Chapter 4

Functional Field Integral

In this chapter, the concept of path integration is generalized to integration over quantum fields. Specifically we will develop an approach to quantum field theory that takes as its starting point an integration over all configurations of a given field, weighted by an appropriate action. To emphasize the importance of the formulation which, methodologiccally, represents the backbone of the remainder of the text, we have pruned the discussion to focus only on the essential elements. This being so, conceptual aspects stand in the foreground and the discussion of applications is postponed to the following chapters.

In this chapter, the concept of path integration will be extended from quantum mechanics to quantum field theory. Our starting point will be from a situation very much analogous to that outlined at the beginning of the previous chapter. Just as there are two different approaches to quantum mechanics, quantum field theory can also be formulated in two different ways; the formalism of canonically quantised field operators, and functional integration. As for the former, although much of the technology needed to efficiently implement this framework — essentially Feynman diagrams — originated in high energy physics, it was with the development of condensed matter physics through the 50s, 60s and 70s that this approach was driven to unprecedented sophistication. The reason is that, almost as a rule, problems in condensed matter investigated at that time necessitated perturbative summations to *infinite* order in the non–trivial content of the theory (typically interactions). This requirement led to the development of advanced techniques to sum (subsets of) the perturbation series in many–body interaction operators to infinite order.

In the 70s, however, essentially *non–perturbative* problems began to attract more and more attention — a still prevailing trend — and it turned out that the formalism of canonically quantised operators was not tailored to this type of physics. By contrast, the alternative approach to many–body problems, functional integration, is ideally suited! The situation is similar to the one described in the last chapter where we saw that the Feynman path integral provided an entire spectrum of novel routes to approaching quantum mechanical problems (controlled semi–classical limits, analogies to classical mechanics, statistical mechanics, concepts of topology and geometry, etc.). Similarly, the introduction of functional field integration into many–body physics spawned plenty of new theoretical developments, many of which were manifestly non–perturbative. Moreover, the advantages of the path integral approach in many–body physics is even more pronounced than in single particle quantum mechanics. Higher dimensionality introduces fields of a more complex internal structure allowing for non–trivial topology while, at the same time, the connections to classical statistical mechanics play a much more important role than in single particle quantum mechanics.

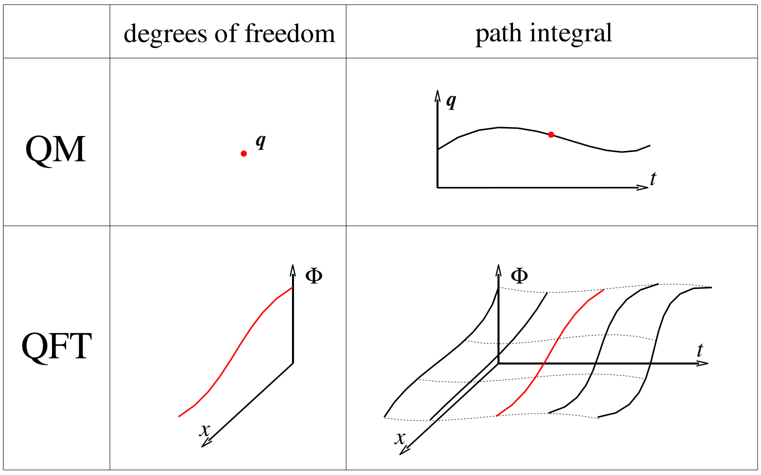

Figure 4.1: The concept of field integration. Upper panels: path integral of quantum mechanics — integration over all time-dependent configurations of a point particle degree of freedom leads to integrals over *curves*. Lower panels: field integral — integration over time dependent configurations of d–dimensional continuum mappings (fields) leads to integrals over generalized $(d+1)$–dimensional *surfaces*.

All of these concepts will begin to play a role in subsequent chapters when applications of the field integral are discussed. Before embarking on the quantitative construction — the subject of the following sections — let us first anticipate the kind of structures that one should expect. In quantum mechanics, we were starting from a single point particle degree of freedom, characterized by some coordinate $\mathbf{q}$ (or some other quantum numbers for that matter). Path integration then meant integration over all time–dependent configurations $\mathbf{q}(t)$, i.e. a set of *curves* $t \mapsto \mathbf{q}(t)$ (see Fig. 4.1 upper panel). By contrast, the degrees of freedom of field theory are continuous objects $\Phi(x)$ by themselves, where x parameterizes some d–dimensional base manifold and Φ takes values in some target manifold (Fig. 4.1, lower panel). The natural generalization of a 'path' integral then implies integration over a single copy of these objects at each instant of time, i.e. we shall have to integrate over generalized *surfaces*, mappings from $(d+1)$–dimensional space–time into the field manifold, $(x,t) \mapsto \Phi(x,t)$. While this notion may sound worrying, it is important to realize that, conceptually, nothing much changes in comparison with the path integral: instead of a one–dimensional manifold — a curve — our object of integration will be a $(d+1)$–dimensional manifold.

We now proceed to formulate these ideas in quantitative terms.

▷ Exercise. If necessary, recapitulate the general construction scheme of path integrals (section 3.2.3) and the connection between quantum fields and second quantized operators.

4.1 Construction of the Many–body Path Integral

The construction of a path integral for field operators follows the general scheme outlined at the end of section 3.2.3. The basic idea is to segment the time evolution of a quantum (many–body) Hamiltonian into infinitesimal time slices and to absorb as much as is possible of the quantum dynamical phase accumulated during the short time propagation into a set of suitably chosen eigenstates. But how should these eigenstates be chosen? In the context of single particle quantum mechanics, the basic structure of the Hamiltonian suggested the choice of a representation in terms of coordinate and momentum eigenstates. Now, given that many particle Hamiltonians are conveniently expressed in terms of creation/annihilation operators, an obvious idea would be to search for eigenstates of *these* operators. Such states indeed exist and are called **coherent states**.

4.1.1 Coherent States (Bosons)

Our goal is, therefore, to find eigenstates of the Fock space (non–Hermitian) operators $a^\dagger$ and a. Although the general form of these states will turn out to be the same for bosons and fermions, there are major differences regarding their algebraic structure. The point is that the anticommutation relations of fermions require that the eigenvalues of an annihilation operator themselves anticommute, i.e. they *cannot* be ordinary numbers. Postponing the introduction of the unfamiliar concept of anticommuting 'numbers' to the next section, we first concentrate on the bosonic case where problems of this kind do not arise.

So what form do the eigenstates $|\phi\rangle$ of the bosonic Fock space operators a, and $a^\dagger$ take? Being a state of the Fock space, an eigenstate $|\phi\rangle$ can be expanded as

$$|\phi\rangle = \sum_{n_1,n_2,\cdots} C_{n_1,n_2,\cdots}|n_1,n_2\cdots\rangle, \qquad |n_1,n_2\cdots\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1}}\frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2}}\cdots|0\rangle\,,$$

where $a_i^\dagger$ creates a boson in state i, $C_{n_1,n_2,\cdots}$ represents a set of expansion coefficients, and $|0\rangle$ represents the vacuum. Here, for reasons of clarity, it is convenient to adopt this convention for the vacuum as opposed to the notation $|\Omega\rangle$ used previously. Furthermore, the many–body state $|n_1,n_2\cdots\rangle$ is indexed by a set of occupation numbers: n_1 in state $|1\rangle$, n_2 in state $|2\rangle$, and so on. Importantly, the state $|\phi\rangle$ can, in principle (and will in practice) contain a superposition of basis states which have different numbers of particles. Now, if the minimum number of particles in state $|\phi\rangle$ is n_0, the minimum of $a_i^\dagger|\phi\rangle$ must be n_0+1: Clearly the *creation* operators $a_i^\dagger$ themselves cannot possess eigenstates.

