \prod_{i=1}^n \int_{-\infty}^{\infty} dy e^{-\frac{1}{2}y^2 D_{ii}} \\ &= e^{\frac{1}{2}J^T A^{-1} J} \prod_{i=1}^n \left(\frac{2\pi}{D_{ii}} \right)^{1/2} \\ &= e^{\frac{1}{2}J^T A^{-1} J} (2\pi)^{n/2} (\det A)^{-1/2}, \end{aligned} \quad (1.825)$$

using $\det D = \det A$.

Wick's theorem

The mean value

$$\langle x_{i_1} \cdots x_{i_k} \rangle = \frac{\int_{-\infty}^{\infty} dx_1 \cdots dx_n x_{i_1} \cdots x_{i_k} e^{-\frac{1}{2}x^T A x}}{\int_{-\infty}^{\infty} dx_1 \cdots dx_n e^{-\frac{1}{2}x^T A x}} \quad (1.826)$$

can be obtained from the generating function (1.823),

$$\begin{aligned} \langle x_{i_1} \cdots x_{i_k} \rangle &= \frac{1}{Z(0)} \frac{\partial}{\partial J_{i_1}} \cdots \frac{\partial}{\partial J_{i_k}} Z(J) \Big|_{J=0} \\ &= \frac{\partial}{\partial J_{i_1}} \cdots \frac{\partial}{\partial J_{i_k}} e^{\frac{1}{2}J^T A^{-1} J} \Big|_{J=0}. \end{aligned} \quad (1.827)$$

We deduce

$$\begin{aligned} \langle x_{i_1} x_{i_2} \rangle &= A_{i_1 i_2}^{-1}, \\ \langle x_{i_1} x_{i_2} x_{i_3} x_{i_4} \rangle &= A_{i_1 i_2}^{-1} A_{i_3 i_4}^{-1} + A_{i_1 i_3}^{-1} A_{i_2 i_4}^{-1} + A_{i_1 i_4}^{-1} A_{i_2 i_3}^{-1}, \end{aligned} \quad (1.828)$$

and more generally

$$\begin{aligned} \langle x_{i_1} \cdots x_{i_{2k}} \rangle &= \sum_{\substack{\text{all possible pairings} \\ p \text{ of } \{i_1, \dots, i_{2k}\}}} \langle x_{i_{p(1)}} x_{i_{p(2)}} \rangle \cdots \langle x_{i_{p(2k-1)}} x_{i_{p(2k)}} \rangle \\ &= \sum_{\substack{\text{all possible pairings} \\ p \text{ of } \{i_1, \dots, i_{2k}\}}} A_{i_{p(1)} i_{p(2)}}^{-1} \cdots A_{i_{p(2k-1)} i_{p(2k)}}^{-1}. \end{aligned} \quad (1.829)$$

This result holds for any Gaussian probability distribution $e^{-\frac{1}{2}x^T A x}$ with zero mean $\langle x_i \rangle = 0$. In field theory, it is known as Wick's theorem and underlies perturbation theory (Sec. 1.5).

⁹⁰Recall that $\int_{-\infty}^{\infty} dy e^{-\frac{a}{2}y^2} = \sqrt{2\pi/a}$ for $a > 0$.

1.E.2 Complex variables

Now we consider the multidimensional integral

$$\begin{aligned} Z(J^*, J) &= \int_{-\infty}^{\infty} \prod_{i=1}^n \frac{dz_i^* dz_i}{2i\pi} e^{-\sum_{i,j} z_i^* A_{ij} z_j + \sum_i (J_i^* z_i + \text{c.c.})} \\ &= \int_{-\infty}^{\infty} \prod_{i=1}^n \frac{dz_i^* dz_i}{2i\pi} e^{-z^\dagger A z + (J^\dagger z + \text{c.c.})} \end{aligned} \quad (1.830)$$

over the complex variables z_i and z_i^* ($i = 1, \dots, n$), where

$$\frac{dz_i^* dz_i}{2i\pi} = \frac{1}{\pi} d\Re(z_i) d\Im(z_i) \quad (1.831)$$

and $z^\dagger = (z_1^*, \dots, z_n^*)$. Let us first assume the complex matrix A to be positive definite Hermitian ($A^\dagger = A$). We can then proceed as in the real case. A can be diagonalized by a unitary transformation: $A = U^\dagger D U$ with U a unitary matrix ($U U^\dagger = U^\dagger U = 1$) and D a diagonal matrix with non-negative real elements ($D_{ii} > 0$). The change of variables

$$z' = U(z - A^{-1}J), \quad z'^\dagger = (z^\dagger - J^\dagger A^{-1})U^\dagger \quad (1.832)$$

has a Jacobian $|\det U|^2 = 1$, and leads to⁹¹

$$Z(J^*, J) = e^{J^\dagger A^{-1}J} \int_{-\infty}^{\infty} \prod_{i=1}^n \frac{dz_i'^* dz_i'}{2i\pi} e^{-z'^\dagger D z'} = e^{J^\dagger A^{-1}J} (\det A)^{-1} \quad (1.833)$$

(using $\det D = \det A$). It can be shown that (1.833) holds for any complex matrix with a positive definite Hermitian part $\frac{1}{2}(A + A^\dagger)$.⁹²

