Lecture 10: FERMIONS IN THE GRASSMANN FORMALISM

We have described methods that allow studying general quantum Bose systems in the grand canonical formulation of statistical physics. One important ingredient was the introduction of generating functions of symmetric wave functions of bosons, as we have shown in section 4.9.

By contrast, in the case of fermion systems, since fermion wave functions are antisymmetric in the exchange of a fermion pair, the construction of generating functions, thus, requires the introduction of an antisymmetric or Grassmann algebra of 'classical functions'.

It is then possible to generalize to Grassmann algebras the notions of derivatives and integrals. This leads to parallel formalisms for bosons and fermions. In particular, one defines a Grassmann path integral for fermions, analogous to the holomorphic path integral for bosons.

In the limit of an infinite number of available fermion states, the formalism allows expressing the partition function of the Fermi gas as an integral over Grassmann fields with anti-periodic boundary conditions.

10.1 Grassmann algebras

A Grassmann algebra $\mathfrak{A}$ on $\mathbb{R}$ or $\mathbb{C}$ (real or complex numbers) is an associative algebra generated by a unit (denoted by 1 in what follows) and a set of generators $\{\theta_i\}$ that satisfy the anti-commutation relations

$$\theta_i\theta_j + \theta_j\theta_i = 0 \qquad \forall i, j\,.$$

(In what follows, unless stated otherwise, we consider only complex algebras and when we speak of generators, we omit the unit that plays a special role.)

As a consequence:

(i) If the number n of generators is finite, the elements of the algebra form a vector space of finite dimension 2^n over $\mathbb{R}$ or $\mathbb{C}$. All elements can be written as linear combinations of the elements A_ν, $\nu = 1, \dots, 2^n$:

$$A_\nu \in \{1 \text{ and } \{\theta_{i_1}\theta_{i_2}\dots\theta_{i_p}\} \text{ with } i_1 < i_2 < \cdots < i_p\,,\ 1 \le p \le n\}. \quad (10.1)$$

(*ii*) $\mathfrak{A}$ is a graded algebra: to each monomial $\theta_{i_1}\theta_{i_2}\cdots\theta_{i_p}$, one can associate an integer p that counts the number of generators in a product. In particular, if A_p and A_q are two monomials of degree p and q, respectively, then

$$A_p A_q = (-1)^{pq} A_q A_p \,.$$

(*iii*) Elements of $\mathfrak{A}$ are invertible if and only if in the expansion on the basis (10.1) the term of degree zero does not vanish.

For example, the element $1+\theta$ is invertible and its inverse is $1-\theta$; in contrast θ is not invertible. The inverse can be calculated by expanding in a formal power series starting from the inverse of the term of degree zero.

(*iv*) All elements in a Grassmann algebra, considered as functions of a generator θ_i, are first degree polynomials, that is, affine functions.

10.1.1 Reflection

In the algebra $\mathfrak{A}$, one can define an automorphism P, which thus satisfies

$$\mathrm{P}(A+B) = \mathrm{P}(A) + \mathrm{P}(B), \quad \mathrm{P}(AB) = \mathrm{P}(A)\mathrm{P}(B),$$
$$\mathrm{P}(\lambda A) = \lambda \mathrm{P}(A) \quad \forall A, B \in \mathfrak{A}\,, \quad \lambda \in \mathbb{C}\,,$$

which has the nature of a reflection:

$$\mathrm{P}(\theta_i) = -\theta_i \;\Rightarrow\; \mathrm{P}^2 = \mathbf{1}\,. \tag{10.2}$$

Acting on a monomial of degree p, it yields

$$\mathrm{P}(\theta_{i_1} \cdots \theta_{i_p}) = (-1)^p \theta_{i_1} \cdots \theta_{i_p}\,.$$

The vector space generated by the elements of $\mathfrak{A}$ can be divided into the sum of two vector spaces $\mathfrak{A}^\pm$ containing the even and odd elements:

$$\mathrm{P}(\mathfrak{A}^\pm) = \pm\mathfrak{A}^\pm.$$

Note also the property

$$A\theta_i = \theta_i \mathrm{P}(A). \tag{10.3}$$

When A_+ belongs to $\mathfrak{A}^+$, it commutes with all elements of $\mathfrak{A}$:

$$A_+ \in \mathfrak{A}^+ \;\Rightarrow\; A_+ B = B A_+\,,\; \forall B\,.$$

In particular, $\mathfrak{A}^+$ can be identified with the maximal commutative subalgebra of $\mathfrak{A}$.

On the other hand, if A_-, B_- both belong to $\mathfrak{A}^-$, they anti-commute:

$$A_- \text{ and } B_- \in \mathfrak{A}^- \;\Rightarrow\; A_- B_- + B_- A_- = 0\,.$$

As a consequence, all elements of $\mathfrak{A}^-$ are nilpotent with a vanishing square.

10.1.2 Formal complex conjugation

In quantum mechanics, one needs mainly Grassmann algebras $\mathfrak{A}$ with an even number of generators, which can be divided into two subsets $\{\theta_i\}$ and $\{\bar{\theta}_i\}$, $i = 1, \ldots, n$. One can then define in the algebra generated by $\{\theta_i, \bar{\theta}_i\}$ the analogue of the formal complex conjugation of the holomorphic representation. The operation that plays the role of complex conjugation, and we denote by $A \mapsto \bar{A}$, actually has properties analogous to the hermitian conjugation for matrices or operators:

$$\begin{cases} \theta_i \leftrightarrow \bar{\theta}_i \,, \\ \overline{(\lambda A_1 + \mu A_2)} = \lambda^* \bar{A}_1 + \mu^* \bar{A}_2 \,, \\ \overline{A_1 A_2} = \bar{A}_2 \bar{A}_1 \,, \quad \forall\, A_1 \,, A_2 \in \mathfrak{A} \text{ and } \lambda \,, \mu \in \mathbb{C} \,, \end{cases} \tag{10.4}$$

where λ^* and μ^* are the complex conjugate of λ and μ, respectively.

Note for example that, as a consequence, $\overline{\theta_i \bar{\theta}_j} = \theta_j \bar{\theta}_i$.

An element such that $\bar{A} = A$ is called formally real.

10.2 Differentiation in Grassmann algebras

In Grassmann algebras, it is possible to define a generalized derivative. However, a too naive definition, would be inconsistent with the non-commutative character of the algebra.

10.2.1 Definition

Considered as functions of a given generator θ_i, all elements A of $\mathfrak{A}$ can be written as (in general, after some commutations)

$$A = A_1 + \theta_i A_2 \,,$$

where A_1 and A_2 do not depend on θ_i. One then defines the derivative with respect to θ_i by

$$\frac{\partial A}{\partial \theta_i} = A_2 \,. \tag{10.5}$$

The operator $\partial/\partial\theta_i$ is nilpotent with vanishing square: $(\partial/\partial\theta_i)^2 = 0$.

Left and right differentiation. Equation (10.5) defines a left derivative in the sense that the action of $\partial/\partial\theta_i$ consists in commuting θ_i to the left in all monomials before suppressing it. In a similar way, one could define a right derivative by commuting θ_i to the right before suppressing it.

Derivative of sums and products. It follows from the definition (10.5) that the derivative ($\mathrm{D} \equiv \partial/\partial\theta_i$) is a linear operation

$$\mathrm{D}(\lambda A + \mu B) = \lambda \mathrm{D}(A) + \mu \mathrm{D}(B) \quad \forall A, B \in \mathfrak{A}\,, \quad \lambda, \mu \in \mathbb{C}\,,$$

but the derivative of a product does not satisfy the usual Leibnitz rule $\mathrm{D}(AB) = A\mathrm{D}(B) + \mathrm{D}(A)B$. Using the remark (10.3), one verifies that this rule is replaced by

$$\mathrm{D}(AB) = \mathrm{P}(A)\mathrm{D}(B) + \mathrm{D}(A)B\,, \tag{10.6}$$

a rule that is consistent for any associative algebra and homomorphism P.

Chain rule. The Grassmann derivative implies a special form of chain rule. If $\sigma(\theta)$ belongs to $\mathfrak{A}^-$ and $x(\theta)$ belongs to $\mathfrak{A}^+$, one finds

$$\frac{\partial}{\partial\theta} f(\sigma, x) = \frac{\partial\sigma}{\partial\theta}\frac{\partial f}{\partial\sigma} + \frac{\partial x}{\partial\theta}\frac{\partial f}{\partial x} \,. \tag{10.7}$$

The verification is simple since F is necessarily an affine function of σ, and σ and x are affine functions of θ.

Note that in the second term on the right hand side, the ordering of factors is important.

10.2.2 Operator algebra

The identity and the nilpotent differentiation operators $\partial/\partial\theta_i$, combined with the generators θ_i considered as operators acting on $\mathfrak{A}$ by left-multiplication, generate an operator algebra $\mathfrak{C}_n$ acting on $\mathfrak{A}$ whose generators satisfy the anti-commutation relations

$$\theta_i\theta_j + \theta_j\theta_i = 0\,,\ \frac{\partial}{\partial\theta_i}\frac{\partial}{\partial\theta_j} + \frac{\partial}{\partial\theta_j}\frac{\partial}{\partial\theta_i} = 0\,,\ \theta_i\frac{\partial}{\partial\theta_j} + \frac{\partial}{\partial\theta_j}\theta_i = \delta_{ij}\,. \tag{10.8}$$

The operators

$$\mathrm{D}_i^{\pm} = \frac{\partial}{\partial\theta_i} \pm \theta_i$$

then satisfy the anti-commutation relations ($\{U, V\} \equiv UV + VU$)

$$\{\mathrm{D}_i^{\pm}, \mathrm{D}_j^{\pm}\} = \pm 2\delta_{ij}\,,\ \ \{\mathrm{D}_i^{+}, \mathrm{D}_j^{-}\} = 0\,.$$

This representation shows that the algebra can be expressed as the direct sum of two Clifford algebras.