However, with annihilation operators this problem does not arise. Indeed, the annihilation operators do possess eigenstates known as **bosonic coherent states**

$$\boxed{|\phi\rangle \equiv \exp\left[\sum_i \phi_i a_i^\dagger\right]|0\rangle} \tag{4.1}$$

where the elements of $\phi = \{\phi_i\}$ represent a set of complex numbers. The states $|\phi\rangle$ are eigenstates in the sense that, for all i,

$$\boxed{a_i|\phi\rangle = \phi_i|\phi\rangle} \tag{4.2}$$

i.e. they simultaneously diagonalise all annihilation operators. Noting that a_i and $a_j^\dagger$, with $j \neq i$, commute, Eq. (4.2) can be verified by showing that $a\exp(\phi a^\dagger)|0\rangle = \phi\exp(\phi a^\dagger)|0\rangle$.[1] Although not crucial to the practice of functional field integration, in the construction of the many–body path integral, it will be useful to assimilate some further properties of coherent states.

- ▷ By taking the Hermitian conjugate of Eq. (4.2), we find that the 'bra' associated with the 'ket' $|\phi\rangle$ is a left eigenstate of the set of creation operators, i.e. for all i,

$$\langle\phi|a_i^\dagger = \langle\phi|\bar{\phi}_i \tag{4.3}$$

  where $\bar{\phi}_i$ is the complex conjugate of ϕ_i, and $\langle\phi| = \langle 0|\exp[\sum_i \bar{\phi}_i a_i]$.

- ▷ It is a straightforward matter — e.g. by a Taylor expansion of Eq. (4.1) — to show that the action of a creation operator on a coherent state yields the identity

$$a_i^\dagger|\phi\rangle = \partial_{\phi_i}|\phi\rangle. \tag{4.4}$$

  Reassuringly, it may be confirmed that Eqs. (4.4) and (4.2) are consistent with the commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$: $[a_i, a_j^\dagger]|\phi\rangle = (\partial_{\phi_j}\phi_i - \phi_i\partial_{\phi_j})|\phi\rangle = \delta_{ij}|\phi\rangle$.

- ▷ Making use of the relation $\langle\theta|\phi\rangle = \langle 0|e^{\sum_i \bar{\theta}_i a_i}|\phi\rangle = e^{\sum_i \bar{\theta}_i \phi_i}\langle 0|\phi\rangle$ one finds that the overlap between two coherent states is given by

$$\langle\theta|\phi\rangle = \exp\left[\sum_i \bar{\theta}_i\phi_i\right] \tag{4.5}$$

- ▷ From this result, one can infer that the norm of a coherent state is given by

$$\langle\phi|\phi\rangle = \exp\left[\sum_i \bar{\phi}_i\phi_i\right] \tag{4.6}$$

- ▷ Most importantly, the coherent states form a complete — in fact an overcomplete — set of states in Fock space:

$$\boxed{\int \prod_i \frac{d\bar{\phi}_i d\phi_i}{\pi} e^{-\sum_i \bar{\phi}_i\phi_i}|\phi\rangle\langle\phi| = \mathbf{1}_{\mathcal{F}},} \tag{4.7}$$

  where $d\bar{\phi}_i d\phi_i = d\mathrm{Re}\,\phi_i d\mathrm{Im}\,\phi_i$, and $\mathbf{1}_{\mathcal{F}}$ represents the unit operator or identity in the Fock space.

[1] Using the result $[a, (a^\dagger)^n] = n(a^\dagger)^{n-1}$ (cf. Eq. **??**) a Taylor expansion shows $a\exp(\phi a^\dagger)|0\rangle = [a, \exp(\phi a^\dagger)]|0\rangle = \sum_{n=0}^\infty \frac{\phi^n}{n!}[a, (a^\dagger)^n]|0\rangle = \sum_{n=1}^\infty \frac{n\phi^n}{n!}(a^\dagger)^{n-1}|0\rangle = \phi\sum_{n=1}^\infty \frac{\phi^{n-1}}{(n-1)!}(a^\dagger)^{n-1}|0\rangle = \phi\exp(\phi a^\dagger)|0\rangle$.

▷ INFO. The proof of Eq. (4.7) proceeds by straightforward application of Schur's lemma (cf. our discussion of the completeness of the spin coherent states in the previous chapter): The operator family $\{a_i\}$, $\{a_i^\dagger\}$ acts irreducibly in Fock space. According to Schur's lemma, the proportionality of the left hand side of Eq. (4.7) to the unit operator is, therefore, equivalent to its commutativity with all creation and annihilation operators. Indeed, this property is easily confirmed:

$$a_i \int d(\bar\phi,\phi) e^{-\sum_i \bar\phi_i \phi_i} |\phi\rangle\langle\phi| = \int d(\bar\phi,\phi) e^{-\sum_i \bar\phi_i \phi_i} \phi_i |\phi\rangle\langle\phi| = -\int d(\bar\phi,\phi) \left(\partial_{\bar\phi_i} e^{-\sum_i \bar\phi_i\phi_i}\right) |\phi\rangle\langle\phi|$$
$$\overset{\text{by parts}}{=} \int d(\bar\phi,\phi) e^{-\sum_i \bar\phi_i\phi_i} |\phi\rangle \left(\partial_{\bar\phi_i}\langle\phi|\right) = \int d(\bar\phi,\phi) e^{-\sum_i \bar\phi_i\phi_i} |\phi\rangle\langle\phi| a_i, \tag{4.8}$$

where, for brevity, we have set $d(\bar\phi,\phi) \equiv \prod_i d\bar\phi_i d\phi_i/\pi$. Taking the adjoint of Eq. (4.8), one may further check that the left hand side of (4.7) commutes with the set of creation operators, i.e. it must be proportional to the unit operator. To fix the constant of proportionality, one may simply take the overlap with the vacuum:

$$\int d(\bar\phi,\phi) e^{-\sum_i \bar\phi_i\phi_i} \langle 0|\phi\rangle\langle\phi|0\rangle = \int d(\bar\phi,\phi) e^{-\sum_i \bar\phi_i\phi_i} = 1, \tag{4.9}$$

where the last equality follows from Eq. (3.11). Taken together, Eqs. (4.8) and (4.9) prove (4.7). Note that the coherent states are overcomplete in the sense that they are not mutually orthogonal (see Eq. (4.5)). The exponential weight $e^{-\sum_i \bar\phi_i\phi_i}$ appearing in the resolution of the identity compensates for the overcounting achieved by integrating over the whole set of coherent states.

With these definitions we have all that we need to construct the many–body path integral for the bosonic system. However, before doing so, we will first introduce the fermionic version of the coherent state. This will allow us to construct the path integrals for bosons and fermions simultaneously, thereby emphasising the similarity of their structure.

4.1.2 Coherent States (Fermions)

Surprisingly, much of the formalism above generalises to the fermionic case: As before, it is evident that creation operators cannot possess eigenstates. Following the bosonic system, let us suppose that the annihilation operators are characterised by a set of coherent states such that, for all i,

$$\boxed{a_i|\eta\rangle = \eta_i|\eta\rangle} \tag{4.10}$$

where η_i is the eigenvalue. Although the structure of this equation appears to be equivalent to its bosonic counterpart (4.2) it has one frustrating feature: Anticommutativity of the fermionic operators, $[a_i, a_j]_+ = 0$, where $i \neq j$, implies that the eigenvalues η_i also have to anticommute,

$$\boxed{\eta_i\eta_j = -\eta_j\eta_i} \tag{4.11}$$

Clearly, these objects cannot be ordinary numbers. In order to define a fermionic version of coherent states, we now have two choices: We may (a) accept Eq.(4.11) as a working definition and pragmatically explore its consequences, or (b), first try to remove any mystery from the definitions (4.10) and (4.11). This latter task is tackled in the info block below where objects $\{\eta_i\}$ with the desired properties are defined in a mathematically consistent manner. Readers wishing to proceed in a maximally streamlined manner may skip this exposition and directly turn to the more praxis–oriented discussion below.