Wick's theorem

The average value of a monomial can be obtained from the generating function $Z(J^*, J)$,

$$\begin{aligned} \langle z_{i_1} z_{i_1'}^* \dots z_{i_k} z_{i_k'}^* \rangle &= \frac{\int_{-\infty}^{\infty} \prod_{i=1}^n \frac{dz_i^* dz_i}{2i\pi} z_{i_1} z_{i_1'}^* \dots z_{i_k} z_{i_k'}^* e^{-z^\dagger A z}}{\int_{-\infty}^{\infty} \prod_{i=1}^n \frac{dz_i^* dz_i}{2i\pi} e^{-z^\dagger A z}} \\ &= \frac{1}{Z(0,0)} \frac{\partial}{\partial J_{i_1}^*} \frac{\partial}{\partial J_{i_1'}} \dots \frac{\partial}{\partial J_{i_k}^*} \frac{\partial}{\partial J_{i_k'}} Z(J^*, J) \Big|_{J^*=J=0} \\ &= \frac{\partial}{\partial J_{i_1}^*} \frac{\partial}{\partial J_{i_1'}} \dots \frac{\partial}{\partial J_{i_k}^*} \frac{\partial}{\partial J_{i_k'}} e^{J^\dagger A^{-1}J} \Big|_{J^*=J=0}. \end{aligned} \quad (1.834)$$

⁹¹We use $\int_{-\infty}^{\infty} \frac{dz^* dz}{2i\pi} e^{-a|z|^2} = a^{-1}$ for $a > 0$.

⁹²This can be understood by noting that, contrary to the case of the real Gaussian integral, the result (1.833) is an algebraic function of the matrix elements A_{ij} and can therefore be analytically continued to any complex matrix with a positive definite Hermitian part [4].

Note that only monomials with equal number of z_i and z_i^* factors have a non-vanishing average. From (1.834), we obtain

$$\begin{aligned} \langle z_{i_1} z_{i'_1}^* \cdots z_{i_k} z_{i'_k}^* \rangle &= \prod_{j=1}^k \frac{\partial}{\partial J_{i_j}^*} \left(\sum_{l_1} J_{l_1}^* A_{l_1 i'_1}^{-1} \right) \cdots \left(\sum_{l_k} J_{l_k}^* A_{l_k i'_k}^{-1} \right) e^{J^\dagger A^{-1} J} \Big|_{J^*=J=0} \\ &= \sum_{p \in S_k} A_{i_{p(1)} i'_1}^{-1} \cdots A_{i_{p(k)} i'_k}^{-1}, \end{aligned} \quad (1.835)$$

where the sum is over all permutations p of $\{1, \dots, k\}$.

1.E.3 Grassmannian integrals

In order to establish the analog results for Grassmann variables, we first need to derive the law of change of variables in a Grassmannian integral.

Change of variables

Let us consider the integral

$$I = \int d\theta f(\theta) \quad (1.836)$$

with θ a Grassmann variable, and perform the change of variables $\theta = a\theta' + b$ with a and b c-numbers. Since integration and derivation are identical for Grassmann numbers (Sec. 1.3.2), we obtain

$$I = \frac{\partial}{\partial \theta} f(\theta) = \frac{\partial \theta'}{\partial \theta} \frac{\partial f}{\partial \theta'} = \frac{1}{a} \frac{\partial f}{\partial \theta'} = \frac{1}{a} \int d\theta' f(a\theta' + b) \quad (1.837)$$

using the chain rule for differentiation of Grassmann variables [Eq. (1.226)]. The Jacobian of the transformation is therefore a^{-1} instead of a for ordinary variables.

This result can be generalized to a multidimensional integral,

$$\begin{aligned} I &= \int d\theta_1 \cdots d\theta_n f(\theta_1 \cdots \theta_n) \\ &= \prod_{i=1}^n \frac{\partial}{\partial \theta_i} f(\theta_1 \cdots \theta_n) \\ &= \prod_{i=1}^n \left(\sum_j \frac{\partial \theta'_j}{\partial \theta_i} \frac{\partial}{\partial \theta'_j} \right) f(\theta_1 \cdots \theta_n). \end{aligned} \quad (1.838)$$

For a linear transformation $\theta'_i = \sum_j M_{ij} \theta_j$, we obtain

$$I = \prod_{i=1}^n \left(\sum_j M_{ji} \frac{\partial}{\partial \theta'_j} \right) f(\theta_1 \cdots \theta_n). \quad (1.839)$$

Since the differential operators $\partial/\partial \theta'_j$ anticommute, the differential operator acting on $f(\theta_1 \cdots \theta_n)$ is proportional to $\partial_{\theta'_1} \cdots \partial_{\theta'_n}$, and the prefactor is easily seen to be the determinant of the matrix M ,

$$I = \det \left(\frac{\partial \theta'_i}{\partial \theta_j} \right) \prod_{i=1}^n \frac{\partial}{\partial \theta'_i} f(\theta_1 \cdots \theta_n) = \det \left(\frac{\partial \theta'_i}{\partial \theta_j} \right) \int \prod_{i=1}^n d\theta'_i f(\theta_1 \cdots \theta_n), \quad (1.840)$$

i.e.

$$\prod_{i=1}^n d\theta_i = \det \left(\frac{\partial \theta'_i}{\partial \theta_j} \right) \prod_{i=1}^n d\theta'_i. \quad (1.841)$$

The Jacobian is the inverse of the determinant $\det(\partial \theta_i / \partial \theta'_j)$.

Gaussian integrals

The one-dimensional Gaussian integral over a pair of complex Grassmann variables reads

$$\int d^* \theta d\theta e^{-a\theta^* \theta} = \int d\theta^* d\theta (1 - a\theta^* \theta) = a \quad (1.842)$$

for any c-number a . This result is easily generalized to the multidimensional Gaussian integral

$$Z = \int \prod_{i=1}^n d\theta_i^* d\theta_i e^{-\sum_{i,j} \theta_i^* A_{ij} \theta_j}, \quad (1.843)$$

where A is an arbitrary complex matrix. With the linear transformation $\theta'_i = \sum_j A_{ij} \theta_j$, we obtain

$$Z = \det(A) \int \prod_{i=1}^n d\theta_i^* d\theta'_i e^{-\sum_i \theta_i^* \theta'_i} = \det(A) \prod_{i=1}^n \int d\theta_i^* d\theta'_i (1 - \theta_i^* \theta'_i) = \det(A). \quad (1.844)$$

Note that for ordinary complex variables, one would obtain $(\det A)^{-1}$.