10.3 Integration in Grassmann algebras

The integration over Grassmann variables, which we denote by the integration symbol, is defined to be an operation identical to differentiation:

$$\int \mathrm{d}\theta_i \, A \equiv \frac{\partial}{\partial \theta_i} A, \ \forall A \in \mathfrak{A} \,. \tag{10.9}$$

One may, thus, wonder whether it is really useful to introduce two symbols, integral and derivative, for one unique operation. Still one verifies that this operation has also the formal properties that one expects from integration in the case of definite integrals (without boundary terms):

(*i*) The operation is linear.

(*ii*) The integral of a total derivative vanishes, a property that legitimates integration by parts.

(*iii*) After integration over a variable, an expression does not depend on this variable any more.

(*iv*) A factor in a product that does not depend on the integration variable can be factorized in front of the integration sign.

Then, the choice of using the integration or differentiation symbol depends on the context, and allows constructing for fermions a formalism quite parallel to the formalism for bosons described in section 4, as we will show.

Change of variables. We consider the integral

$$\int \mathrm{d}\theta\, f(\theta),$$

and change variables, setting (the change of variables is necessarily affine)

$$\theta = \theta' A + B\,. \tag{10.10}$$

We demand that parity, in the sense of the reflection (10.2), is conserved: since $\mathrm{P}(\theta) = -\theta$,

$$\mathrm{P}(\theta') = -\theta' \ \Leftrightarrow\ \theta' \in \mathfrak{A}^- \ \Rightarrow\ A \in \mathfrak{A}^+\,,\ B \in \mathfrak{A}^-\,.$$

Moreover, the element A must be invertible and, thus, its term of degree zero in the Grassmann variables must be non-vanishing. These conditions, in fact, imply that θ and θ' are two equivalent generators in the algebra.

Then, using the definition (10.9), one finds

$$\int \mathrm{d}\theta\, f(\theta) = A^{-1} \int \mathrm{d}\theta'\, f(\theta' A + B) = \int \mathrm{d}\theta' \left(\frac{\partial\theta}{\partial\theta'}\right)^{-1} f\big(\theta(\theta')\big), \qquad (10.11)$$

where the latter form is independent of the special parametrization (10.10). This is a very important property of Grassmann integrals: the Jacobian is $(\partial\theta/\partial\theta')^{-1}$, instead of $\partial\theta/\partial\theta'$ in the case of real or complex variables.

This difference is also a reflection of the identity between differentiation and integration in Grassmann algebras.

Generalization. More generally, we now show that the change of variables

$$\theta_i = \theta_i(\theta'), \;\; \theta'_i \in \mathfrak{A}^-,$$

where the matrix $\partial\theta_i/\partial\theta'_j$ is invertible (which is equivalent to the invertibility of the matrix of the terms of degree zero), generates a Jacobian that is the inverse of the determinant of $\partial\theta_i/\partial\theta'_j$:

$$\mathrm{d}\theta_1 \ldots \mathrm{d}\theta_n = \mathrm{d}\theta'_1 \ldots \mathrm{d}\theta'_n J(\boldsymbol{\theta}') \tag{10.12}$$

with

$$J = \det \frac{\partial\theta'_i}{\partial\theta_j} = \left(\det \frac{\partial\theta_i}{\partial\theta'_j}\right)^{-1}. \tag{10.13}$$

Notice that the determinant is defined because all elements of the matrix $\partial\theta_i/\partial\theta'_j$ belong to the commutative sub-algebra $\mathfrak{A}^+$.

The result can be derived by changing variables one at a time and using equation (10.11) repeatedly: $\theta_1 \mapsto \theta'_1$ then $\theta_2 \mapsto \theta'_2$ until, finally, $\theta_n \mapsto \theta'_n$. One then verifies

$$J = \left.\frac{\partial \theta'_1}{\partial \theta_1}\right|_{\theta_2,\ldots,\theta_n} \left.\frac{\partial \theta'_2}{\partial \theta_2}\right|_{\theta'_1,\theta_3,\ldots,\theta_n} \cdots \left.\frac{\partial \theta'_{n-1}}{\partial \theta_{n-1}}\right|_{\theta'_1,\ldots,\theta'_{n-2},\theta_n} \left.\frac{\partial \theta'_n}{\partial \theta_n}\right|_{\theta'_1,\ldots,\theta'_{n-1}} .$$

One recognizes one form of the Jacobian for complex variables, but for the change of variables $\theta'_i \mapsto \theta_i$. Indeed, if one introduces the matrices

$$M^{(p)}_{ij} = \frac{\partial \theta'_i}{\partial \theta_j}\,, \ i,j \le p \le n\,,$$

one verifies, using the chain rule (10.7), the recursion relation

$$\begin{aligned}\left.\frac{\partial \theta'_n}{\partial \theta_n}\right|_{\theta'_1,\ldots,\theta'_{n-1}} &= \left.\frac{\partial \theta'_n}{\partial \theta_n}\right|_{\theta_1,\ldots,\theta_{n-1}} - \sum_{i,j<n} \frac{\partial \theta'_n}{\partial \theta_i} \left[M^{n-1}\right]^{-1}_{ij} \frac{\partial \theta'_j}{\partial \theta_n} \\ &= \det M^{(n)} [M^{(n-1)}]^{-1} .\end{aligned}$$

The expression (10.13) follows.

Example. The following example allows a direct verification of equation (10.12). One starts from the identity

$$1 = \int \mathrm{d}\theta_1 \dots \mathrm{d}\theta_n \, \theta_n \dots \theta_1 \, .$$

After the linear change of variables

$$\theta_i = \sum_j a_{ij} \theta'_j \, ,$$

the result then relies on the identity

$$\theta_n \dots \theta_1 = \theta'_n \dots \theta'_1 \, \det \mathbf{a} \, .$$

10.3.1 Integration and complex conjugation

In what follows, we consider algebras with a double family of generators $\{\theta_i, \bar{\theta}_i\}$, $i = 1, \ldots, n$, related by the complex conjugation defined in (10.4). In these algebras, one considers integrals of the form

$$I = \int \mathrm{d}\theta \, \mathrm{d}\bar{\theta} \, f(\theta, \bar{\theta}),$$

where the pair $\theta, \bar{\theta}$ stands for any pair of conjugate generators, which are the direct analogues of the complex integrals of lecture 4.

Expanding the function f on θ and $\bar{\theta}$ in the form

$$f = a_0 + \theta a_1 + \bar{\theta} b_1 + \bar{\theta}\theta a_2 \,,$$

where the coefficients belong to the algebra, one can integrate and finds $I = a_2$. One now integrates the complex conjugate function:

$$J = \int \mathrm{d}\theta \, \mathrm{d}\bar{\theta} \, \overline{f(\theta, \bar{\theta})}.$$

With the same parametrization

$$\overline{f(\theta,\bar\theta)}=\bar a_0+\bar a_1\bar\theta+\bar b_1\theta+\bar a_2\bar\theta\theta\,,$$

and, thus, since $\bar\theta\theta$ commutes with $\bar a_2$, $J=\bar a_2=\bar I$. The integral of the conjugate function is the conjugate of the integral of the function. One can thus consider the measure $\mathrm{d}\theta_i\mathrm{d}\bar\theta_i$ as being invariant under complex conjugation.

In particular, the integral of a formally real function $(f=\bar f)$ is also formally real.

In what follows, we also meet integrals of the form

$$I=\int \mathrm{d}\theta\mathrm{d}\bar\theta\;\mathrm{e}^{\bar\theta\theta}\,f(\theta,\bar\theta)=a_0+a_2\,.$$

Again, the substitution $f\mapsto\bar f$ leads to the conjugate result.

10.4 Gaussian integrals. Expectation values. Wick's theorem

We now define Gaussian integrals with an integration over two families of generators $\{\theta_i, \bar{\theta}_i\}$, $1 = 1, \ldots, n$, analogues of the complex Gaussian integrals of section 4.1.

10.4.1 Gaussian integrals

As in the case of complex variables, we first calculate Gaussian integrals, and for the same reason: one often tries to reduce any integral to a formal sum of a finite or an infinite number of Gaussian integrals.

We first consider the integral

$$\mathcal{Z}(\mathbf{K}) = \int \mathrm{d}\theta_1 \mathrm{d}\bar{\theta}_1 \mathrm{d}\theta_2 \mathrm{d}\bar{\theta}_2 \ldots \mathrm{d}\theta_n \mathrm{d}\bar{\theta}_n \exp\left(\sum_{i,j=1}^{n} \bar{\theta}_i K_{ij} \theta_j\right). \qquad (10.14)$$

According to the rules of Grassmann integration, the result is simply the coefficient of the product $\bar{\theta}_n \theta_n \ldots \bar{\theta}_1 \theta_1$ in the expansion of the integrand.

The argument of the exponential function contains only terms belonging to $\mathfrak{A}^+$, which commute. The integrand can thus be written as

$$\begin{aligned}\exp\left(\sum_{i,j=1}^{n}\bar{\theta}_i K_{ij}\theta_j\right) &= \prod_{i=1}^{n}\exp\left(\bar{\theta}_i\sum_{j=1}^{n}K_{ij}\theta_j\right)\\ &= \prod_{i=1}^{n}\left(1+\bar{\theta}_i\sum_{j_i=1}^{n}K_{ij_i}\theta_{j_i}\right).\end{aligned}$$

Expanding the product, one observes that in each factor only the term proportional to $\bar{\theta}_i$ contributes to the integral. It thus remains to integrate

$$\prod_{i=1}^{n}\bar{\theta}_i\left(\sum_{j_i=1}^{n}K_{ij_i}\theta_{j_i}\right).$$

The terms that give a non-vanishing contribution to the integral, are those that contain the product $\theta_n\ldots\theta_2\theta_1$ up to a permutation of the factors θ_j.

They have the form

$$\sum_{\substack{\text{permutations}\\ \{j_1\ldots j_n\}}} K_{nj_n}K_{n-1j_{n-1}}\ldots K_{1j_1}\bar{\theta}_n\theta_{j_n}\ldots\bar{\theta}_1\theta_{j_1}.$$

A commutation of the generators to cast all products into some standard order, for example $\bar{\theta}_n\theta_n\ldots\bar{\theta}_1\theta_1$, yields a sign, the signature of the permutation, and one then recognizes in the coefficient the determinant of the matrix $\mathbf{K}$. Thus,

$$\mathcal{Z}(\mathbf{K}) = \det \mathbf{K}\,. \tag{10.15}$$

This result is the inverse of the result (4.3), obtained by an integration over complex variables.