▷ INFO. There is a mathematical structure ideally suited to generalize the concept of ordinary number(fields), namely **algebras**. An algebra $\mathcal{A}$ is a vector space endowed with a multiplication rule $\mathcal{A} \times \mathcal{A} \to \mathcal{A}$. So, let us *construct* an algebra $\mathcal{A}$ by starting out from a set of elements, or generators, $\eta_i \in \mathcal{A}, i = 1, \ldots N$, and imposing the rules:

(i) The elements η_i can be added and multiplied by complex numbers, viz.

$$c_0 + c_i\eta_i + c_j\eta_j, \in \mathcal{A} \qquad c_0, c_i, c_j \in \mathbb{C}\,, \tag{4.12}$$

i.e. $\mathcal{A}$ is a complex vectorspace.

(ii) The product, $\mathcal{A} \times \mathcal{A} \to \mathcal{A}, (\eta_i, \eta_j) \mapsto \eta_i\eta_j$, is associative and anticommutative, i.e. it obeys the anti–commutation relation (4.11). Because of the associativity of this operation, there is no ambiguity when it comes to forming products of higher order, i.e. $(\eta_i\eta_j)\eta_k = \eta_i(\eta_j\eta_k) \equiv \eta_i\eta_j\eta_k$. The definition requires that products of odd order in the number of generators anti–commute, while (even,even) and (even,odd) combinations commute (exercise).

By virtue of (i) and (ii), the set $\mathcal{A}$ of all linear combinations $c_0+\sum_{n=1}^{\infty}\sum_{i_1,\cdots i_n=1}^{N} c_{i_1,\ldots,i_n}\eta_{i_1}\ldots\eta_{i_n}$, $c_0, c_{i_1,\ldots,i_n} \in \mathbb{C}$ spans a finite–dimensional associative algebra $\mathcal{A}$,[2] known as the **Grassmann algebra**[3] (and sometimes also the **exterior algebra**).

For completeness we mention that Grassmann algebras find a number of realizations in mathematics, the most basic being exterior multiplication in linear algabra: Given an N–dimensional vector space V, let V^* be the dual space, i.e. the space of all linear mappings, or 'forms' $\Lambda : V \to \mathbb{C}, v \mapsto \Lambda(v)$, where $v \in V$. (Like V, V^* is a vector space of dimension N.) Next, define exterior multiplication through, $(\Lambda, \Lambda') \to \Lambda \wedge \Lambda'$, where $\Lambda \wedge \Lambda'$ is the mapping

$$\begin{aligned} \Lambda \wedge \Lambda' : V \times V &\to \mathbb{C} \\ (v, v') &\mapsto \Lambda(v)\Lambda'(v') - \Lambda(v')\Lambda'(v). \end{aligned}$$

This operation is manifestly anti–commutative: $\Lambda\wedge\Lambda' = -\Lambda\wedge\Lambda'$. Identifying the N linear basis forms $\Lambda_i \leftrightarrow \eta_i$ with generators and $\wedge$ with the product, we see that the space of exterior forms of a vector space forms a Grassmann algebra.

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[2] ...whose dimension can be shown to be 2^N (exercise)

[3] **Hermann Günter Grassmann** 1809–1877: credited for inventing what is now called Exterior Algebra.

Apart from their anomalous commutation properties, the generators $\{\eta_i\}$, and their product generalizations $\{\eta_i\eta_j, \eta_i\eta_j\eta_k, \ldots\}$ resemble ordinary, albeit anti-commutative numbers. (In practice, the algebraic structure underlying their definition can safely be ignored. All we will need to work with these objects is the basic rule (4.11) and the property (4.12).) We emphasize that $\mathcal{A}$ not only contains anticommuting but also commuting elements, i.e. linear combinations of an *even* number of Grassmann numbers η_i are overall commutative. (This mimics the behaviour of the Fock space algebra: products of an even number of annihilation operators $a_i a_j \ldots$ commute with all other linear combinations of operators a_i. In spite of this similarity, the 'numbers' η_i must not be confused with the Fock space operators; there is nothing on which they act.)

To make practical use of the new concept, we need to go beyond the level of pure arithmetic. Specifically, we need to introduce functions of anti–commuting numbers, and elements of calculus. Remarkably, most of the concepts of calculus not only naturally generalize to anti–commuting number fields, but contrary to what one might expect, the anti–commutative generalization of differentiation, integration, etc. turns out to be much *simpler* than in ordinary calculus.

▷ Functions of Grassmann numbers are defined via their Taylor expansion:

$$\xi_1, \ldots, \xi_k \in \mathcal{A}: \qquad f(\xi_1, \ldots, \xi_k) = \sum_{n=0}^{\infty} \sum_{i_1, \cdots i_n = 1}^{k} \frac{1}{n!} \frac{\partial^n f}{\partial \xi_{i_1} \ldots \partial \xi_{i_n}}\bigg|_{\xi=0} \xi_{i_n} \ldots \xi_{i_1}, \tag{4.13}$$

where f is an analytic function. Note that the anticommutation properties of the algebra implies that the series terminates after a *finite* number of terms. For example, in the simple case where η is first order in the generators of the algebra, $N = 1$, and $f(\eta) = f(0) + f'(0)\eta$ (since $\eta^2 = 0$).

▷ Differentiation with respect to Grassmann numbers is defined by

$$\boxed{\partial_{\eta_i} \eta_j = \delta_{ij}} \tag{4.14}$$

Note that in order to be consistent with the commutation relations, the differential operator ∂_{η_i} must itself be anti–commutative. In particular, $\partial_{\eta_i} \eta_j \eta_i \stackrel{i\neq j}{=} -\eta_j$.

▷ Integration over Grassmann variables is defined by

$$\boxed{\int d\eta_i = 0, \qquad \int d\eta_i \eta_i = 1} \tag{4.15}$$

Note that the definitions (4.13), (4.14) and (4.15) imply that the action of *Grassmann differentiation and integration are effectively identical*, viz.

$$\int d\eta f(\eta) = \int d\eta (f(0) + f'(0)\eta) = f'(0) = \partial_\eta f(\eta)\,.$$

With this background, let us now proceed to apply the Grassmann algebra to the construction of fermion coherent states. To this end we need to enlarge the algebra even further so as to allow for a multiplication of Grassmann numbers by fermion operators. In order to be consistent with the anticommutation relations, we need to require that fermion operators and Grassmann generators anticommute,

$$[\eta_i, a_j]_+ = 0\,. \tag{4.16}$$

It then becomes a straightforward matter to demonstrate that **fermionic coherent states** are defined by

$$\boxed{|\eta\rangle = \exp\left[-\sum_i \eta_i a_i^\dagger\right]|0\rangle} \tag{4.17}$$

i.e. by a structure perfectly analogous to the bosonic states (4.1).[4] It is a straightforward matter — and also a good exercise — to demonstrate that the properties (4.3), (4.4), (4.5), (4.6) and, most importantly, (4.7) carry over to the fermionic case. One merely has to identify a_i with a fermionic operator and replace the complex variables ϕ_i by $\eta_i \in \mathcal{A}$. Apart from a few sign changes and the $\mathcal{A}$–valued arguments, the fermionic coherent states differ only in two respects from their bosonic counterpart: firstly, the Grassmann variables $\bar\eta_i$ appearing in the adjoint of a fermion coherent state,

$$\langle\eta| = \langle 0|\exp\left[-\sum_i a_i\bar\eta_i\right] = \langle 0|\exp\left[\sum_i \bar\eta_i a_i\right]\,,$$

are *not* related to the η_is of the state $|\eta\rangle$ via some kind of complex conjugation. Rather η_i and $\bar\eta_i$ are strictly independent variables.[5] Secondly, the Grassmann version of a Gaussian integral (exercise), $\int d\bar\eta d\eta\, e^{-\bar\eta\eta} = 1$ does not contain the factors of π characteristic of standard Gaussian integrals. Thus, the measure of the fermionic analogue of Eq. (4.7) does not contain a π in the denominator.

For the sake of future reference, the most important properties of Fock space coherent states are summarised in table 4.1.