The generalized Gaussian integral

$$Z(J^*, J) = \int \prod_{i=1}^n d\theta_i^* d\theta_i e^{-\theta^{\dagger} A \theta + (J^{\dagger} \theta + \text{c.c.})} = \det(A) e^{J^{\dagger} A^{-1} J} \quad (1.845)$$

(J_i^* and J_i are anticommuting numbers) is easily calculated using the change of variables $\theta = \theta' + A^{-1} J$ and $\theta^{\dagger} = \theta'^{\dagger} + J^{\dagger} A^{-1}$.

Wick's theorem

As with complex variables, the average value

$$\begin{aligned} \langle \theta_{i_1} \cdots \theta_{i_k} \theta_{i'_k}^* \cdots \theta_{i'_1}^* \rangle &= \frac{\int \prod_{i=1}^n d\theta_i^* d\theta_i \theta_{i_1} \cdots \theta_{i_k} \theta_{i'_k}^* \cdots \theta_{i'_1}^* e^{-\theta^{\dagger} A \theta}}{\int \prod_{i=1}^n d\theta_i^* d\theta_i e^{-\theta^{\dagger} A \theta}} \\ &= \frac{(-1)^n}{Z(0,0)} \frac{\partial}{\partial J_{i_1}^*} \cdots \frac{\partial}{\partial J_{i_k}^*} \frac{\partial}{\partial J_{i'_k}} \cdots \frac{\partial}{\partial J_{i'_1}} Z(J, J^*) \Big|_{J^*=J=0} \end{aligned} \quad (1.846)$$

can be obtained from the generating function (1.845). This yields

$$\begin{aligned} &\langle \theta_{i_1} \cdots \theta_{i_k} \theta_{i'_k}^* \cdots \theta_{i'_1}^* \rangle \\ &= \frac{\partial}{\partial J_{i_1}^*} \cdots \frac{\partial}{\partial J_{i_k}^*} \left(\sum_{l_k} J_{l_k}^* A_{l_k i'_k}^{-1} \right) \cdots \left(\sum_{l_1} J_{l_1}^* A_{l_1 i'_1}^{-1} \right) e^{J^{\dagger} A^{-1} J} \Big|_{J^*=J=0} \\ &= \sum_{p \in S_k} \epsilon_p A_{i_{p(k)} i'_k}^{-1} \cdots A_{i_{p(1)} i'_1}^{-1}, \end{aligned} \quad (1.847)$$

where ϵ_p denotes the signature of the permutation p .

“Real” Grassmannian Gaussian integrals

We can also consider integrals of the type

$$Z = \int d\theta_1 \cdots d\theta_{2n} e^{-\frac{1}{2}\theta^T A \theta}, \quad (1.848)$$

where A is an antisymmetric matrix: $A_{ij} = -A_{ji}$.⁹³ Expanding the exponential in (1.848) and retaining the only non-vanishing term, we obtain

$$\begin{aligned} Z &= \frac{(-1)^n}{2^n n!} \int d\theta_1 \cdots d\theta_{2n} \left(\sum_{i,j=1}^{2n} \theta_i A_{ij} \theta_j \right)^n \\ &= \frac{1}{2^n n!} \sum_{p \in S_{2n}} \epsilon_p A_{p(1),p(2)} \cdots A_{p(2n-1),p(2n)}, \end{aligned} \quad (1.849)$$

where ϵ_p is the signature of the permutation p . The quantity in the rhs is called the Pfaffian of the matrix A ,

$$Z = \text{Pf}(A). \quad (1.850)$$

The Pfaffian is related in a simple way to the determinant. To see this, we consider the square of Z ,

$$Z^2 = \int d\theta_1 \cdots d\theta_{2n} d\theta'_1 \cdots d\theta'_{2n} e^{-\frac{1}{2}\theta^T A \theta - \frac{1}{2}\theta'^T A \theta'}. \quad (1.851)$$

The change of variables

$$\begin{aligned} \eta_k &= \frac{1}{\sqrt{2}}(\theta_k + i\theta'_k), \\ \eta_k^* &= \frac{1}{\sqrt{2}}(\theta_k - i\theta'_k) \end{aligned} \quad (1.852)$$

gives

$$\begin{aligned} d\theta_1 \cdots d\theta_{2n} d\theta'_1 \cdots d\theta'_{2n} &= (-1)^n d\theta_1 d\theta'_1 \cdots d\theta_{2n} d\theta'_{2n} \\ &= (-1)^n J d\eta_1^* d\eta_1 \cdots d\eta_{2n}^* d\eta_{2n}, \end{aligned} \quad (1.853)$$

where J is the Jacobian of the transformation $\theta_k, \theta'_k \rightarrow \eta_k^*, \eta_k$. Since

$$\det \left(\frac{\partial(\eta_k^*, \eta_k)}{\partial(\theta_k, \theta'_k)} \right) = \det \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} = i, \quad (1.854)$$

we find $J = i^{2n} = (-1)^n$ and therefore

$$Z^2 = \int d\eta_1^* d\eta_1 \cdots d\eta_{2n}^* d\eta_{2n} e^{-\eta^\dagger A \eta} = \det(A), \quad (1.855)$$

i.e.

$$\text{Pf}(A)^2 = \det A. \quad (1.856)$$

⁹³If A is not antisymmetric, only its antisymmetric part contributes since the product $\theta_i \theta_j$ is antisymmetric.