This calculation is mainly a verification since, for $\det \mathbf{K} \neq 0$, one can also change variables,

$$\theta_i \mapsto \theta'_i = \sum_j K_{ij}\theta_j$$

and use the form (10.12) of the Jacobian. One verifies

$$\begin{aligned}\mathcal{Z}(\mathbf{K}) &= \det \mathbf{K} \int \mathrm{d}\theta'_1 \mathrm{d}\bar{\theta}_1 \ldots \mathrm{d}\theta'_n \mathrm{d}\bar{\theta}_n \exp\left(\sum_{i=1}^{n} \bar{\theta}_i \theta'_i\right) \\ &= \det \mathbf{K} \int \prod_{i=1}^{n} \mathrm{d}\theta'_i \mathrm{d}\bar{\theta}_i \left(1 + \bar{\theta}_i \theta'_i\right) = \det \mathbf{K}\,.\end{aligned}$$

Real quadratic form. From the definition (10.4) of formal complex conjugation, it follows that the conjugate of a quadratic form is given by

$$\sum_{i,j=1}^{n} \overline{\bar{\theta}_i K_{ij} \theta_j} = \sum_{i,j=1}^{n} \bar{\theta}_j K^*_{ij} \theta_i = \sum_{i,j=1}^{n} \bar{\theta}_i K^\dagger_{ij} \theta_j \,.$$

If the matrix $\mathbf{K}$ is hermitian, the quadratic form is formally real (invariant under formal complex conjugation). Then, the result of the integral is real since

$$\det \mathbf{K} = \det \mathbf{K}^\dagger = (\det \mathbf{K})^*,$$

in agreement with the discussion of section 10.3.1. In particular, if the matrix $\mathbf{K}$ is positive, the Gaussian integrand can be used to define a scalar product (see section 10.7.1).

10.4.2 General Gaussian integrals

We introduce another copy of the Grassmann algebra $\mathfrak{A}$ whose generators we denote by η_i and $\bar{\eta}_i$, and consider the Grassmann algebra generated by the set $\{\theta, \bar{\theta}, \eta, \bar{\eta}\}$. Adapting the strategy of section 4.1, we first evaluate the integral

$$\mathcal{Z}_{\mathrm{G}}(\eta, \bar{\eta}) = \int \left(\prod_i \mathrm{d}\theta_i \mathrm{d}\bar{\theta}_i \right) \exp E_{\mathrm{G}}(\theta, \bar{\theta}, \eta, \bar{\eta}) \tag{10.16}$$

with

$$E_{\mathrm{G}}(\theta, \bar{\theta}, \eta, \bar{\eta}) = \sum_{i,j=1}^{n} \bar{\theta}_i K_{ij} \theta_j + \sum_{i=1}^{n} \left(\bar{\eta}_i \theta_i + \bar{\theta}_i \eta_i \right), \tag{10.17}$$

where E_{G}, thus, is an element of the direct sum of the two copies of the initial Grassmann algebra. Moreover, we assume $\det \mathbf{K} \neq 0$.

To eliminate the terms linear in θ and $\bar{\theta}$, we solve the equations

$$\frac{\partial E_{\mathrm{G}}}{\partial \theta_i} = 0\,, \quad \frac{\partial E_{\mathrm{G}}}{\partial \bar{\theta}_i} = 0\,.$$

Introducing the inverse matrix $\mathbf{\Delta} = \mathbf{K}^{-1}$, one can write the solutions $\theta^{\mathrm{s}}, \bar{\theta}^{\mathrm{s}}$ as

$$\theta^{\mathrm{s}}_i = -\sum_j \Delta_{ij}\eta_j \,, \ \ \bar{\theta}^{\mathrm{s}}_i = -\sum_j \bar{\eta}_j \Delta_{ji} \,.$$

After the change of variables, $\{\theta_i\} \mapsto \{\theta'_i\}$ with

$$\theta_i = \theta'_i - \sum_j \Delta_{ij}\eta_j \,, \ \ \bar{\theta}_i = \bar{\theta}'_i - \sum_j \bar{\eta}_j \Delta_{ji} \,.$$

the resulting integral takes the form (10.14) already calculated (equation (10.15)). The complete result is

$$\mathcal{Z}_{\mathrm{G}}(\eta, \bar{\eta}) = \det \mathbf{K} \, \exp\Bigg(- \sum_{i,j=1}^{n} \bar{\eta}_i \Delta_{ij} \eta_j \Bigg). \tag{10.18}$$

10.4.3 Gaussian expectation values

We now define expectation values $\langle \bullet \rangle$ with respect to the normalized Gaussian measure proportional to the integrand in (10.14) by

$$\langle \bar{\theta}_{i_1} \theta_{j_1} \bar{\theta}_{i_2} \theta_{j_2} \dots \bar{\theta}_{i_p} \theta_{j_p} \rangle \\ = (\det \mathbf{K})^{-1} \int \Big(\prod_i \mathrm{d}\theta_i \mathrm{d}\bar{\theta}_i \Big) \bar{\theta}_{i_1} \theta_{j_1} \dots \bar{\theta}_{i_p} \theta_{j_p} \exp \Big(\sum_{i,j=1}^{n} \bar{\theta}_i K_{ij} \theta_j \Big) \quad (10.19)$$

with $p \leq n$.

All expectation values with an unequal number of θ and $\bar{\theta}$ vanish since the measure is invariant under the $U(1)$ transformation

$$\theta_i \mapsto \mathrm{e}^{i\alpha} \theta_i \,, \quad \bar{\theta}_i \mapsto \mathrm{e}^{-i\alpha} \bar{\theta}_i \,.$$

Differentiating the integral (10.16) with respect to η_i and $\bar{\eta}_i$ and using

$$\frac{\partial}{\partial \eta_i}\,\mathrm{e}^{E_{\mathrm{G}}} = -\bar{\theta}_i\,\mathrm{e}^{E_{\mathrm{G}}}, \quad \frac{\partial}{\partial \bar{\eta}_i}\,\mathrm{e}^{E_{\mathrm{G}}} = \theta_i\,\mathrm{e}^{E_{\mathrm{G}}}\,,$$

(notice the sign in the first equation) one verifies that the function $\mathcal{Z}_{\mathrm{G}}$ given by expression (10.16) is a generating function of the expectation values (10.19).

Repeatedly differentiating the integral (10.16) with respect to η and $\bar{\eta}$ (the order matters) and setting then $\eta = \bar{\eta} = 0$, one derives the identity

$$\det \mathbf{K}\left\langle \bar{\theta}_{i_1}\theta_{j_1}\bar{\theta}_{i_2}\theta_{j_2}\ldots\bar{\theta}_{i_p}\theta_{j_p}\right\rangle = \left[\frac{\partial}{\partial\bar{\eta}_{j_1}}\frac{\partial}{\partial\eta_{i_1}}\cdots\frac{\partial}{\partial\bar{\eta}_{j_p}}\frac{\partial}{\partial\eta_{i_p}}\mathcal{Z}_{\mathrm{G}}(\eta,\bar{\eta})\right]\Bigg|_{\eta=\bar{\eta}=0}.$$

One then substitutes for $\mathcal{Z}_{\mathrm{G}}$ the explicit expression (10.18) and obtains

$$\begin{aligned}&\left\langle \bar{\theta}_{i_1}\theta_{j_1}\bar{\theta}_{i_2}\theta_{j_2}\ldots\bar{\theta}_{i_p}\theta_{j_p}\right\rangle\\ &\quad = \left\{\frac{\partial}{\partial\bar{\eta}_{j_1}}\frac{\partial}{\partial\eta_{i_1}}\cdots\frac{\partial}{\partial\bar{\eta}_{j_p}}\frac{\partial}{\partial\eta_{i_p}}\exp\left[-\sum_{i,j=1}^{n}\bar{\eta}_j\Delta_{ji}\eta_i\right]\right\}\Bigg|_{\eta=\bar{\eta}=0}.\end{aligned}$$

10.4.4 Wick's theorem

Second moment or two-point function. In the example of the second moment, one obtains

$$\left\langle \bar{\theta}_i \theta_j \right\rangle = \frac{\partial}{\partial \bar{\eta}_j} \frac{\partial}{\partial \eta_i} \exp\left(- \sum_{i,j=1}^{n} \bar{\eta}_i \Delta_{ij} \eta_j \right) \Bigg|_{\eta=\bar{\eta}=0} . \tag{10.20}$$

It follows

$$\left\langle \bar{\theta}_i \theta_j \right\rangle = \Delta_{ji} \, .$$

Differentiating systematically with respect to the generators η and $\bar{\eta}$, one obtains all expectation values and can prove Wick's theorem for Grassmann variables.

Fermion Wick's theorem. All variables η and $\bar{\eta}$ that are not differentiated can immediately be suppressed. The matrix $\boldsymbol{\Delta}$ is then reduced to a $p \times p$ matrix with elements $\Delta_{j_l i_k}$. The identity between differentiation and integration then allows reducing the explicit calculation to a Gaussian integration. One concludes

$$\begin{aligned}\left\langle \bar{\theta}_{i_1}\theta_{j_1} \ldots \bar{\theta}_{i_p}\theta_{j_p} \right\rangle = \det \Delta_{j_l i_k} &= \sum_{\substack{\text{permutations}\\ P \text{ of } \{j_1 \ldots j_p\}}} \epsilon(P)\Delta_{j_{P_1} i_1}\Delta_{j_{P_2} i_2} \ldots \Delta_{j_{P_p} i_p} \\ &= \sum_{\substack{\text{permutations}\\ P \text{ of } \{j_1 \ldots j_p\}}} \epsilon(P) \left\langle \bar{\theta}_{i_1}\theta_{j_{P_1}} \right\rangle \left\langle \bar{\theta}_{i_2}\theta_{j_{P_2}} \right\rangle \cdots \left\langle \bar{\theta}_{i_p}\theta_{j_{P_p}} \right\rangle ,\end{aligned} \tag{10.21}$$

where $\epsilon(P) = \pm 1$ is the signature of the permutation P.