[4]To prove that the states (4.17) indeed fulfil the defining relation (4.10), we note that $a_i \exp(-\eta_i a_i^\dagger)|0\rangle \overset{(4.13)}{=} a_i(1-\eta_i a_i^\dagger)|0\rangle \overset{(4.16)}{=} \eta_i a_i a_i^\dagger|0\rangle = \eta_i|0\rangle = \eta_i(1-\eta_i a_i^\dagger)|0\rangle = \eta_i\exp(-\eta_i a_i^\dagger)|0\rangle$. This, in combination with the fact that a_i and $\eta_j a_j^\dagger$ $(i \neq j)$ commute proves (4.10). Note that the proof has actually been simpler than in the bosonic case. The fermionic Taylor series terminates after the first contribution. This observation is representative of a general rule: Grassmann calculus is simpler than standard calculus; all series are finite, integrals always converge, etc.

[5]In the literature, complex conjugation of Grassmann variables is sometimes defined. Although appealing from an aesthetic point of view — symmetry between bosons and fermions — this concept is problematic. The difficulties become apparent when **supersymmetric theories** are considered, i.e. theories where operator algebras contain both bosons and fermions (the so–called super–algebras). It is not possible to introduce a complex conjugation that leads to compatibility with the commutation relations of a super–algebra. It therefore seems to be better to abandon the concept of Grassmann complex conjugation altogether. Note that although, in the bosonic case, complex conjugation is inevitable (in order to define convergent Gaussian integrals, say), no such need arises in the fermionic case.

Definition	$\|\psi\rangle = \exp\left[\zeta \sum_i \psi_i a_i^\dagger\right] \|0\rangle$
Action of a_i	$a_i\|\psi\rangle = \psi_i\|\psi\rangle, \qquad \langle\psi\|a_i = \partial_{\bar\psi_i}\langle\psi\|$
Action of $a_i^\dagger$	$a_i^\dagger\|\psi\rangle = \zeta\partial_{\psi_i}\|\psi\rangle, \qquad \langle\psi\|a_i^\dagger = \langle\psi\|\bar\psi_i$
Overlap	$\langle\psi'\|\psi\rangle = \exp\left[\sum_i \bar\psi_i'\psi_i\right]$
Completeness	$\int d(\bar\psi,\psi)\, e^{-\sum_i \bar\psi_i\psi_i}\|\psi\rangle\langle\psi\| = \mathbf{1}_{\mathcal{F}}$

Table 4.1: Basic properties of coherent states for bosons ($\zeta = 1$, $\psi_i \in \mathbb{C}$) and fermions ($\zeta = -1$, $\psi_i \in \mathcal{A}$). In the last line, the integration measure is defined as $d(\bar\psi,\psi) \equiv \prod_i \frac{d\bar\psi_i d\psi_i}{\pi^{(1+\zeta)/2}}$.

$\triangleright$ INFO. **Grassmann Gaussian Integration:** Finally, before turning to the development of the functional field integral, it is useful to digress on the generalization of higher dimensional Gaussian integrals for Grassmann variables. The prototype of all Grassmann Gaussian integration formulae is the identity

$$\boxed{\int d\bar\eta d\eta\, e^{-\bar\eta a \eta} = a} \tag{4.18}$$

where $a \in \mathbb{C}$ takes arbitrary values. Eq. (4.18) is derived by a first order Taylor expansion of the exponential and application of Eq. (4.15). The multi–dimensional generalization of (4.18) is given by

$$\int d(\bar\phi,\phi) e^{-\bar\phi^T \mathbf{A}\phi} = \det \mathbf{A}\,, \tag{4.19}$$

where $\bar\phi$ and ϕ are N–component vectors of Grassmann variables, the measure $d(\bar\phi,\phi) \equiv \prod_{i=1}^N d\bar\phi_i d\phi_i$, and $\mathbf{A}$ may be an *arbitrary* complex matrix. For matrices that are unitarily diagonalisable, $\mathbf{A} = \mathbf{U}^\dagger\mathbf{D}\mathbf{U}$, with $\mathbf{U}$ unitary, and $\mathbf{D}$ diagonal, Eq. (4.19) is proven in the same way as its complex counterpart (3.17): One changes variables $\phi \to \mathbf{U}^\dagger\phi$, $\bar\phi \to \mathbf{U}^T\bar\phi$. Since $\det\mathbf{U} = 1$, the transform leaves the measure invariant (see below) and leaves us with N decoupled integrals of the type (4.18). The resulting product of N eigenvalues is just the determinant of $\mathbf{A}$ (cf. the later discussion of the partition function of the non–interacting gas). For general (non–diagonalisable) $\mathbf{A}$, the identity is established by a straightforward expansion of the exponent. The expansion terminates at Nth order and, by commuting through integration variables, it may be shown that the resulting Nth order polynomial of matrix elements of $\mathbf{A}$ is the determinant.[6]

Keeping the analogy with ordinary commuting variables, the Grassmann version of Eq. (3.18) reads

$$\int d(\bar{\phi},\phi)e^{-\bar{\phi}^T\mathbf{A}\phi+\bar{\nu}^T\cdot\phi+\bar{\phi}^T\cdot\nu} = e^{\bar{\nu}^T\mathbf{A}^{-1}\nu}\det\mathbf{A} \tag{4.22}$$

To prove the latter, we note that $\int d\eta f(\eta) = \int d\eta f(\eta+\nu)$, i.e. in Grassmann integration one can shift variables as in the ordinary case. The proof of the Gaussian relation above thus proceeds in complete analogy to the complex case. As with Eq. (3.18), Eq. (4.22) can also be employed to generate further integration formulae. Defining $\langle\cdots\rangle \equiv \det\mathbf{A}^{-1}\int d(\bar{\phi},\phi)e^{-\bar{\phi}^T\mathbf{A}\phi}(\cdots)$, and expanding both the left and the right hand side of (4.22) to leading order in the 'monomial' $\bar{\nu}_j\nu_i$, one obtains $\langle\eta_j\bar{\eta}_i\rangle = A^{-1}_{ji}$. Finally, the N–fold iteration of this procedure gives

$$\boxed{\langle\eta_{j_1}\eta_{j_2}\ldots\eta_{j_n}\bar{\eta}_{i_1}\bar{\eta}_{i_2}\ldots\bar{\eta}_{i_n}\rangle = \sum_P(\text{ sgn } P)\,A^{-1}_{j_1 i_{P_1}}\ldots A^{-1}_{j_n i_{P_n}}}$$

where the signum of the permutation accounts for the sign changes accompanying the interchange of Grassmann variables. Finally, as with Gaussian integration over commuting variables, by taking $N\to\infty$, the Grassmann integration can be translated to a Gaussian functional integral.

4.2 Field Integral for the Quantum Partition Function

Having introduced the coherent states, we will see that the construction of path integrals for many–body systems no longer presents substantial difficulties. However, be-

[6]As with ordinary integrals, Grassmann integrals can also be subjected to **variable transforms**. Suppose we are given an integral $\int d(\bar{\phi},\phi)f(\bar{\phi},\phi)$ and wish to change variables according to

$$\bar{\nu} = \mathbf{M}\bar{\phi},\quad \nu = \mathbf{M}'\phi\,, \tag{4.20}$$

where, for simplicity, $\mathbf{M}$ and $\mathbf{M}'$ are complex matrices (i.e. we here restrict ourselves to linear transforms). One can show that

$$\bar{\nu}_1\ldots\bar{\nu}_N = (\det\mathbf{M})\bar{\phi}_1\ldots\bar{\phi}_N, \qquad \nu_1\ldots\nu_N = (\det\mathbf{M}')\phi_1\ldots\phi_N\,. \tag{4.21}$$