In most cases of interest, we can use $Z = \pm(\det A)^{1/2}$, since the sign of Z either does not matter (e.g. when calculating average values $\langle \theta_{i_1} \cdots \theta_{i_k} \rangle$) or can be easily determined.

The result for the generalized Gaussian integral

$$Z(J) = \int d\theta_1 \cdots d\theta_{2n} e^{-\frac{1}{2}\theta^T A \theta + J^T \theta} = \pm \sqrt{\det A} e^{-\frac{1}{2}J^T A^{-1} J} \quad (1.857)$$

(note the minus sign in the exponential) is derived from the change of variables $\theta = \theta' - A^{-1}J$. Equation (1.857) implies that Wick's theorem for real Grassmann variables reads

$$\langle \theta_{i_1} \cdots \theta_{i_{2k}} \rangle = \sum_{\substack{\text{all possible pairings} \\ p \text{ of } \{i_1, \dots, i_{2k}\}}} \epsilon_p A_{i_{p(1)} i_{p(2)}}^{-1} \cdots A_{i_{p(2k-1)} i_{p(2k)}}^{-1}. \quad (1.858)$$

Except for the signature ϵ_p of the permutation, this result is similar to the one obtained for real variables [Eq. (1.829)].

1.E.4 Gaussian functional integrals

Since functional integrals can be defined as the continuum limit of ordinary integrals (Secs. 1.1 and 1.4), the preceding results generalize straightforwardly to Gaussian functional integrals, i.e.

$$\begin{aligned} Z[J] &= \int \mathcal{D}[\phi] e^{-\frac{1}{2} \int d^d x d^d y \phi(\mathbf{x}) A(\mathbf{x}, \mathbf{y}) \phi(\mathbf{y}) + \int d^d x J(\mathbf{x}) \phi(\mathbf{x})} \\ &= (\det A)^{-1/2} e^{\frac{1}{2} \int d^d x d^d y J(\mathbf{x}) A^{-1}(\mathbf{x}, \mathbf{y}) J(\mathbf{y})} \end{aligned} \quad (1.859)$$

for a real field $\phi(\mathbf{x})$ coupled to a real external “source” $J(\mathbf{x})$, and

$$\begin{aligned} Z[J^*, J] &= \int \mathcal{D}[\psi^*, \psi] e^{-\int d^d x d^d y \psi^*(\mathbf{x}) A(\mathbf{x}, \mathbf{y}) \psi(\mathbf{y}) + \int d^d x [J^*(\mathbf{x}) \psi(\mathbf{x}) + \text{c.c.}]} \\ &= (\det A)^{-\zeta} e^{\int d^d x d^d y J^*(\mathbf{x}) A^{-1}(\mathbf{x}, \mathbf{y}) J(\mathbf{y})} \end{aligned} \quad (1.860)$$

for a complex ($\zeta = 1$) or Grassmann ($\zeta = -1$) field which couples to an external source of the same type. For a (real) Grassmannian field $\psi(\mathbf{x})$ coupled to a Grassmannian source $J(\mathbf{x})$, one finds

$$\begin{aligned} Z[J] &= \int \mathcal{D}[\psi] e^{-\frac{1}{2} \int d^d x d^d y \psi(\mathbf{x}) A(\mathbf{x}, \mathbf{y}) \psi(\mathbf{y}) + \int d^d x J(\mathbf{x}) \psi(\mathbf{x})} \\ &= \pm (\det A)^{1/2} e^{-\frac{1}{2} \int d^d x d^d y J(\mathbf{x}) A^{-1}(\mathbf{x}, \mathbf{y}) J(\mathbf{y})} \end{aligned} \quad (1.861)$$

(note the minus sign in the exponential). Equations (1.859-1.861) hold up to a multiplicative constant which depends on the precise definition of the functional integral measure $\mathcal{D}[\cdot]$.

The inverse A^{-1} of the operator A is defined by

$$\int d^d z A(\mathbf{x}, \mathbf{z}) A^{-1}(\mathbf{z}, \mathbf{y}) = \int d^d z A^{-1}(\mathbf{x}, \mathbf{z}) A(\mathbf{z}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}). \quad (1.862)$$

$\det A$ denotes the determinant of the operator A . A useful identity is

$$\det A = \exp(\ln \det A) = \exp(\text{Tr} \ln A), \quad (1.863)$$

where $\text{Tr}(A)$ denotes the trace of the operator A . When A can be written as $A = 1 + K$,

$$\text{Tr} \ln A = \text{Tr} \ln(1 + K) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \text{Tr}(K^n) \quad (1.864)$$

(provided K^n exists for any n), where

$$\text{Tr}(K^n) = \int d^d x_1 \cdots d^d x_n K(\mathbf{x}_1, \mathbf{x}_2) K(\mathbf{x}_2, \mathbf{x}_3) \cdots K(\mathbf{x}_n, \mathbf{x}_1). \quad (1.865)$$