This result, which is the form Wick's theorem assumes in the case of 'complex' Grassmann variables, differs from expression (4.8a), obtained in the case of usual complex variables, only by the signature.

10.5 Perturbative expansion: a quartic perturbation

To calculate expectation values with the weight $\mathrm{e}^{-\mathcal{S}(\theta,\bar\theta)}/\mathcal{Z}$, where

$$\mathcal{S}(\theta,\bar\theta) = -\sum_{i,j=1}^{n} K_{ij}\bar\theta_i\theta_j - V(\bar\theta,\theta)$$

with K_{ij} hermitian and $V \in \mathfrak{A}_+$ real and where the normalization $\mathcal{Z}$ is given by the integral

$$\mathcal{Z} = \int \prod_i \mathrm{d}\bar\theta_i \mathrm{d}\theta_i \; \mathrm{e}^{-\mathcal{S}(\theta,\bar\theta)}, \tag{10.22}$$

one can expand in powers of the polynomial V and then calculate Gaussian expectation values using Wick's theorem in the form (10.21).

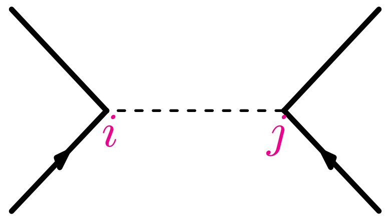

Fig. 10.1 – Faithful Feynman diagram: the interaction vertex , full lines corresponding to Δ (fermions), dotted lines to V.

Quartic perturbation. We consider the example of a quartic perturbation (Fig. 10.1) such that

$$\mathcal{S}(\theta,\bar{\theta}) = -\sum_{i,j=1}^{n} K_{ij}\bar{\theta}_i\theta_j - \tfrac{1}{2}\sum_{i,j} V_{ij}\bar{\theta}_i\theta_i\bar{\theta}_j\theta_j\,, \tag{10.23}$$

where $V_{ij} = V_{ji}$ is real and K_{ij} hermitian.

The normalization. The first terms of the expansion in powers of V of $\ln \mathcal{Z}$, where $\mathcal{Z}$ is the normalization integral (10.22), has the form

$$\ln \mathcal{Z} - \ln \det \mathbf{K} = \tfrac{1}{2} \sum_{i,j} V_{ij} \left\langle \bar{\theta}_i \theta_i \bar{\theta}_j \theta_j \right\rangle_{0,\mathrm{c}} + \tfrac{1}{8} \sum_{i,j,k,l} V_{ij} V_{kl} \left\langle \bar{\theta}_i \theta_i \bar{\theta}_j \theta_j \bar{\theta}_k \theta_k \bar{\theta}_l \theta_l \right\rangle_{0,\mathrm{c}} + O(V^3)\,,$$

where $\langle \bullet \rangle_{0,\mathrm{c}}$ denotes connected part of the Gaussian expectation value (cumulant expansion).

Using Wick's theorem, one obtains

$$\begin{aligned}\ln \mathcal{Z} - \ln \det \mathbf{K} &= \tfrac{1}{2} \sum_{i,j} V_{ij} \left(\Delta_{ii} \Delta_{jj} - \Delta_{ji} \Delta_{ij} \right) \\ &+ \tfrac{1}{4} \sum_{i,j,k,l} V_{ij} V_{kl} \left[2\Delta_{ki} \left(-\Delta_{ik} \Delta_{jj} \Delta_{ll} + 2\Delta_{il} \Delta_{lk} \Delta_{jj} - \Delta_{ij} \Delta_{jl} \Delta_{lk} \right) \right. \\ &\left. + \Delta_{ik} \Delta_{ki} \Delta_{lj} \Delta_{jl} - \Delta_{ki} \Delta_{il} \Delta_{lj} \Delta_{jk} \right] + O(V^3).\end{aligned}$$

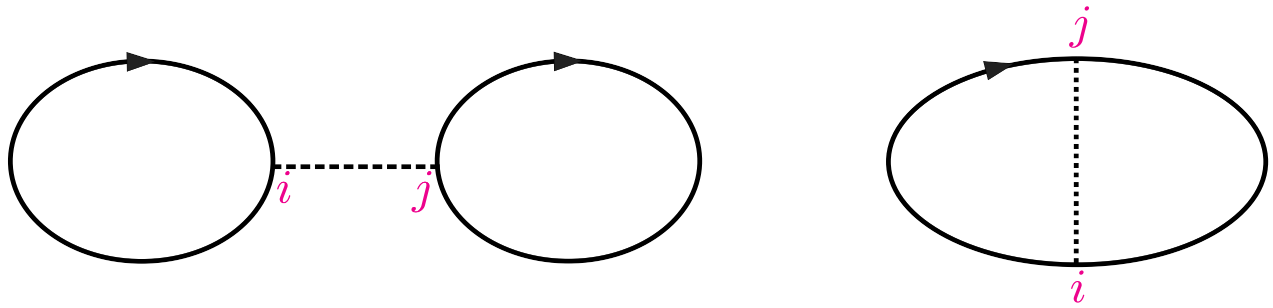

Fig. 10.2 – Faithful Feynman diagrams: the contributions of order V, full lines corresponding to Δ (fermions), dotted lines to V.

In this expression, the signs have an interpretation in terms of the parity of the number of fermion loops in Feynman diagrams (see Fig. 10.2).

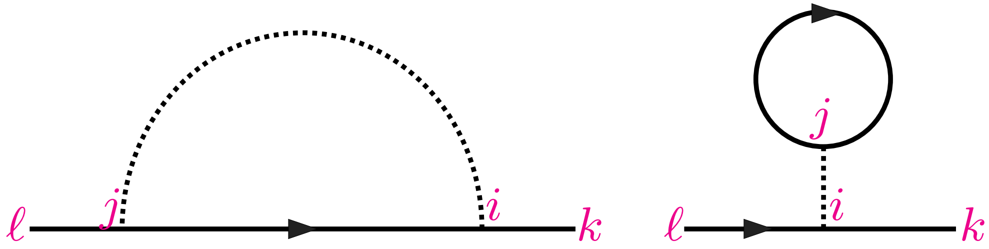

Fig. 10.3 – Faithful Feynman diagrams: the contributions of order V, full lines corresponding to Δ (fermions), dotted lines to V.

Two-point expectation value. At order V^2, after division by the normalization $\mathcal{Z}$, which corresponds to the cancellation of disconnected diagrams,

$$\begin{aligned}\left\langle \bar{\theta}_k \theta_\ell \right\rangle = \Delta_{\ell k} &+ \tfrac{1}{2} \sum_{i,j} V_{ij} \left\langle \bar{\theta}_k \theta_\ell \bar{\theta}_i \theta_i \bar{\theta}_j \theta_j \right\rangle_{0,\mathrm{c}} \\ &+ \tfrac{1}{8} \sum_{i,j,a,b} V_{ij} V_{ab} \left\langle \bar{\theta}_k \theta_\ell \bar{\theta}_i \theta_i \bar{\theta}_j \theta_j \bar{\theta}_a \theta_a \bar{\theta}_b \theta_b \right\rangle_{0,\mathrm{c}} + O(V^3),\end{aligned}$$

where $\langle \bullet \rangle_{0,\mathrm{c}}$ again denotes connected part of Gaussian expectation values.

Application of Wick's theorem then leads to (the diagrams of order V are displayed in Fig. 10.3)

$$\begin{aligned}\langle\bar{\theta}_k\theta_\ell\rangle = \Delta_{\ell k} &+ \sum_{i,j} V_{ij}\left(\Delta_{\ell j}\Delta_{ji}\Delta_{ik} - \Delta_{\ell i}\Delta_{ik}\Delta_{jj}\right)\\
&+ \sum_{i,j,a,b}\left(\Delta_{\ell j}V_{jb}\Delta_{bb}\Delta_{ji}V_{ia}\Delta_{aa}\Delta_{ik} - \Delta_{\ell j}V_{jb}\Delta_{bb}\Delta_{ja}V_{ia}\Delta_{ai}\Delta_{ik}\right.\\
&- \Delta_{\ell j}V_{bj}\Delta_{jb}\Delta_{bi}V_{ia}\Delta_{aa}\Delta_{ik} + \Delta_{\ell j}V_{bj}\Delta_{jb}\Delta_{ba}V_{ia}\Delta_{ai}\Delta_{ik}\\
&+ \Delta_{\ell i}V_{ia}\Delta_{aj}V_{jb}\Delta_{bb}\Delta_{ja}\Delta_{ik} - \Delta_{\ell j}V_{ji}\Delta_{ja}V_{ab}\Delta_{bb}\Delta_{ai}\Delta_{ik}\\
&- \Delta_{\ell i}V_{ia}\Delta_{aj}V_{jb}\Delta_{jb}\Delta_{ba}\Delta_{ik} + \Delta_{\ell j}V_{ji}\Delta_{ja}V_{ab}\Delta_{ab}\Delta_{bi}\Delta_{ik}\\
&\left.-\Delta_{\ell j}V_{jb}\Delta_{ab}\Delta_{ba}V_{ai}\Delta_{ji}\Delta_{ik} + \Delta_{\ell j}V_{ja}\Delta_{jb}V_{bi}\Delta_{ba}\Delta_{ai}\Delta_{ik}\right)\\
&+ O(V^3). \qquad (10.24)\end{aligned}$$

10.6 Generating functions

General expectation values can then be generated from the function

$$\mathcal{Z}(\eta,\bar{\eta}) = \int \left(\prod_i \mathrm{d}\bar{\theta}_i \mathrm{d}\theta_i\right) \mathrm{e}^{E(\theta,\bar{\theta},\bar{\eta},\eta)}$$

with

$$E(\theta,\bar{\theta},\bar{\eta},\eta) = -\mathcal{S}(\theta,\bar{\theta}) + \sum_{i=1}^{n} \left(\bar{\eta}_i\theta_i + \bar{\theta}_i\eta_i\right).$$

From the remarks (*cf.* definition (10.16)),

$$\frac{\partial}{\partial\bar{\eta}_k}\mathcal{Z}(\eta,\bar{\eta}) = \int \left(\prod_i \mathrm{d}\theta_i \mathrm{d}\bar{\theta}_i\right) \theta_k \exp E(\theta,\bar{\theta},\eta,\bar{\eta}), \tag{10.25}$$

$$\frac{\partial}{\partial\eta_k}\mathcal{Z}(\eta,\bar{\eta}) = -\int \left(\prod_i \mathrm{d}\theta_i \mathrm{d}\bar{\theta}_i\right) \bar{\theta}_k \exp E(\theta,\bar{\theta},\eta,\bar{\eta}), \tag{10.26}$$

(notice the sign in equation (10.26)), all expectation values can be derived from $\mathcal{Z}(\eta,\bar{\eta})$.