(There are different ways to prove this identity. The most straightforward is by explicitly expanding (4.20) in components and commuting all Grassmann variables to the right. A more elegant way is to argue that the coefficient relating the right and the left hand sides of (4.21) must be an Nth order polynomial of matrix elements of $\mathbf{M}$. In order to be consistent with the anti–commutation behaviour of Grassmann variables, the polynomial must obey commutation relations which uniquely characterise a determinant. Excercise: Check the relation for $N=2$.) On the other hand, the integral of the new variables must obey the defining relation, $\int d\bar{\nu}\bar{\nu}_1\ldots\bar{\nu}_N = \int d\nu\nu_1\ldots\nu_N = (-)^{N+1}$, where $d\bar{\nu} = \prod_{i=1}^N d\bar{\nu}_i$ and the sign on the right hand side is attributed to ordering of the integrand, viz. $\int d\nu_1 d\nu_2\nu_1\nu_2 = -\int d\nu_1\nu_1\int d\nu_2\nu_2 = -1$. Together Eqs. (4.21) and (4.20) enforce the identities $d\bar{\nu} = (\det\mathbf{M})^{-1}d\bar{\phi}$, $d\nu = (\det\mathbf{M}')^{-1}d\phi$, which combine to give

$$\int d(\bar{\phi},\phi)f(\bar{\phi},\phi) = \det(\mathbf{M}\mathbf{M}')\int d(\bar{\nu},\nu')f(\bar{\phi}(\bar{\nu}),\phi(\nu))\,.$$

fore proceeding, we should address the question; what does the phrase 'path–integral for many–body systems' actually mean? In the next chapter we will see that much of the information about a quantum many–particle systems is encoded in expectation values of products of creation and annihilation operators, i.e. expressions of the structure $\langle a^\dagger a \ldots \rangle$. By an analogy to be explained then, objects of this type are generally called **correlation functions**. More important for our present discussion, at any finite temperature, the average $\langle \ldots \rangle$ entering the definition of the correlation function runs over the quantum Gibbs[7] distribution $\hat\rho \equiv e^{-\beta(\hat H - \mu \hat N)}/\mathcal{Z}$, where, as usual,

$$\mathcal{Z} = \mathrm{tr}\; e^{-\beta(\hat H - \mu \hat N)} = \sum_n \langle n | e^{-\beta(\hat H - \mu \hat N)} | n \rangle \,, \tag{4.23}$$

is the quantum partition function, $\beta \equiv 1/T$, μ denotes the chemical potential, and the sum extends over a complete set of Fock space states $\{|n\rangle\}$. (For the time being we neither specify the statistics of the system — bosonic or fermionic — nor the structure of the Hamiltonian.)

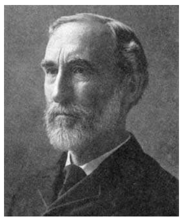
Ultimately, we will want to construct and evaluate the path integral representations of many–body correlation functions. Later we will see that all of these representations can be derived by a few straightforward manipulations form a prototypical path integral, namely that for $\mathcal{Z}$. Further, the (path integral of the) partition function is of importance in its own right: It contains much of the information needed to characterise the thermodynamic properties of a many–body quantum system.[8] We thus begin our journey into many–body field theory with a construction of the path integral for $\mathcal{Z}$.

To prepare the representation of the partition function (4.23) in terms of coherent states, one must insert the resolution of identity

$$\mathcal{Z} = \int d(\bar\psi, \psi)\, e^{-\sum_i \bar\psi_i \psi_i} \sum_n \langle n | \psi \rangle \langle \psi | e^{-\beta(\hat H - \mu \hat N)} | n \rangle \,. \tag{4.24}$$

We now wish to get rid of the — now redundant — Fock space summation over $|n\rangle$ (another resolution of identity). To bring the summation to the form $\sum_n |n\rangle\langle n| = \mathbf{1}_{\mathcal{F}}$,

[7] **Josiah Willard Gibbs** 1839–1903: credited with the development of chemical thermodynamics, he introduced concepts of free energy and chemical potential.



[8] In fact, the statement above is not entirely correct. Strictly speaking thermodynamic properties involve the **thermodynamic potential** $\Omega = -T \ln \mathcal{Z}$ rather than the partition function itself. At first sight it seems that the difference between the two is artificial — one might first calculate $\mathcal{Z}$ and then take the logarithm. However, typically, one is unable to determine $\mathcal{Z}$ in closed form, but rather one has to perform a perturbative expansion, i.e. the result of a calculation of $\mathcal{Z}$ will take the form of a series in some small parameter ϵ. Now a problem arises when the logarithm of the series is taken. In particular, the Taylor series expansion of $\mathcal{Z}$ to a given order in ϵ does *not* automatically determine the expansion of Ω to the same order. Fortunately, the situation is not all that bad. It turns out that the logarithm essentially rearranges the combinatorial structure of the perturbation series in an order known as a **cumulant expansion**.

one must commute the factor $\langle n|\psi\rangle$ to the right hand side. However, in performing this seemingly innocuous operation, we must be careful not to miss a sign change whose presence will have important consequences for the structure of the fermionic path integral: Indeed, it may be checked that, whilst for bosons, $\langle n|\psi\rangle\langle\psi|n\rangle = \langle\psi|n\rangle\langle n|\psi\rangle$, the fermionic coherent states change sign upon permutation, $\langle n|\psi\rangle\langle\psi|n\rangle = \langle -\psi|n\rangle\langle n|\psi\rangle$ (i.e. $\langle -\psi| \equiv \exp\left(-\sum_i \bar{\psi}_i a_i\right)$). The presence of the sign is a direct consequence of the anti–commutation relations between Grassmann variables and Fock space operators (exercise). Note that, as both $\hat{H}$ and $\hat{N}$ contain elements even in the creation/annihilation operators, the sign is insensitive to the presence of the Boltzmann factor in (4.24). Making use of the sign factor ζ, the result of the interchange can be formulated as the general expression

$$\begin{aligned}\mathcal{Z} &= \int d(\bar{\psi},\psi)\, e^{-\sum_i \bar{\psi}_i\psi_i} \sum_n \langle\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle\langle n|\psi\rangle \\ &= \int d(\bar{\psi},\psi)\, e^{-\sum_i \bar{\psi}_i\psi_i} \langle\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle\,, \end{aligned} \qquad (4.25)$$

where the equality is based on the identity $\sum_n |n\rangle\langle n| = \mathbf{1}_{\mathcal{F}}$. Eq. (4.25) can now be directly subjected to the general construction scheme of the path integral.

To be concrete, let us assume that the Hamiltonian is limited to a maximum of two–body interactions (cf. Eqs. (2.5) and (2.9)),

$$\hat{H}(a^\dagger,a) = \sum_{ij} h_{ij} a_i^\dagger a_j + \sum_{ijkl} V_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l\,. \qquad (4.26)$$

Note that, to facilitate the construction of the field integral, it is helpful to arrange for all of the annihilation operators to stand to the right of the creation operators. Fock space operators of this structure are said to be **normal ordered**.[9] The reason for emphasising normal ordering is that such an operator can be readily diagonalised by means of coherent states: Dividing the 'time interval' β into N segments and inserting coherent state resolutions of identity (steps 1, 2 and 3 of the general scheme), Eq. (4.25) assumes the form

$$\mathcal{Z} = \int_{\substack{\bar{\psi}^0=\zeta\bar{\psi}^N \\ \psi^0=\zeta\psi^N}} \prod_{n=0}^{N} d(\bar{\psi}^n,\psi^n)\, e^{-\delta\sum_{n=0}^{N-1}\left[\delta^{-1}(\bar{\psi}^n-\bar{\psi}^{n+1})\cdot\psi^n + H(\bar{\psi}^{n+1},\psi^n)-\mu N(\bar{\psi}^{n+1},\psi^n)\right]}\,, \qquad (4.27)$$

where $\delta = \beta/N$ and $\frac{\langle\psi|\hat{H}(a^\dagger,a)|\psi'\rangle}{\langle\psi|\psi'\rangle} = \sum_{ij} h_{ij}\bar{\psi}_i\psi'_j + \sum_{ijkl} V_{ijkl}\,\bar{\psi}_i\bar{\psi}_j\psi'_k\psi'_l \equiv H(\bar{\psi},\psi')$, (similarly $N(\bar{\psi},\psi')$). Here, in writing Eq. (4.27), we have adopted the shorthand $\psi^n = \{\psi_i^n\}$, etc. Finally, sending $N\to\infty$ and taking limits analogous to those leading from (3.5) to

[9]More generally, an operator is defined to be 'normal ordered' with respect to a given vacuum state $|0\rangle$, if and only if, it annihilates $|0\rangle$. Note that the vacuum need not necessarily be defined as a zero particle state. If the vacuum contains particles, normal ordering need not lead to a representation where all annihilators stand to the right. If, for whatever reason, one is given a Hamiltonian whose structure differs from (4.26), one can always affect a normal ordered form at the expense of introducing commutator terms. For example, normal ordering the quartic term leads to the appearance of a quadratic contribution which can be absorbed into $h_{\alpha\beta}$.