Wick's theorem

The various forms of Wick's theorem derived in the previous sections translate into

$$\begin{aligned} \langle \phi(\mathbf{x}_1) \cdots \phi(\mathbf{x}_{2k}) \rangle &= \sum_{\substack{\text{all possible pairings} \\ p \text{ of } \{\mathbf{x}_1, \dots, \mathbf{x}_{2k}\}}} A^{-1}(\mathbf{x}_{p(1)}, \mathbf{x}_{p(2)}) \cdots A^{-1}(\mathbf{x}_{p(2k-1)}, \mathbf{x}_{p(2k)}), \\ \langle \psi(\mathbf{x}_1) \cdots \psi(\mathbf{x}_k) \psi^*(\mathbf{x}'_k) \cdots \psi^*(\mathbf{x}'_1) \rangle &= \sum_{p \in S_k} \zeta^p A^{-1}(\mathbf{x}_1, \mathbf{x}'_{p(1)}) \cdots A^{-1}(\mathbf{x}_k, \mathbf{x}'_{p(k)}), \\ \langle \psi(\mathbf{x}_1) \cdots \psi(\mathbf{x}_{2k}) \rangle &= \sum_{\substack{\text{all possible pairings} \\ p \text{ of } \{\mathbf{x}_1, \dots, \mathbf{x}_{2k}\}}} \epsilon_p A^{-1}(\mathbf{x}_{p(1)}, \mathbf{x}_{p(2)}) \cdots A^{-1}(\mathbf{x}_{p(2k-1)}, \mathbf{x}_{p(2k)}), \end{aligned} \quad (1.866)$$

where the averages are obtained from the generating functionals (1.859), (1.860) and (1.861), respectively. ζ^p equals one for bosons and the signature of the permutation p for fermions.

Finally we note that Wick's theorem for complex variables can be generalized from the result

$$\begin{aligned} Z[J^*, J] &= \int \mathcal{D}[\psi^*, \psi] e^{-\frac{1}{2} \int d^d x d^d y (\psi^*(\mathbf{x}), \psi(\mathbf{x})) A(\mathbf{x}, \mathbf{y}) \begin{pmatrix} \psi(\mathbf{y}) \\ \psi^*(\mathbf{y}) \end{pmatrix} + \int d^d x (J^*(\mathbf{x}), J(\mathbf{x})) \begin{pmatrix} \psi(\mathbf{x}) \\ \psi^*(\mathbf{x}) \end{pmatrix}} \\ &= \pm (\det A)^{-1/2} e^{\frac{1}{2} \int d^d x d^d y (J^*(\mathbf{x}), J(\mathbf{x})) A^{-1}(\mathbf{x}, \mathbf{y}) \begin{pmatrix} J(\mathbf{x}) \\ J^*(\mathbf{x}) \end{pmatrix}}. \end{aligned} \quad (1.867)$$

Contrary to the case previously discussed, the matrix $A(\mathbf{x}, \mathbf{y})$ in (1.867) can connect $\psi(\mathbf{x})$ and $\psi(\mathbf{y})$, or $\psi^*(\mathbf{x})$ and $\psi^*(\mathbf{y})$. Thus the averages $\langle \psi(\mathbf{x}) \psi(\mathbf{y}) \rangle$ and $\langle \psi^*(\mathbf{x}) \psi^*(\mathbf{y}) \rangle$ can be nonzero. Wick's theorem is otherwise unchanged: the average of a product of ψ and ψ^* fields is given by the sum of all possible pairings.

1.F Matsubara frequency sums

In this Appendix, we describe the standard methods to carry out summations over Matsubara frequencies ω_n and discuss explicitly a few examples.

General method

We consider the Matsubara sum

$$S = \frac{1}{\beta} \sum_{\omega_n} f(i\omega_n), \quad (1.868)$$

where f is some function. To compute S , we consider the integral

$$I = \int_{(\mathcal{C})} \frac{dz}{2i\pi} f(z) n_{\zeta}(z) \quad (1.869)$$

along some path (\mathcal{C}) in the complex plane, where

$$n_{\zeta}(z) = \frac{1}{e^{\beta z} - \zeta} = \begin{cases} n_B(z) & (\text{bosons}), \\ n_F(z) & (\text{fermions}). \end{cases} \quad (1.870)$$

Since $n_{\zeta}(z)$ has simple poles at the imaginary frequencies $z = i\omega_n$ (with residue ζ/β), the integral I will be related to S if the integration path (\mathcal{C}) is suitably chosen.

Example 1

As a first example, we consider the sum

$$S = \frac{1}{\beta} \sum_{\omega_n} \frac{e^{i\omega_n \eta}}{i\omega_n - \xi} \quad (\eta \rightarrow 0^+). \quad (1.871)$$

S can be calculated from the integral

$$I = \oint_{(\mathcal{C})} \frac{dz}{2i\pi} \frac{e^{z\eta}}{z - \xi} n_{\zeta}(z) \quad (1.872)$$

along a circle (\mathcal{C}) of radius $R \rightarrow \infty$ around the origin $z = 0$ in the complex plane. In the limit $|z| \rightarrow \infty$, the function $e^{z\eta} n_{\zeta}(z)$ is exponentially suppressed⁹⁴ so that the integral I vanishes for $R \rightarrow \infty$. Now we can also evaluate I by the residue theorem. Besides the poles of $n_{\zeta}(z)$ at the Matsubara frequencies ω_n , there is a pole at $z = \xi$, and

$$I = \sum_{\omega_n} \text{Res}(i\omega_n) + \text{Res}(\xi) = \zeta S + n_{\zeta}(\xi) = 0, \quad (1.873)$$

i.e.

$$\frac{1}{\beta} \sum_{\omega_n} \frac{e^{i\omega_n \eta}}{i\omega_n - \xi} = \begin{cases} -n_B(\xi) & (\text{bosons}), \\ n_F(\xi) & (\text{fermions}). \end{cases} \quad (1.874)$$

⁹⁴Note that this property depends crucially on the factor $e^{z\eta}$ when $\Re(z) < 0$.