10.6.1 Cumulants. Legendre transformation

Cumulants or connected functions. The function

$$\mathcal{W}(\eta,\bar{\eta})=\ln\mathcal{Z}(\eta,\bar{\eta}),$$

is the generating function of cumulants, to which only connected Feynman diagrams contribute.

Legendre transformation. Then, one can introduce its Legendre transform $\Gamma(\theta,\bar{\theta})$ defined by

$$\mathcal{W}(\eta,\bar{\eta})+\Gamma(\theta,\bar{\theta})=\sum_{i=1}^{n}\left(\bar{\eta}_i\theta_i+\bar{\theta}_i\eta_i\right)$$

$$\theta_i=\frac{\partial\mathcal{W}}{\partial\bar{\eta}_i}\,,\qquad \bar{\theta}_i=-\frac{\partial\mathcal{W}}{\partial\eta_i}\,.$$

To $\Gamma(\theta,\bar{\theta})$, only one-line irreducible Feynman diagrams contribute.

10.6.2 Loop expansion

At leading order (tree approximation), one substitutes in E the solutions $\theta_i^{\mathrm{s}}, \bar{\theta}_i^{\mathrm{s}}$ of

$$\frac{\partial E}{\partial \bar{\theta}_i} = \eta_i - \frac{\partial \mathcal{S}}{\partial \bar{\theta}_i} = 0\,, \quad \frac{\partial E}{\partial \theta_i} = -\bar{\eta}_i - \frac{\partial \mathcal{S}}{\partial \theta_i} = 0\,.$$

Then,

$$\mathcal{W}(\eta, \bar{\eta}) = -\mathcal{S}(\theta^{\mathrm{s}}, \bar{\theta}^{\mathrm{s}}) + \sum_{i=1} \left(\bar{\eta}_i \theta_i^{\mathrm{s}} + \bar{\theta}_i^{\mathrm{s}} \eta_i\right)$$

and, thus,

$$\Gamma(\theta, \bar{\theta}) = \mathcal{S}(\theta, \bar{\theta}).$$

Higher orders are obtained by expanding around $\theta^{\mathrm{s}}, \bar{\theta}^{\mathrm{s}}$, keeping the quadratic form in the exponential and expanding terms of higher degree. This generates Gaussian expectation values, which correspond to a loop expansion.

One-loop contribution. The one-loop contribution $\Gamma_1(\theta, \bar{\theta})$ to Γ expanded to order $(\bar{\theta}\theta)^2$ is

$$\begin{aligned}\Gamma_1(\theta, \bar{\theta}) = \sum_{a,b} V_{ab} \left[\Delta_{ab}\bar{\theta}_b\theta_a - \Delta_{bb}\bar{\theta}_a\theta_a\right) \\ + \sum_{a,b,c,d} \left(-\tfrac{1}{2}\Delta_{ab}\Delta_{ba}V_{ac}V_{bd}\bar{\theta}_c\theta_c\bar{\theta}_d\theta_d + \Delta_{ab}\Delta_{bd}V_{bc}V_{da}\bar{\theta}_c\theta_c\bar{\theta}_a\theta_d\right. \\ \left. -\tfrac{1}{2}\Delta_{ac}\Delta_{bd}\left(V_{cb}V_{da} + V_{ab}V_{cd}\right)\bar{\theta}_b\theta_c\bar{\theta}_a\theta_d\right] .\end{aligned}$$

Two-point function. The properties of the Legendre transformation imply

$$\frac{\partial^2\Gamma}{\partial\bar{\theta}_\ell\partial\theta_k} = [\langle\bar{\theta}\theta\rangle]^{-1}_{\ell k}$$

in the sense of matrices. This quantity has a simpler expansion than the two-point cumulant $\langle\bar{\theta}\theta\rangle$, involving only one-line irreducible diagrams.

Using expression (10.24), one finds

$$
\begin{aligned}
[\langle\bar{\theta}\theta\rangle]^{-1}_{\ell k} = K_{\ell k} - V_{k\ell}\Delta_{\ell k} + \delta_{\ell k}\sum_j V_{\ell j}\Delta_{jj} \\
&+ \sum_{a,b}\Big[V_{\ell k}\Delta_{\ell a}V_{ab}\left(\Delta_{bb}\Delta_{ak} - \Delta_{ab}\Delta_{bk}\right) \\
&+ V_{\ell b}\Delta_{ab}V_{ak}\left(\Delta_{ba}\Delta_{\ell k} - \Delta_{\ell a}\Delta_{bk}\right)\Big] \\
&+ \delta_{k\ell}\sum_{a,b,j} V_{\ell a}\Delta_{aj}V_{jb}\left(\Delta_{jb}\Delta_{ba} - \Delta_{bb}\Delta_{ja}\right) + O(V^3),
\end{aligned}
$$

a form consistent to order V^2 with the expansion of Γ_1.

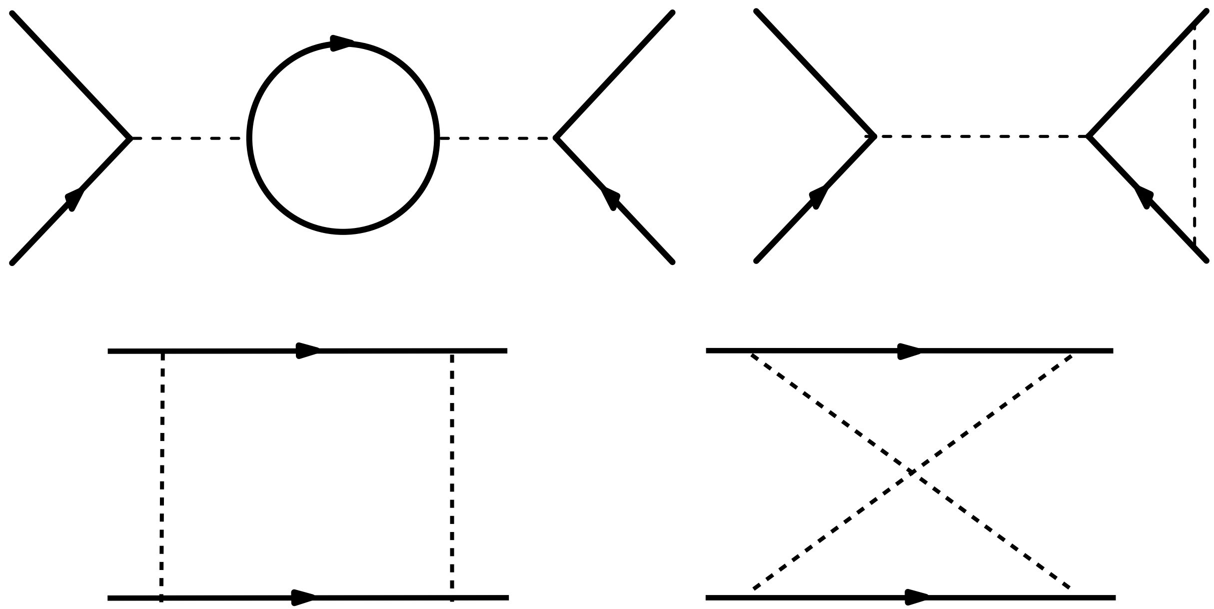

Fig. 10.4 – Faithful Feynman diagrams: contributions of order V^2 to the four-point vertex function, full lines corresponding to Δ (fermions), dotted lines to V.

Four-point expectation value. We give here only the one-line irreducible (1LI) contributions corresponding to vertex functions in QFT. We define

$$\Gamma^{(4)}_{ijk\ell} = \frac{\partial^4 \Gamma}{\partial\bar\theta_\ell \partial\theta_k \partial\bar\theta_j \partial\theta_i}.$$

With this convention,

$$
\begin{aligned}
\Gamma^{(4)}_{ijk\ell} = {} & V_{ik}\left(\delta_{i\ell}\delta_{jk} - \delta_{ij}\delta_{k\ell}\right) + \Delta_{ji}\Delta_{\ell k}\left(V_{i\ell}V_{jk} + V_{j\ell}V_{ik}\right) \\
& - \Delta_{jk}\Delta_{\ell i}\left(V_{k\ell}V_{ij} + V_{j\ell}V_{ik}\right) \\
& \sum_a \Big(\delta_{ij}V_{ia}\Delta_{ka}\Delta_{a\ell}V_{k\ell} - \delta_{kj}V_{ka}\Delta_{ia}\Delta_{a\ell}V_{i\ell} \\
& - \delta_{i\ell}V_{ia}\Delta_{ka}\Delta_{aj}V_{kj} + \delta_{k\ell}V_{ka}\Delta_{ia}\Delta_{aj}V_{ij}\Big) \\
& - \sum_{a,b}\Delta_{ab}\Delta_{ba}V_{ai}V_{bk}\left(\delta_{ij}\delta_{k\ell} - \delta_{i\ell}\delta_{jk}\right) + O(V^3).
\end{aligned}
\tag{10.27}
$$

10.7 Fermion vector space and operators: one state

The Grassmann formalism that we have just described allows handling fermions in a way quite analogous to bosons with the holomorphic formalism.

Using the holomorphic formalism, we have defined in section 4.3 a scalar product between analytic functions (equation (4.10)). This scalar product then allows constructing a Hilbert space of analytic functions. From the quantum viewpoint, the coefficients of the Taylor series expansion correspond to the components of the state vector on states with a given number of particles (see section 4.9). Quantum operators are then represented by multiplications and differentiations acting on these analytic functions.