(3.6) we obtain the continuum version of the path integral,[10]

$$\boxed{\mathcal{Z} = \int D(\bar\psi,\psi) e^{-S[\bar\psi,\psi]}, \qquad S[\bar\psi,\psi] = \int_0^\beta d\tau \left[\bar\psi\partial_\tau\psi + H(\bar\psi,\psi) - \mu N(\bar\psi,\psi)\right]} \tag{4.28}$$

where $D(\bar\psi,\psi) = \lim_{N\to\infty}\prod_{n=1}^N d(\bar\psi^n,\psi^n)$, and the fields satisfy the boundary condition

$$\bar\psi(0) = \zeta\bar\psi(\beta), \quad \psi(0) = \zeta\psi(\beta)\,. \tag{4.29}$$

Written in a more explicit form, the action associated with the general pair–interaction Hamiltonian (4.26) can be cast in the form

$$S = \int_0^\beta d\tau \left[\sum_{ij}\bar\psi_i(\tau)\left[(\partial_\tau - \mu)\delta_{ij} + h_{ij}\right]\psi_j(\tau) + \sum_{ijkl} V_{ijkl}\bar\psi_i(\tau)\bar\psi_j(\tau)\psi_k(\tau)\psi_l(\tau)\right]\,. \tag{4.30}$$

Notice that the structure of the action fits nicely into the general scheme discused in the previous chapter. By analogy, one would expect that the exponent of the many–body path integral carries the significance of the Hamiltonian action, $S \sim \int(p\dot q - H)$, where (q,p) symbolically stands for a set of generalized coordinates and momenta. In the present case, the natural pair of canonically conjugate operators is $(a, a^\dagger)$. One would then interpret the eigenvalues $(\psi,\bar\psi)$ as 'coordinates' (much as (q,p) are the eigenvalues of the operators $(\hat q,\hat p)$). Adopting this interpretation, we see that the exponent of the path integral indeed has the canonical form of a Hamiltonian action and, therefore, is easy to memorize.

Eqs. (4.28) and (4.30) define the **functional integral in the time representation** (in the sense that the fields are functions of a time variable). In practice we shall mostly find it useful to represent the action in an alternative, Fourier conjugate representation. To this end, note that, due to the boundary conditions (4.29), the functions $\psi(\tau)$ can be interpreted as functions on the entire Euclidean time axis which are periodic/antiperiodic on the interval $[0,\beta]$. As such they can be represented in terms of a Fourier series,

$$\psi(\tau) = \frac{1}{\sqrt\beta}\sum_{\omega_n}\psi_n e^{-i\omega_n\tau}, \qquad \psi_n = \frac{1}{\sqrt\beta}\int_0^\beta d\tau\psi(\tau)e^{i\omega_n\tau}\,,$$

where

$$\omega_n = \begin{cases} 2n\pi T, & \text{bosons,} \\ (2n+1)\pi T, & \text{fermions} \end{cases}, \qquad n\in\mathbb{Z} \tag{4.31}$$

are known as **Matsubara frequencies**. Substituting this representation into (4.28) and (4.30), we obtain $\mathcal{Z} = \int D(\bar\psi,\psi)e^{-S[\bar\psi,\psi]}$, where $D(\bar\psi,\psi) = \prod_n d(\bar\psi_n,\psi_n)$ defines the

[10] Whereas the bosonic continuum limit is indeed perfectly equivalent to the one taken in constructing the quantum mechanical path integral ($\lim_{\delta\to0}\delta^{-1}(\bar\psi^{n+1}-\bar\psi^n) = \partial_\tau|_{\tau=n\delta}$ gives an ordinary derivative etc.), a novelty arises in the fermionic case. The notion of replacing differences by derivatives is purely symbolic for Grassmann variables. There is no sense in which $\bar\psi^{n+1}-\bar\psi^n$ is small. The symbol $\partial_\tau\bar\psi$ rather denotes the formal (and well defined expression) $\lim_{\delta\to0}\delta^{-1}(\bar\psi^{n+1}-\bar\psi^n)$.

measure (for each Matsubara index n we have an integration over a coherent state basis $\{|\psi_n\rangle\}$),[11] and the action takes the form

$$S[\bar\psi,\psi] = \sum_{ij,\omega_n} \bar\psi_{in}\left[(-i\omega_n-\mu)\,\delta_{ij}+h_{ij}\right]\psi_{jn} + \frac{1}{\beta}\sum_{ijkl,\{\omega_{n_i}} V_{ijkl}\,\bar\psi_{in_1}\bar\psi_{jn_2}\psi_{kn_3}\psi_{ln_4}\delta_{n_1+n_2,n_3+n_4} \quad (4.32)$$

Here we have used the identity $\int_0^\tau d\tau e^{-i\omega_n\tau} = \beta\delta_{\omega_n,0}$. Eq. (4.32) defines the **frequency representation of the action**.[12]

▷ INFO. In performing calculations in the Matsubara representation, one sometimes runs into convergence problems (which will manifest themselves in the form of ill–convergent Matsubara frequency summations): In such cases it will be important to remember that Eq. (4.32) does not actually represent the precise form of the action. What is missing is a convergence generating factor whose presence follows from the way in which the integral was constructed, and which will save us in cases of non–convergent sums (except, of course, in cases where divergences have a physical origin). More precisely, since the fields $\bar\psi$ are evaluated infinitesimally later than the operators ψ (cf. Eq. (4.27)), the h and μ–dependent contributions to the action acquire a factor $\exp(-i\omega_n\delta)$, δ infinitesimal. Similarly, the V contribution acquires a factor $\exp(-i(\omega_{n_1}+\omega_{n_2})\delta)$. In cases where the convergence is not critical, we will omit these contributions. However, once in a while it is necessary to remember their presence.

4.2.1 Partition Function of Non–Interacting Gas

As a first exercise, let us consider the quantum partition function of the non–interacting gas. (Later, this object will prove useful as a 'reference' in the development of weakly interacting theories.) In some sense, the field integral formulation of the non–interacting partition function has a status similar to that of the path integral for the quantum harmonic osciallator: The direct quantum mechanical solution of the problem is straightforward and application of the full artillery of the field integral seems somewhat ludicrous. From a pedagogical point of view, however, the free partition function is a good problem; it provides us with the welcome opportunity to introduce a number of practical concepts of field integration within a comparatively simple setting. Moreover, the field integral representation of the free partition function will be an important operational building block for our subsequent analysis of interacting problems.

Consider, then the partition function (4.28) with $H_0(\bar\psi,\psi)=\sum_{ij}\bar\psi_i\,H_{0,ij}\,\psi_j$. Diagonalising H_0 by a unitary transformation U, $H_0 = UDU^\dagger$ and transforming integration variables $U^\dagger\psi\equiv\phi$, the action assumes the form, $S=\sum_a\sum_{\omega_n}\bar\phi_{an}(-i\omega_n+\xi_a)\phi_{an}$, where $\xi_a\equiv\epsilon_a-\mu$ and ϵ_a are the single particle eigenvalues. Remembering that the fields $\phi_a(\tau)$

[11]Notice, however, that the fields ψ_n carry dimension $[\text{energy}]^{-1/2}$, i.e. the frequency coherent state integral is normalized as $\int d(\bar\psi_n,\psi_n)\,e^{-\bar\psi_n\epsilon\psi_n}=(\beta\epsilon)^{-\zeta}$.