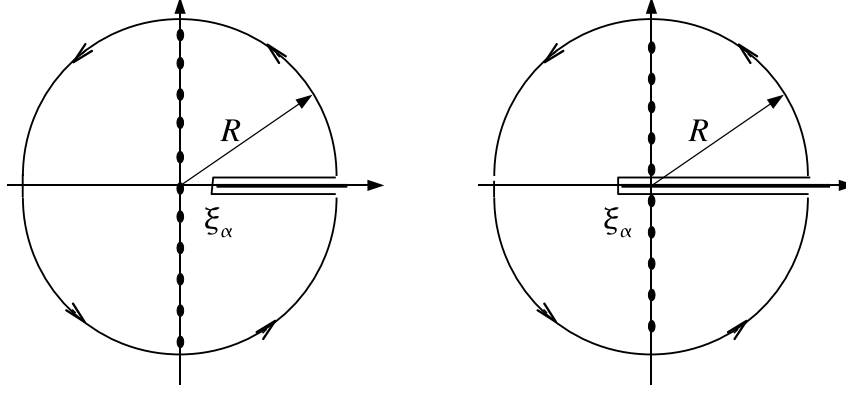


Figure 1.17: Integration contour (\mathcal{C}) in equation (1.876) for bosons (left) and fermions (right). The thick line on the real axis shows the branch cut of the function $\ln(-z + \xi_\alpha)$ and the black dots the positions of the imaginary frequencies $i\omega_n$. In the bosonic case, the branch cut is always located on the positive part of the real axis.

Example 2

As a second example, we consider the grand potential of non-interacting bosons or fermions (Sec. 1.4.2),

$$\Omega_0 = \frac{\zeta}{\beta} \sum_{\alpha, \omega_n} \ln(-i\omega_n + \xi_\alpha) e^{i\omega_n \eta}, \quad (1.875)$$

which can be calculated from the integral

$$I_\alpha = \oint_{(\mathcal{C})} \frac{dz}{2i\pi} n_\zeta(z) \ln(-z + \xi_\alpha) e^{z\eta}. \quad (1.876)$$

The contour (\mathcal{C}) is chosen such as to avoid the branch cut of the function $\ln(-z + \xi_\alpha)$ (Fig. 1.17). For non-interacting bosons, the chemical potential is always smaller than $\min_\alpha(\epsilon_\alpha)$. When $\mu \rightarrow \min_\alpha(\epsilon_\alpha)$, there is Bose-Einstein condensation. The condition $\xi_\alpha = \epsilon_\alpha - \mu > 0$ implies that there is no overlap between the branch cut of $\ln(-z + \xi_\alpha)$ and the Matsubara frequency $\omega_{n=0} = 0$. Again, the function $e^{z\eta} n_\zeta(z)$ ensures that the circular parts of (\mathcal{C}) do not contribute to I_α in the limit $R \rightarrow \infty$. We therefore obtain

$$\begin{aligned} I_\alpha &= \int_{\xi_\alpha}^{\infty} \frac{d\epsilon}{2i\pi} n_\zeta(\epsilon) \ln(-\epsilon - i\eta + \xi_\alpha) + \int_{\infty}^{\xi_\alpha} \frac{d\epsilon}{2i\pi} n_\zeta(\epsilon) \ln(-\epsilon + i\eta + \xi_\alpha) \\ &= \int_{\xi_\alpha}^{\infty} \frac{d\epsilon}{2i\pi} n_\zeta(\epsilon) [\ln(-\epsilon - i\eta + \xi_\alpha) - \text{c.c.}]. \end{aligned} \quad (1.877)$$

Using

$$n_\zeta(\epsilon) = \frac{\zeta}{\beta} \frac{d}{d\epsilon} \ln |1 - \zeta e^{-\beta\epsilon}| \quad (1.878)$$

and integrating by part,

$$\begin{aligned}
 I_\alpha &= -\frac{\zeta}{\beta} \int_{\xi_\alpha}^{\infty} \frac{d\epsilon}{2i\pi} \ln |1 - \zeta e^{-\beta\epsilon}| \frac{d}{d\epsilon} [\ln(-\epsilon - i\eta + \xi_\alpha) - \text{c.c.}] \\
 &= -\frac{\zeta}{\beta} \int_{\xi_\alpha}^{\infty} \frac{d\epsilon}{2i\pi} \ln |1 - \zeta e^{-\beta\epsilon}| [-2i\pi\delta(\epsilon - \xi_\alpha)] \\
 &= \frac{\zeta}{\beta} \ln(1 - \zeta e^{-\beta\xi_\alpha})
 \end{aligned} \tag{1.879}$$

since $\xi_\alpha > 0$ for bosons ($\zeta = 1$). On the other hand, the residue theorem gives

$$I_\alpha = \frac{\zeta}{\beta} \sum_{\omega_n} \ln(-i\omega_n + \xi_\alpha) e^{i\omega_n \eta}. \tag{1.880}$$

From (1.879) and (1.880), we finally deduce

$$\Omega_0 = \frac{\zeta}{\beta} \sum_{\alpha} \ln(1 - \zeta e^{-\beta\xi_\alpha}), \tag{1.881}$$

which is the familiar result for non-interacting particles (Sec. 1.C.5).