Following an analogous scheme, we first define Grassmann 'analytic' functions. These functions form a vector space in which we define a scalar product. Quantum operators are then represented by elements of the algebra of multiplication and differential operators acting on these functions.

A noticeable difference with the boson case is that the Hilbert space for identical particles obeying the Fermi–Dirac statistics (*i.e.*, fermions) and that can occupy only one state, reduces to a two-dimensional complex vector space, as a direct consequence of the Pauli principle: a state can only be empty (state with zero particle or vacuum) or occupied once.

Therefore, the Grassmann formalism is not really necessary to deal with this situation. However, the situation changes drastically when fermions can occupy a large number of states, and this provides the justification.

Finally, unlike the case of bosons, there is an algebraic and physical symmetry between filled and empty state, the latter being only defined by the lowest energy.

10.7.1 Grassmann analytic functions and scalar product

We first consider a Grassmann algebra $\mathfrak{A}$ with only two generators $\theta, \bar{\theta}$. We define a Grassmann analytic function as an element of the algebra that depends only on the variable θ and thus

$$\frac{\partial \psi}{\partial \bar{\theta}} = 0 \, .$$

Grassmann analytic functions form a subalgebra $\mathfrak{A}_{\mathrm{an.}}$ of the algebra $\mathfrak{A}$. Analytic functions $\psi(\theta)$ are automatically affine functions since

$$\psi(\theta) = \psi_0 + \psi_1 \theta \, , \;\; \psi_0, \psi_1 \in \mathbb{C}^2 \, .$$

These functions span a complex two-dimensional vector space isomorphic to the space of the vectors (ψ_0, ψ_1), ψ_0 and ψ_1 being the components of the vector on the empty and one-particle state, respectively. By choosing θ to be a generator of a Grassmann algebra $\mathfrak{A}$, one ensures that a state can be occupied only once since $\theta^2 = 0$, in agreement with the Fermi–Dirac statistics.

The function complex conjugate to the function ψ is (*cf.*, the definition (10.4))

$$\overline{\psi(\theta)} \equiv \psi_0^* + \psi_1^* \bar{\theta} \,.$$

As for analytic functions of usual complex variables, one then defines a scalar product between functions of θ:

$$(\psi, \xi) = \int \mathrm{d}\theta \, \mathrm{d}\bar{\theta} \, \mathrm{e}^{\bar{\theta}\theta} \; \overline{\psi(\theta)} \, \xi(\theta). \qquad (10.28)$$

Parametrizing the function ξ as

$$\xi(\theta) = \xi_0 + \xi_1 \theta \,,$$

one verifies that the integral leads to the usual scalar product of the two corresponding complex vectors (ψ_0, ψ_1) and (ξ_0, ξ_1):

$$(\psi, \xi) = \psi_0^* \xi_0 + \psi_1^* \xi_1 \,.$$

Note, for later purpose, that the same scalar product is obtained from the expression

$$(\psi,\xi)=\int \mathrm{d}\bar{\theta}\mathrm{d}\theta\ \mathrm{e}^{\theta\bar{\theta}}\ \xi(\theta)\ \overline{\psi(\theta)}, \tag{10.29}$$

as one verifies by explicit calculation.

If we normalize the functions ψ by the scalar product (10.28): $\|\psi\|^2=(\psi,\psi)=1$, $|\psi_0|^2$ and $|\psi_1|^2$ represent the respective probability for a quantum system to be in empty state (vacuum) or occupied state.

10.7.2 Operators

On functions $\psi(\theta)$ acts the operator algebra $\mathfrak{C}_1$ (section 10.2.2), which here reduces to linear combinations of 1, θ, $\partial/\partial\theta$ and $\theta\partial/\partial\theta$. The identity and the three Pauli matrices can be represented by

$$1\mapsto \mathbf{1}\,,\ \frac{\partial}{\partial\theta}+\theta\mapsto\sigma_1\,,\ \frac{\partial}{\partial\theta}-\theta\mapsto i\sigma_2\,,\ \frac{\partial}{\partial\theta}\theta-\theta\frac{\partial}{\partial\theta}\mapsto\sigma_3\,.$$

Hermitian conjugation. We consider the scalar product

$$(\psi, \partial\xi/\partial\theta) = \int \mathrm{d}\theta \mathrm{d}\bar{\theta}\ \mathrm{e}^{\bar{\theta}\theta}\ \overline{\psi(\theta)}\ \frac{\partial\xi(\theta)}{\partial\theta}.$$

Using the identity

$$\frac{\partial}{\partial\theta}\,\mathrm{e}^{\bar{\theta}\theta}\,\xi(\theta) = \mathrm{e}^{\bar{\theta}\theta}\left(\frac{\partial\xi(\theta)}{\partial\theta} - \bar{\theta}\xi\right),$$

and integrating by parts, one infers (the same method has been used in section 4.4.1)

$$(\psi, \partial\xi/\partial\theta) = (\theta\psi, \xi),$$

which shows that the operators θ and $\partial/\partial\theta$ are hermitian conjugate and thus $\theta\partial/\partial\theta$ is hermitian.

Reflection. The reflection operator (10.2) is represented by

$$\mathrm{P} \mapsto 1 - \theta\frac{\partial}{\partial\theta}\,.$$

Note that operators corresponding to physical observables must respect the fermion character and thus commute with P. This implies here that they are linear combinations of 1 and $\theta\partial/\partial\theta$.

10.7.3 A few operators

We list below a few operators relevant for what follows.

Occupation number. We define the occupation number operator (here also the particle number operator):

$$\mathbf{n} \equiv \theta \frac{\partial}{\partial\theta} \;\Rightarrow\; \mathbf{n}^2 = \mathbf{n}\,. \tag{10.30}$$

Indeed, its eigenvectors and eigenvalues are

$$\mathbf{n}\,1 = 0\,, \quad \mathbf{n}\,\theta = \theta\,.$$

It is hermitian with respect to the scalar product (10.28) and commutes with P.

Hamiltonian. An operator that commutes with P is necessarily proportional to $\mathbf{n}$, up to an additive constant. We thus define the Hamiltonian H_0 as (in this first part we set $\hbar = 1$)

$$H_0 = \omega\,\mathbf{n}\,,\quad \omega > 0\,, \tag{10.31}$$

and this is the most general Hamiltonian,up to an additive constant, with only one fermion state. H_0 conserves the number of particles and is hermitian. The condition $\omega > 0$ ensures that $\psi(\theta) = 1$ is the ground state and thus the empty state. Otherwise, one has to redefine the basis, which includes exchanging the roles of θ and $\partial/\partial\theta$.

Statistical operator. The statistical operator $U_0(t) = \mathrm{e}^{-H_0 t}$ can then be inferred from the property (10.30). One finds

$$U_0(t) \equiv \mathrm{e}^{-H_0 t} = \mathrm{e}^{-\omega t\mathbf{n}} = \mathbf{1} + \left(\mathrm{e}^{-\omega t} - 1\right)\mathbf{n}\,. \tag{10.32}$$

10.7.4 Annihilation and creation operators

The operators θ and $\partial/\partial\theta$ form a representation of the algebra of the fermion creation and annihilation operators $a^\dagger$ and a, with the correspondence

$$a^\dagger \mapsto \theta\,,\ a \mapsto \frac{\partial}{\partial\theta}\,.$$

Indeed, they are hermitian conjugate and satisfy the anticommutation relations

$$a^2 = a^{\dagger 2} = 0\,,\ aa^\dagger + a^\dagger a = 1\,, \tag{10.33}$$

which, clearly, encode the Pauli principle.

In terms of creation and annihilation operators, the Hamiltonian (10.31) reads

$$H_0 = \omega a^\dagger a\,.$$

The correspondence between the normalized eigenvectors $|0\rangle$, the ground state, and the occupied state $|1\rangle = a^\dagger\,|0\rangle$ is then

$$|0\rangle \mapsto 1\,,\ |1\rangle \mapsto \theta\,.$$

10.8 General Grassmann analytic functions

The generalization to fermions that can occupy a finite number N of states requires introducing Grassmann analytic functions of N generators θ_i.

We thus consider a Grassmann algebra $\mathfrak{A}$ with generators $\{\theta_i, \bar{\theta}_i\}$. We define Grassmann analytic functions as elements of the algebra that depend only on the variables θ_i and thus satisfy

$$\frac{\partial \psi}{\partial \bar{\theta}_i} = 0\,, \ \forall i\,.$$

They form a subalgebra $\mathfrak{A}_{\text{an.}}$ of the algebra $\mathfrak{A}$.

The complex conjugation is defined as in (10.4) (*i.e.*, as the hermitian conjugation of operators). Then, as a straightforward generalization of the definition (10.28), the scalar product of two functions ψ and ξ is defined by

$$(\psi, \xi) = \int \Big(\prod_i \mathrm{d}\theta_i \mathrm{d}\bar{\theta}_i\Big) \exp\Big(\sum_i \bar{\theta}_i \theta_i\Big)\, \overline{\psi(\theta)}\, \xi(\theta). \tag{10.34}$$

Since

$$\overline{\left(\overline{\psi(\theta)}\,\xi(\theta)\right)} = \overline{\xi(\theta)}\,\psi(\theta),$$

it follows from the remarks of section 10.3.1, that

$$(\psi, \xi)^* = (\xi, \psi).$$

To prove that the scalar product defines a positive norm $\|\psi\|$, one can expand all elements of the algebra $\mathfrak{A}_{\text{an.}}$, considered as a complex vector space, on the basis of the 2^N distinct monomials $A_\nu(\boldsymbol{\theta})$, $\nu = 1, \ldots, 2^N$ (*cf.* equation (10.1)):

$$\{A_\nu(\boldsymbol{\theta})\} = \{1, \theta_{i_1}\theta_{i_2}\ldots\theta_{i_p}\,,\ \forall\ 1 \le p \le N \text{ and } \forall\ i_1 < i_2 < \cdots < i_p\}.$$

The evaluation of the scalar product (A_μ, A_ν) follows from the evaluation of the integral (10.19) with $K_{ij} = \delta_{ij}$. Using Wick's theorem (10.21), one obtains

$$(A_\mu, A_\nu) = \delta_{\mu\nu}\,.$$

The monomials $A_\nu(\boldsymbol{\theta})$ thus form an orthonormal basis. As a consequence, if one expands

$$\psi = \sum_\nu \psi_\nu A_\nu \,, \;\; \xi = \sum_\nu \xi_\nu A_\nu \,,$$

where ψ_ν, ξ_ν are two complex vectors in $\mathbb{C}^{2^N}$, one finds

$$(\psi, \xi) = \sum_\nu \psi^*_\nu \xi_\nu \,,$$

that is, the usual scalar product of the two vectors.