[12]As for the signs of the Matsubara indices appearing in Eq. (4.32), note that the Fourier representation of $\bar\psi$ is defined as $\bar\psi(\tau)=\frac{1}{\sqrt\beta}\sum_n\bar\psi_n e^{+i\omega_n\tau}$, $\bar\psi_n=\frac{1}{\sqrt\beta}\int_0^\beta d\tau\,\bar\psi(\tau)e^{-i\omega_n\tau}$. In the bosonic case, this sign convention is motivated by $\bar\psi$ being the complex conjugate of ψ. For reasons of notational symmetry, this convention is also adopted in the fermionic case.

are independent integration variables (exercise: why does the transformation $\psi \to \phi$ have a Jacobian of unity?), we find that the partition function decouples, $\mathcal{Z} = \prod_a \mathcal{Z}_a$, where

$$\mathcal{Z}_a = \int D(\bar{\phi}_a, \phi_a)\, e^{-\sum_n \bar{\phi}_{an}(-i\omega_n+\xi_a)\phi_{an}} = \prod_n [\beta(-i\omega_n + \xi_a)]^{-\zeta}, \tag{4.33}$$

and the last equality follows from the fact that the integrals over ϕ_{an} are one–dimensional complex or Grassmann Gaussian integrals. Here, let us recall our convention defining $\zeta = 1(-1)$ for bosonic (fermionic) fields. At this stage, we have left all aspects of field integration behind us and reduced the problem to one of computing an infinite product over factors $i\omega_n - \xi_a$. Since products are usually more difficult to get under control than sums, we take the logarithm of $\mathcal{Z}$ to obtain the free energy

$$F = -T \ln \mathcal{Z} = -T\zeta \sum_{an} \ln[\beta(-i\omega_n + \xi_a)]. \tag{4.34}$$

▷ INFO. Before proceeding with this expression, let us take a second look at the intermediate identity (4.33). Our calcuation showed the partition function to be the product over all eigenvalues of the operator $-i\hat{\omega} + \hat{H} - \mu\hat{N}$ defining the action of the non-interacting system (here, $\hat{\omega} = \{\omega_n \delta_{nn'}\}$). As such, it can be written compactly as:

$$\boxed{\mathcal{Z} = \det\left[\beta(-i\hat{\omega} + \hat{H} - \mu\hat{N})\right]^{-\zeta}} \tag{4.35}$$

This result was derived by first converting to an eigenvalue integration and then performing the one–dimensional integrals over 'eigencomponents' ϕ_{an}. While technically straightforward, that — explicitly representation-dependent — procedure is not well suited to generalization to more complex problems. (Keep in mind that later on we will want to embed the free action of the non–interacting problem into the more general framework of an interacting theory.)

Indeed, it is not necessary to refer to an eigenbasis at all: In the bosonic case, Eq. (3.17) tells us that Gaussian integration over a bilinear $\sim \bar{\phi}\hat{X}\phi$ generates the inverse determinant of $\hat{X}$. Similarly, as we have seen, Gaussian integration extends to the Grassmann case with the determinants appearing in the numerator rather than in the denominator (as exemplified by (4.35)). (As a matter of fact, (4.33) is already a proof of this relation.)

We now have to face up to a technical problem: How do we compute Matsubara sums of the form $\sum_n \ln(i\omega_n - x)$? Indeed, it takes little imagination to foresee that sums of the type $\sum_{n_1,n_2,\ldots} X(\omega_{n_1}, \omega_{n_2}, \ldots)$, where X symbolically stands for some function, will be a recurrent structure in the analysis of functional integrals. A good ansatz would be to argue that, for sufficiently low temperatures (i.e. temperatures smaller than any other characteristic energy scale in the problem), the sum can be traded for an integral, viz. $T\sum_n \to \int d\omega/(2\pi)$. However, this approximation is too crude to capture much of the characteristic temperature dependence in which one is usually interested. Yet there exists an alternative, and much more accurate way of computing sums over Matsubara frequencies:

▷ INFO. Consider a single **Matsubara frequency summation**,

$$S \equiv \sum_n h(\omega_n)\,, \tag{4.36}$$

where h is some function and ω_n may be either bosonic or fermionic (cf. Eq. (4.31)). The basic idea behind the standard scheme of evaluating sums of this type is to introduce a complex auxiliary function $g(z)$ that has simple poles at $z = i\omega_n$. The sum S then emerges as the sum of residues obtained by integrating the product gh along a suitably chosen path in the complex plane. Typical choices of g include

$$g(z) = \begin{cases} \dfrac{\beta}{\exp(\beta z) - 1}, & \text{bosons} \\ \dfrac{\beta}{\exp(\beta z) + 1}, & \text{fermions} \end{cases} \quad \text{and} \quad g(z) = \begin{cases} \dfrac{\beta}{2}\coth(\beta z/2), & \text{bosons} \\ \dfrac{\beta}{2}\tanh(\beta z/2), & \text{fermions} \end{cases} \tag{4.37}$$

where, in much of this section, we will employ the functions of the first column. (Notice the similarity between these functions and the familiar Fermi and Bose distribution functions.) In practice, the choice of the counting function is mostly a matter of taste, save for some cases where one of the two options is dictated by convergence criteria.

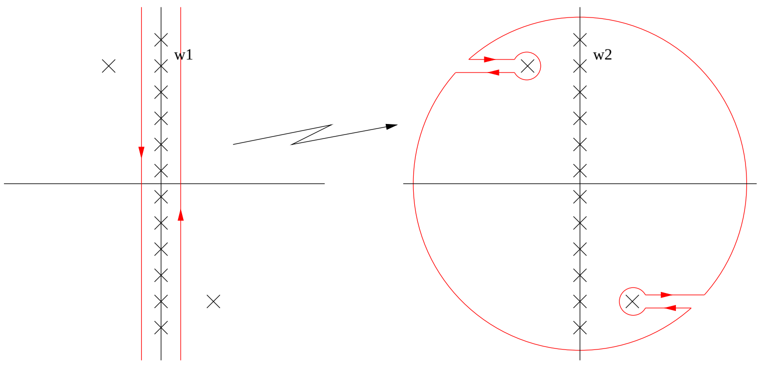


Figure 4.2: Left: the integration contour employed in calculating the sum (4.36). Right: the deformed integration contour.

Integration over the path shown in the left part of Fig. 4.2 then produces

$$\frac{\zeta}{2\pi i}\oint dz g(z) h(-iz) = \zeta \sum_n \mathrm{Res}\,(g(z)h(-iz))|_{z=i\omega_n} = \sum_n h(\omega_n) = S\,,$$

where, in the third identity, we have used the fact that the 'counting functions' g are chosen so as to have residue ζ and it is assumed that the integration contour closes at $z \to \pm i\infty$. (The difference between using the first and the second column of (4.37) lies in the value of the residue. In the latter case, it is equal to unity rather than ζ.) Now, the integral along a contour in the immediate vicinity of the poles of g is usually intractable. However, as long as we are careful not to cross any singularities of g or the function $h(-iz)$ (the latter symbolically indicated by isolated crosses in the figure[13]) we are free to distort the integration path, ideally to a contour along

[13] Remember that a function that is bounded and analytic in the entire complex plane is constant, i.e. every 'interesting' function will have singularities.

which the integral *can* be performed. Finding a suitable contour is not always straightforward. If the product hg decays sufficiently fast at $|z| \to \infty$ (i.e. faster than z^{-1}), one will ususally try to 'inflate' the original contour to an infinitely large circle (Fig. 4.2, right).[14] The integral along the outer perimeter of the contour then vanishes and one is left with the integral around the singularities of the function h. In the simple case where $h(-iz)$ posesses a number of isolated singularities at $\{z_k\}$ (i.e. the situation indicated in the figure) we thus obtain[15]

$$S = -\frac{\zeta}{2\pi i} \oint h(-iz)g(z) = -\zeta \sum_k \operatorname{Res} h(-iz)g(z)|_{z=z_k}\,, \tag{4.38}$$

i.e. the task of computing the infinite sum S has been reduced to that of evaluating a finite number of residues — a task that is always possible!