Example 3

In some cases, it is possible to compute the Matsubara sum more directly. For instance, the particle-hole susceptibility (Lindhard function) encountered in chapters 4 and 5 reads

$$\chi_{nn}^0(q) = -\frac{2}{\beta V} \sum_k G_0(k) G_0(k+q) \tag{1.882}$$

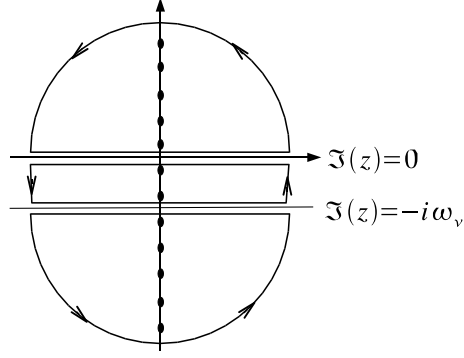
($q = (\mathbf{q}, i\omega_\nu)$), where $G_0(k) = (i\omega_n - \xi_{\mathbf{k}})^{-1}$ is the non-interacting Green function and ω_n a fermionic Matsubara frequency. Adding the factor $e^{i\omega_n \eta}$, which obviously does not change the result, we find

$$\begin{aligned}
 \chi_{nn}^0(q) &= -\frac{2}{\beta V} \sum_k \frac{e^{i\omega_n \eta}}{i\omega_\nu + \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}} \left(\frac{1}{i\omega_n - \xi_{\mathbf{k}}} - \frac{1}{i\omega_n + i\omega_\nu - \xi_{\mathbf{k}+\mathbf{q}}} \right) \\
 &= -\frac{2}{V} \sum_{\mathbf{k}} \frac{n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{i\omega_\nu + \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}},
 \end{aligned} \tag{1.883}$$

making use of (1.874).

Similarly the pairing susceptibility

$$\chi_0(q) = \frac{1}{\beta V} \sum_k G_0(k) G_0(q-k) \tag{1.884}$$

Figure 1.18: Integration contour (\mathcal{C}) in equation (1.887).

which arises in the theory of superconductivity [Eq. (6.187)] is given by

$$\begin{aligned}
 \chi_0(q) &= \frac{1}{\beta V} \sum_k \frac{e^{i\omega_n \eta}}{i\omega_\nu - \xi_{\mathbf{k}} - \xi_{\mathbf{q}-\mathbf{k}}} \left(\frac{1}{i\omega_n - \xi_{\mathbf{k}}} + \frac{1}{i\omega_\nu - i\omega_n - \xi_{\mathbf{q}-\mathbf{k}}} \right) \\
 &= \frac{1}{V} \sum_{\mathbf{k}} \frac{n_F(\xi_{\mathbf{k}}) - n_F(-\xi_{\mathbf{q}-\mathbf{k}})}{i\omega_\nu - \xi_{\mathbf{k}} - \xi_{\mathbf{q}-\mathbf{k}}} \\
 &= \frac{1}{V} \sum_{\mathbf{k}} \frac{n_F(\xi_{\mathbf{k}}) + n_F(\xi_{\mathbf{q}-\mathbf{k}}) - 1}{i\omega_\nu - \xi_{\mathbf{k}} - \xi_{\mathbf{q}-\mathbf{k}}}.
 \end{aligned} \tag{1.885}$$

Suppose that instead of $\chi_{nn}^0(q)$ [Eq. (1.882)], we wish to calculate

$$\tilde{\chi}_{nn}^0(q) = -\frac{2}{\beta V} \sum_k G(k)G(k+q) \tag{1.886}$$

for a fermion system, where $G(k) = [i\omega_n - \xi_{\mathbf{k}} - \Sigma(k)]^{-1}$. The standard method starts from the integral

$$I = \oint_{(\mathcal{C})} \frac{dz}{2i\pi} n_F(z) G(\mathbf{k}, z) G(\mathbf{k} + \mathbf{q}, z + i\omega_\nu). \tag{1.887}$$

Since $G(\mathbf{k}, z)$ can have branch cuts on the real axis $\Im(z) = 0$ (Sec. 3.5), the contour (\mathcal{C}) is chosen as shown in figure 1.18. The circular parts of the contour do not contribute when the radius R of the circle is sent to infinity, and we find

$$\begin{aligned}
 I &= \int_{-\infty}^{\infty} \frac{d\epsilon}{2i\pi} n_F(\epsilon) [G^R(\mathbf{k}, \epsilon) - G^A(\mathbf{k}, \epsilon)] G(\mathbf{k} + \mathbf{q}, \epsilon + i\omega_\nu) \\
 &\quad + \int_{-\infty}^{\infty} \frac{d\epsilon}{2i\pi} n_F(\epsilon) [G^R(\mathbf{k} + \mathbf{q}, \epsilon) - G^A(\mathbf{k} + \mathbf{q}, \epsilon)] G(\mathbf{k}, \epsilon - i\omega_\nu),
 \end{aligned} \tag{1.888}$$

where $G^R(\mathbf{k}, \epsilon) = G^A(\mathbf{k}, \epsilon)^*$ denotes the retarded Green function $G(\mathbf{k}, i\omega_n \rightarrow \epsilon + i\eta)$. $G(\mathbf{k}, z)$ being analytic for $\Im(z) \neq 0$ (Sec. 3.5), the residue theorem gives

$$I = -\frac{1}{\beta} \sum_{\omega_n} G(k)G(k+q), \tag{1.889}$$

which leads to

$$\tilde{\chi}_{nn}^0(q) = -\frac{2}{V} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} d\epsilon n_F(\epsilon) [A(\mathbf{k}, \epsilon) G(\mathbf{k} + \mathbf{q}, \epsilon + i\omega_\nu) + A(\mathbf{k} + \mathbf{q}, \epsilon) G(\mathbf{k}, \epsilon - i\omega_\nu)], \quad (1.890)$$

where $A(\mathbf{k}, \epsilon) = -\frac{1}{\pi} \Im[G^R(\mathbf{k}, \epsilon)]$ is the spectral function of the one-particle Green function (Sec. 3.5).