Again, the same results can be derived from the other form of the scalar product, which generalizes the definition (10.29),

$$(\psi, \xi) = \int \left(\prod_i \mathrm{d}\bar{\theta}_i \mathrm{d}\theta_i \right) \exp\!\left(\sum_i \theta_i \bar{\theta}_i \right) \, \xi(\theta) \, \overline{\psi(\theta)}. \qquad (10.35)$$

10.8.1 Grassmann Dirac's δ-function

In Grassmann algebras, the role of Dirac's δ-function is played by the function $\delta(\theta) \equiv \theta$. Indeed,

$$\int \mathrm{d}\theta\, \theta\psi(\theta) = \psi(0),$$

where $\psi(0)$ means the term of degree zero of the affine function $\psi(\theta)$. This δ-function has a useful integral representation:

$$\delta(\theta) = \int \mathrm{d}\bar{\theta}\ \mathrm{e}^{\bar{\theta}\theta}, \tag{10.36}$$

where $\bar{\theta}$ is an additional variable and, thus, an additional generator of the Grassmann algebra. This representation is analogous to the Fourier representation of the usual δ-function. One verifies directly

$$\psi(0) = \int \mathrm{d}\theta \mathrm{d}\bar{\theta}\ \mathrm{e}^{\bar{\theta}\theta}\, \psi(\theta).$$

10.9 Operators and kernels

Operator algebra. In section 10.2.2 we have introduced the algebra $\mathfrak{C}_N$ of left-differentiation and multiplication operators acting on a Grassmann algebra $\mathfrak{A}_{\mathrm{an.}}$. We have shown in section 10.7.1 that the operators θ_i and $\partial/\partial\theta_i$ are hermitian conjugate.

To be able to construct Grassmann path integrals (in particular, a path integral representation of the partition function), it is necessary to also introduce a kernel representation of operators (*cf.* sections 10.13 and 10.14).

Kernel of the identity. The scalar product (10.34) allows defining an orthonormal basis and, thus, a representation of the identity operator in the form of a kernel:

$$\mathcal{I}(\theta,\bar\theta)=\sum_\nu A_\nu(\theta)\overline{A_\nu(\theta)}=\prod_i(1+\theta_i\bar\theta_i)=\exp\Bigl(-\sum_i\bar\theta_i\theta_i\Bigr). \tag{10.37}$$

A direct verification is based on the representation (10.36) of the δ-function. Indeed,

$$\int \prod_i \left(\mathrm{d}\theta'_i \mathrm{d}\bar{\theta}'_i\right) \mathcal{I}(\theta, \bar{\theta}') \exp\left(\sum_i \bar{\theta}'_i \theta'_i\right) \psi(\theta') \\ = \int \prod_i \left(\mathrm{d}\theta'_i \mathrm{d}\bar{\theta}'_i\right) \exp\left(\sum_i \bar{\theta}'_i (\theta'_i - \theta_i)\right) \psi(\theta') = \psi(\theta). \qquad (10.38)$$

Reflection operator. The reflection operator (10.2) is represented by

$$\mathrm{P} \mapsto \exp\left(\sum_i \bar{\theta}_i \theta_i\right) = \mathcal{I}(-\theta, \bar{\theta}). \qquad (10.39)$$

Indeed, the same calculation shows that

$$[\mathrm{P}\psi](\theta) = \psi(-\theta).$$

Normal order. Using the anti-commutation relations, one can write all elements of the operator algebra $\mathfrak{C}_N$ as a linear combination of monomials in which all differential operators are on the right: the is called the normal order.

Action of kernels on functions. We can act on both sides of identity (10.38) with operators written in normal order. On the right hand side, one obtains their kernel representation by acting on $\mathcal{I}(\theta, \bar{\theta}')$,

$$\theta_{i_1}\theta_{i_2}\dots\theta_{i_p}\frac{\partial}{\partial\theta_{j_1}}\frac{\partial}{\partial\theta_{j_2}}\dots\frac{\partial}{\partial\theta_{j_q}}\mathcal{I}(\theta,\bar{\theta}) = \theta_{i_1}\theta_{i_2}\dots\theta_{i_p}\bar{\theta}_{j_1}\bar{\theta}_{j_2}\dots\bar{\theta}_{j_q}\mathcal{I}(\theta,\bar{\theta}),$$

which are general elements of the Grassmann algebra $\mathfrak{A}$.

In this representation, the action of an operator $O(\theta, \partial/\partial\theta)$ with kernel

$$\mathcal{O}(\theta, \bar{\theta}) = O(\theta, \bar{\theta})\mathcal{I}(\theta, \bar{\theta}),$$

is given by

$$[\mathcal{O}\psi](\theta) = \int \prod_i \mathrm{d}\theta'_i \mathrm{d}\bar{\theta}'_i \; \mathcal{O}(\theta, \bar{\theta}') \exp\left(\sum_i \bar{\theta}'_i \theta'_i\right) \psi(\theta'). \tag{10.40}$$

As in the holomorphic formalism, we introduce here also the rather suggestive matrix element notation

$$\langle\theta| \, \mathcal{O} \, \left|\bar{\theta}\right\rangle \equiv \mathcal{O}(\theta, \bar{\theta}),$$

without defining precisely the corresponding bra and ket vectors.

Finally, the kernel corresponding to the product $\mathcal{O}_2\mathcal{O}_1$, inferred from acting a second time on a function, is given by

$$\langle\theta| \, \mathcal{O}_2\mathcal{O}_1 \left|\bar{\theta}\right\rangle = \int \prod_i \mathrm{d}\theta'_i \mathrm{d}\bar{\theta}'_i \, \langle\theta| \, \mathcal{O}_2 \left|\bar{\theta}'\right\rangle \exp\left(\sum_i \bar{\theta}'_i \theta'_i\right) \langle\theta'| \, \mathcal{O}_1 \left|\bar{\theta}\right\rangle . \tag{10.41}$$

All operators can be expressed in terms of the elements of the basis (10.1):

$$\langle\theta|\,\mathcal{O}\,|\bar{\theta}\rangle = \sum_{\mu,\nu} \mathcal{O}_{\mu\nu} A_\mu(\theta)\overline{A_\nu(\theta)}, \tag{10.42}$$

where the coefficients $\mathcal{O}_{\mu\nu}$ are the matrix elements of $\mathcal{O}$ in this basis.

Trace. In terms of its kernel, the trace of an operator reads

$$\operatorname{tr}\mathcal{O} = \int \prod_i \mathrm{d}\bar{\theta}_i \mathrm{d}\theta_i \exp\Bigl(-\sum_i \bar{\theta}_i\theta_i\Bigr) \langle\theta|\,\mathcal{O}\,|\bar{\theta}\rangle\,. \tag{10.43}$$

Comparing expressions (10.41) and (10.43), one might be surprised by the interchange between the $\bar{\theta}_i$ and θ_i. The reason for this change can be directly related to the second form (10.35) of the scalar product.

Using expression (10.42), one verifies that the expression yields a trace since

$$\operatorname{tr}\mathcal{O} = \sum_\nu \mathcal{O}_{\nu\nu}\,.$$

Physical observables. Operators associated with physical observables must respect the fermion character. This condition is equivalent to the commutation of operators with the reflection operator (10.2). The latter can be written as

$$\mathrm{P}\mathcal{O}\mathrm{P} = \mathcal{O}\,,$$

which in terms of kernels becomes (using the representation (10.39))

$$\mathcal{O}(\theta,\bar{\theta}) = \mathcal{O}(-\theta,-\bar{\theta}). \tag{10.44}$$

The kernels $\mathcal{O}(\theta,\bar{\theta})$ representing physical operators must belong to the commutative subalgebra $\mathfrak{A}^{+}$.

Hermitian conjugation and kernels. Comparing explicitly the scalar products $(f, \mathcal{O}g)$ and $(\mathcal{O}^\dagger f, g)$, where the action of a operator on a function is given by expression (10.40), one verifies directly that the kernel corresponding to the hermitian conjugate of an operator is its formal complex conjugate in the algebra, as defined in (10.4):

$$\mathcal{O} \mapsto \mathcal{O}(\theta, \bar{\theta}) \ \Rightarrow\ \mathcal{O}^\dagger \mapsto \overline{\mathcal{O}(\theta, \bar{\theta})}.$$

As expected, the identity kernel $\mathcal{I}(\theta, \bar{\theta})$ corresponds to a hermitian operator.

10.10 The one-state example

The representation of the Hamiltonian (10.31) in terms of kernels is obtained by acting with the differential operator on the identity:

$$\langle\theta|H_0|\bar\theta\rangle = \omega\theta\frac{\partial}{\partial\theta}\,\mathrm{e}^{-\bar\theta\theta} = \omega\theta\bar\theta\,\mathrm{e}^{-\bar\theta\theta} = -\omega\bar\theta\theta\,.$$

The matrix elements of the operator $U_0(t)$ satisfy the equation

$$\frac{\partial}{\partial t}\,\langle\theta|U_0(t)|\bar\theta\rangle = -\omega\theta\frac{\partial}{\partial\theta}\,\langle\theta|U_0(t)|\bar\theta\rangle$$

with

$$\langle\theta|U_0(0)|\bar\theta\rangle = \mathrm{e}^{-\bar\theta\theta}\,.$$

One verifies that the solution is

$$\langle\theta|\,U_0(t)\,\left|\bar\theta\right\rangle = \mathrm{e}^{-\bar\theta\theta\,\mathrm{e}^{-\omega t}} = 1+\theta\bar\theta\,\mathrm{e}^{-\omega t}, \tag{10.45}$$

in agreement with expression (10.32).