To illustrate the procedure on a simple example, let us consider the function

$$h(\omega_n) = -\frac{\zeta T}{i\omega_n e^{-i\omega_n \delta} - \xi}\,,$$

where δ is a positive infinitesimal.[16] To evaluate the sum $S = \sum_n h(\omega_n)$, we first observe that the product $h(-iz)g(z)$ has benign convergence properties. Further, the function $h(-iz)$ has a simple pole that, in the limit $\delta \to 0$, lies on the real axis at $z = \xi$. This leads to the result

$$\sum_n h(\omega_n) = \zeta \operatorname{Res} g(z)h(-iz)|_{z=\xi} = -\frac{1}{e^{\beta\xi} - \zeta}\,.$$

We have thus arrived at the important identity

$$\boxed{\zeta T \sum_n \frac{1}{i\omega_n - \xi_a} = \begin{cases} n_{\rm B}(\epsilon_a), & \text{bosons,} \\ n_{\rm F}(\epsilon_a), & \text{fermions} \end{cases}} \tag{4.39}$$

[14] Notice that the condition $\lim_{|z|\to\infty} |hg| < z^{-1}$ is not as restrictive as it may seem. The reason is that the function h will be mostly related to physical observables that approach some limit (or vanish) for large excitation energies. This implies vanishing in at least portions of the complex plane. The convergence properties of g depend on the concrete choice of the counting function. (Exercise: explore the convergence properties of the functions shown in Eq. (4.37).)

[15] If you are confused about signs, note that the contour encircles the singularities of h in a clockwise direction.

[16] Indeed, this choice of h is actually not as artificial as it may seem. The expectation value of the **number of particles** in the grand canonical ensemble is defined through the identity $N \equiv -\partial F/\partial\mu$ where F is the free energy. In the non–interacting case, the latter is given by Eq. (4.34) and, remembering that $\xi_a = \epsilon_a - \mu$, one obtains $N \approx -\zeta T \sum_{an} \frac{1}{i\omega_n - \xi_a}$. Now, why did we write '$\approx$' instead of '$=$'? The reason is that the right hand side, obtained by naive differentiation of (4.34), is ill–convergent. (The sum $\sum_{n=-\infty}^{\infty} \frac{1}{n+x}$, x arbitrary, does not exist!) At this point we have to remember the remark made in the on page 136, i.e., had we carefully treated the discretisation of the field integral, both the logarithm of the free energy and $\partial_\mu F$ would acquire infinitesimal phases $\exp(-i\omega_n\delta)$. As an exercise, try to keep track of the discretisation of the field integral from its definition to Eq. (4.34) to show that the accurate expression for N reads

$$N = -\zeta T \sum_{an} \frac{1}{i\omega_n e^{-i\omega_n\delta} - \xi_a} = \sum_a \sum_n h(\omega_n)|_{\xi=\xi_a}\,,$$

where h is the function introduced above. (Note that the necessity to keep track of the lifebuoy $e^{-i\omega_n\delta}$ does not arise too often. Most Matsubara sums of physical interest relate to functions f that decay faster than z^{-1}.)

where

$$n_{\rm F}(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1}, \qquad n_{\rm B}(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}-1} \tag{4.40}$$

are the Fermi/Bose distribution functions. As a corollary we note that the expectation value for the number of particles in a non–interacting quantum gas assumes the familiar form $N = \sum_a n_{\rm F/B}(\epsilon_a)$.

Before returning to our discussion of the partition function, let us note that life is not always as simple as the example above. More often than not, the function h not only contains isolated singularities but also cuts or worse singularities. Under such circumstances, finding a good choice of the integration contour can be far from straightforward!

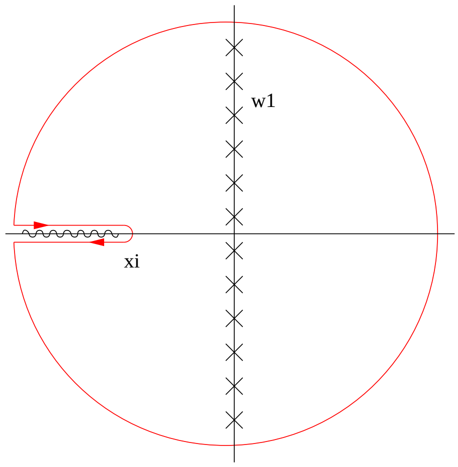


Figure 4.3:

Returning to the problem of computing the sum (4.34), consider for a moment a fixed eigenvalue $\xi_a \equiv a$. In this case, we need to evaluate the sum $S \equiv \sum_n h(\omega_n)$, where $h(\omega_n) \equiv \zeta T \ln[\beta(-i\omega_n + \xi)] = \zeta T \ln[\beta(i\omega_n - \xi)] + C$ and C is an inessential constant. As discussed before, the sum can be represented as $S = -\frac{\zeta}{2\pi i}\oint g(z)h(-iz)$, where $g(z) = \beta(e^{\beta z} - \zeta)^{-1}$ is (β times) the distribution function and the contour encircles the poles of g as in Fig. 4.2, left. Now, there is an essential difference with the example discussed previously, viz. the function $h(-iz) = \zeta T \ln(z - \xi) + C$ has a branch cut along the real axis, $z \in (-\infty, \xi)$ (see the figure). To avoid contact with this singularity one must distort the integration contour as shown in the figure. Noticing that the (suitably regularized, cf. our previous discussion of the particle number N) integral along the perimeter vanishes, we conclude that

$$S = \frac{T}{2\pi i}\int_{-\infty}^{\infty} d\epsilon\, g(\epsilon)\left(\ln(\epsilon^+ - \xi) - \ln(\epsilon^- - \xi)\right),$$

where $\epsilon^\pm = \epsilon \pm i\eta$, η is a positive infinitesimal, and we have used the fact that $g(\epsilon^\pm) \simeq g(\epsilon)$ is continuous across the cut. (Also, without changing the value of the integral (exercise: why?), we have enlarged the integration interval from $(-\infty, \xi]$ to $(-\infty, \infty)$). To evaluate the integral, we observe that $g(\epsilon) = -\zeta\partial_\epsilon \ln\left(1-\zeta e^{-\beta\epsilon}\right)$ and integrate by parts:

$$S = -\frac{\zeta T}{2\pi i}\int d\epsilon \, \ln\left(1-\zeta e^{-\beta\epsilon}\right)\left(\frac{1}{\epsilon^+ - \xi} - \frac{1}{\epsilon^- - \xi}\right) \overset{(3.58)}{=} \zeta T \ln\left(1-\zeta e^{-\beta\xi}\right) .$$

Insertion of this result into Eq. (4.34) finally obtains the familiar expression

$$F = \zeta T \sum_a \ln\left(1-\zeta e^{-\beta(\epsilon_a-\mu)}\right) \tag{4.41}$$

for the free energy of the non–interacting Fermi/Bose gas. While this result could have been obtained much more straightforwardly by the methods of quantum statistical mechanics, we will shortly see how powerful a tool the methods discussed in this section are when it comes to the analysis of less elementary problems!

4.3 Summary and Outlook

This concludes our preliminary introduction to the field integral. We have learned how to represent the partition function of a quantum many–body system in terms of a generalized path integral. The field integral representation of the partition function will be the basic platform on which all our further developments will be based. In fact, we are now in a position to face up to the main problem addressed in this text: practically none of the 'non–trivial' field integrals in which one might be interested can be executed in closed form. This reflects the fact that, save for a few exceptions, interacting many–body problems do not admit closed solutions. In the following chapter, we will introduce approximation stratgies for addressing interacting theories by exploring some physical applications of the field integral.