Alternatively, one can use the spectral representation

$$\begin{aligned} \frac{1}{\beta} \sum_{\omega_n} G(k) G(k+q) &= \frac{1}{\beta} \sum_{\omega_n} \int_{-\infty}^{\infty} d\epsilon d\epsilon' \frac{A(\mathbf{k}, \epsilon) A(\mathbf{k} + \mathbf{q}, \epsilon')}{(i\omega_n - \epsilon)(i\omega_n + i\omega_\nu - \epsilon')} \\ &= \int_{-\infty}^{\infty} d\epsilon d\epsilon' A(\mathbf{k}, \epsilon) A(\mathbf{k} + \mathbf{q}, \epsilon') \frac{n_F(\epsilon) - n_F(\epsilon' + i\omega_\nu)}{i\omega_\nu + \epsilon - \epsilon'}, \end{aligned} \quad (1.891)$$

where we have used (1.874). Using again the spectral representation, equation (1.891) can be rewritten as

$$\begin{aligned} \frac{1}{\beta} \sum_{\omega_n} G(k) G(k+q) &= \int_{-\infty}^{\infty} d\epsilon n_F(\epsilon) [A(\mathbf{k}, \epsilon) G(\mathbf{k} + \mathbf{q}, \epsilon + i\omega_\nu) \\ &\quad + A(\mathbf{k} + \mathbf{q}, \epsilon) G(\mathbf{k}, \epsilon - i\omega_\nu)], \end{aligned} \quad (1.892)$$

which leads to (1.890).

Example 4

Finally, we note that it is sometimes possible to express Matsubara sums in terms of special functions. For example, the coefficient of the quartic term in the Ginzburg-Landau expansion of the free energy of a superconductor [Eq. (6.238)] depends on the Matsubara sum

$$S = \frac{1}{\beta} \sum_{\omega_n} \frac{1}{|\omega_n|^3} = \frac{1}{4\pi^3 T^2} \sum_{n=0}^{\infty} \frac{1}{(n + \frac{1}{2})^3} = \frac{1}{4\pi^3 T^2} \zeta\left(3, \frac{1}{2}\right), \quad (1.893)$$

where

$$\zeta(z, q) = \sum_{n=0}^{\infty} \frac{1}{(n+q)^z} \quad (1.894)$$

is the generalized Riemann Zeta function. Using $\zeta(z, 1/2) = (2^z - 1)\zeta(z)$ where

$$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z} \quad (1.895)$$

is the Riemann Zeta function, we finally obtain

$$S = \frac{7\zeta(3)}{4\pi^3 T^2}, \quad (1.896)$$

with $\zeta(3) \simeq 1.20$.

Guide to the bibliography

- Many aspects of Feynman's path integral [1, 2] are reviewed in Schulman's book [3] (see also Refs. [4, 5]).
- Most textbooks on quantum field theory (e.g. Refs. [5, 6, 7, 8]) discuss the functional integral formalism, perturbation theory, as well as the effective action (the generating functional of 1PI vertices).
- Functional integrals in non-relativistic systems and their applications to condensed-matter physics are discussed in [9, 10].
- The Luttinger-Ward functional (the generating functional of 2PI vertices) was introduced in Refs. [11, 12, 13, 14] in condensed-matter physics and generalized to relativistic field theories in [15].
- The quantization of the electromagnetic field is presented in detail in [16].
- The “traditional” approach (based on the operator formalism) to quantum statistical physics is described in Refs. [17, 18, 19].

Bibliography

- [1] R. P. Feynman, *Rev. Mod. Phys.* **20**, 367 (1948).
- [2] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGrawHill, New York, 1965).
- [3] L. S. Schulman, *Techniques and Applications of Path integration* (Dover, 2005).
- [4] J. Zinn-Justin, *Intégrale de chemin en mécanique quantique: Introduction* (EDP Sciences, 2003).
- [5] H. Kleinert, *Path integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets* (World Scientific, 2005).
- [6] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, Third Edition (Clarendon Press, Oxford, 1996).
- [7] M. E. Peskin and D. V. Schroeder, *An introduction to Quantum Field Theory* (Westview Press, 1995).
- [8] S. Weinberg, *The Theory of Quantum Fields*, Vols. I and II (Cambridge University Press, 1995).
- [9] J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Addison-Wesley, 1988).
- [10] A. Atland and B. Simons, *Condensed-Matter Field Theory* (Cambridge University Press, 2006).
- [11] J. M. Luttinger, *Phys. Rev.* **118**, 1417 (1960).
- [12] G. Baym and L. P. Kadanoff, *Phys. Rev.* **124**, 287 (1961).
- [13] G. Baym, *Phys. Rev.* **127**, 1391 (1962).
- [14] C. De Dominicis and P. C. Martin, *J. Math. Phys.* **5**, 14 and 31 (1964).
- [15] J. M. Cornwall, R. Jackiw and E. Tomboulis, *Phys. Rev. D* **10**, 2428 (1974).
- [16] C. Cohen-Tannoudji, J. Dupont-Roc, and G. Grynberg, *Photons and Atoms* (Wiley, 1989).

- [17] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, 1975).
- [18] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (Dover, 2003).
- [19] G. D. Mahan, *Many-particle physics*, 2nd edition (Plenum press, New York, 1990).
- [20] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, Massachussets, 1950).
- [21] T. Kibble, *Classical Mechanics* (Imperial College Press, London, 2004).
- [22] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, 1955).
- [23] A. Messiah, *Quantum mechanics*, Vols. I and II (North-Holland, Amsterdam, 1962).
- [24] C. Cohen-Tannoudji, B. Diu, and F. Laloë, Vols. I and II *Quantum Mechanics* (Wiley and Herman, Paris, 1977).
- [25] R. Shankar, *Principles of Quantum Mechanics*, second edition (Plenum Press, New York, 1994).
- [26] R. Balian, *From Microphysics to Macrophysics*, Vols. I and II (Springer-Verlag, 1991).