Replacing in (10.41) $\mathcal{O}_1$ and $\mathcal{O}_2$ by $U(t_1)$ and $U(t_2)$, respectively, one can also verify directly the semi-group property.

The kernels of the physical operators H_0 and $U_0(t)$ belong to the commutative subalgebra $\mathfrak{A}^+$. Moreover, since the operators are hermitian, the kernels are indeed formally real in the sense of the conjugation (10.4).

Using the explicit expression (10.45) and the definition (10.43) of the trace, one can calculate the partition function. One finds the expected result

$$\mathcal{Z}_0(\beta) = \operatorname{tr} U_0(\beta) = \int \mathrm{d}\bar{\theta}\mathrm{d}\theta \; \mathrm{e}^{-\bar{\theta}\theta}\, \mathrm{e}^{-\bar{\theta}\theta\, \mathrm{e}^{-\omega\beta}} = 1 + \mathrm{e}^{-\omega\beta} \,. \tag{10.46}$$

Remark. The action of the operator U_0 on a function $\psi(\theta)$ is given by

$$\begin{aligned}[U_0(t)\psi](\theta) &= \int \mathrm{d}\theta' \mathrm{d}\bar{\theta}' \, \mathrm{e}^{-\bar{\theta}'\theta\, \mathrm{e}^{-\omega t}}\, \mathrm{e}^{\bar{\theta}'\theta'}\, \psi(\theta') \\ &= \psi(\mathrm{e}^{-\omega t}\,\theta),\end{aligned} \tag{10.47}$$

where the equation (10.36) has been used. Note the analogy with equation (4.27).

10.11 Many-fermion states. Hamiltonians

We now describe fermion state vectors when identical fermions, thus obeying the Pauli principle, can occupy an arbitrary finite number of quantum states, generalizing the discussion of section 10.7.

10.11.1 Fermion states

One-particle states. A fermion state is defined by a vector, which we denote by ψ_i, which belongs to a complex vector space $\mathfrak{H}_1$ of finite dimension N.

Many-particle states. A state vector describing n identical fermions is a complex vector $\psi_{i_1 i_2 \ldots i_n}$, where the indices i_k take N values. The Pauli principle for fermions implies that the vector $\psi_{i_1 i_2 \ldots i_n}$ is antisymmetric in all permutations of the indices

$$\psi_{i_1 i_2 \ldots i_k i_{k+1} \ldots i_n} = -\psi_{i_1 i_2 \ldots i_{k+1} i_k \ldots i_n} \quad \forall k\,.$$

The vectors $\psi_{i_1 i_2 \ldots i_n}$ are, thus, antisymmetric tensors with n indices, and belong to a complex vector space $\mathfrak{H}_n$ of dimension $\binom{N}{n}$.

10.11.2 Hamiltonians

Independent particle Hamiltonian. A one-particle (or one-body) Hamiltonian $\mathbf{H}^{(1)}$ is defined by its action on a one-particle state: it is then represented by a hermitian $N \times N$ matrix $H^{(1)}_{ij}$, which can be diagonalized. We denote by ω_i its eigenvalues ($\omega_i > 0$). Then,

$$[\mathbf{H}^{(1)}\,\psi]_i = \omega_i \psi_i\,.$$

Its action on n-particle states is additive:

$$[\mathbf{H}^{(1)}\,\psi]_{i_1 i_2 \ldots i_n} = \sum_\ell \omega_{i_\ell}\,\psi_{i_1 i_2 \ldots i_n}\,.$$

When the complete Hamiltonian reduces to a one-particle Hamiltonian, the fermions do not interact: one then speaks of independent particles.

Pair interaction. A pair or two-body interaction $\mathbf{H}^{(2)}$ is defined by its action on a two-particle state:

$$[\mathbf{H}^{(2)}\,\psi]_{i_1 i_2} = \sum_{j_1, j_2} H^{(2)}_{i_1 i_2, j_1 j_2} \psi_{j_1 j_2}\,,$$

where $H^{(2)}_{i_1 i_2, j_1 j_2}$ is a hermitian matrix that satisfies

$$H^{(2)}_{i_1 i_2, j_1 j_2} = H^{(2)}_{i_2 i_1, j_2 j_1} = (H^{(2)}_{j_1 j_2, i_1 i_2})^*$$

and, thus, is an internal mapping in the vector space $\mathfrak{H}_2$ of antisymmetric tensors. It is, of course, possible following the same strategy to define many-particle interactions but we restrict the discussion here to the two-body interaction, for simplicity.

The action of $\mathbf{H}^{(2)}$ on an n-particle state then is given by

$$[\mathbf{H}^{(2)}\,\psi]_{i_1 i_2 \ldots i_n} = \frac{1}{2} \sum_{\ell \neq m} \sum_{j,k} H^{(2)}_{i_\ell i_m, jk} \psi_{i_1 i_2 \ldots i_{\ell-1} j i_{\ell+1} \ldots i_{m-1} k\, i_{m+1} \ldots i_n}\,.$$

On the same model, one can construct many-body interactions.

10.12 Second quantization representation

In statistical physics, the grand canonical formulation implies dealing with a variable number of particles. We thus consider the set of state vectors corresponding to an arbitrary number of identical fermions that belong to the space $\oplus_n \mathfrak{H}_n$, $n = 0, 1, \ldots$ ($\mathfrak{H}_0$ is the vacuum), and associate to them a generating function. The tensors $\psi_{i_1 i_2 \ldots i_n}$ being antisymmetric, we must introduce a Grassmann algebra with N generators θ_i. We then show how quantum operators can be represented when acting on the Grassmann algebra and generalize the one-state construction of section 10.7 by using the formalism described in section 10.8.

10.12.1 State representation

A generating function of state vectors has the form

$$\Psi(\theta)=\sum_{n=0}^{N}\frac{1}{n!}\sum_{i_1,i_2,\ldots,i_n}\theta_{i_1}\theta_{i_2}\ldots\theta_{i_n}\psi_{i_1 i_2\ldots i_n}\,.$$

With our assumptions, $\Psi(\theta)$ is a polynomial of degree N. Notice, conversely, that the function $\Psi(\theta)$ can only generate antisymmetric tensors.

The function $\Psi(\theta)$ can be considered as a Grassmann analytic function. Such functions form a vector space that can be endowed with the scalar product (10.34) (thus the denomination second quantization). The norm of Ψ is given by

$$\|\Psi\|^2=(\Psi,\Psi)=\sum_{n=0}^{N}\frac{1}{n!}\sum_{i_1,i_2,\ldots,i_n}|\psi_{i_1 i_2\ldots i_n}|^2\,.$$

If the function Ψ has unit norm, the quantity $\frac{1}{n!}\sum_{i_1,i_2,\ldots,i_n}|\psi_{i_1 i_2\ldots i_n}|^2$ is the probability to find the quantum system in an n-fermion state.

10.12.2 Occupation number

In this framework, one can introduce the operators occupation number of the state i, whose action on $\Psi(\theta)$ is given by (definition (10.30))

$$\mathbf{n}_i = \theta_i \frac{\partial}{\partial\theta_i} \;\Rightarrow\; \mathbf{n}_i^2 = \mathbf{n}_i\,, \quad [\mathbf{n}_i, \mathbf{n}_j] = 0\,. \tag{10.48}$$

The sum

$$\mathbf{N} = \sum_i \mathbf{n}_i \tag{10.49}$$

is the operator total number of particles.

10.12.3 Hamiltonian

As in the Bose case, we note that

$$\sum_j \theta_j \omega_j \frac{\partial \Psi(\theta)}{\partial \theta_j} = \sum_n \frac{1}{(n-1)!} \sum_j \theta_j \omega_j \sum_{i_2, i_3, \ldots, i_n} \theta_{i_2} \theta_{i_3} \ldots \theta_{i_n} \psi_{j i_2 \ldots i_n}$$
$$= \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{i_1, i_2, \ldots, i_n} \theta_{i_1} \theta_{i_2} \ldots \theta_{i_n} \sum_\ell \omega_{i_\ell} \, \psi_{i_1 i_2 \ldots i_n} .$$

The representation of the one-particle Hamiltonian $\mathbf{H}^{(1)}$ acting on the generating functions $\Psi(\theta)$ thus is

$$\mathbf{H}^{(1)} \equiv \sum_i \theta_i \omega_i \frac{\partial}{\partial \theta_i} = \sum_i \omega_i \, \mathbf{n}_i .$$

An analogous calculation shows that the two-body interaction is represented by

$$\mathbf{H}^{(2)} = \tfrac{1}{2} \sum_{i_1, i_2, j_1, j_2} \theta_{i_1} \theta_{i_2} H^{(2)}_{i_1 i_2, j_1 j_2} \frac{\partial^2}{\partial \theta_{j_1} \partial \theta_{j_2}} .$$

The total Hamiltonian $\mathbf{H} = \mathbf{H}^{(1)} + \mathbf{H}^{(2)}$ is hermitian with respect to the scalar product (10.34). It has a representation analogous to the Hamiltonians of the holomorphic representation and the general strategy described in sections 4.9 and 4.10 can again be followed here.

The Hamiltonian $\mathbf{H}$ conserves the number of particles. One thus verifies that the particle number operator $\mathbf{N}$ (equation (10.49)) commutes with $\mathbf{H}$:

$$[\mathbf{N}, \mathbf{H}] = 0\,.$$

Chemical potential. Since the Hamiltonian conserves the number of particles, in statistical physics one must then introduce a chemical potential μ coupled to $\mathbf{N}$ to be able to vary the average number of particles. In the definition of the partition function, this amounts to the substitution (a modification of $\mathbf{H}^{(1)}$)

$$\mathbf{H} \mapsto \mathbf{H} - \mu\mathbf{N}\,.$$

Remarks.

(*i*) As in the example with only one generator, the Clifford algebra (10.8) is isomorphic to the algebra of creation and annihilation operators $a_i, a_i^\dagger$ for fermions with the correspondence

$$a_i^\dagger \mapsto \theta_i \,, \quad a_i \mapsto \partial/\partial\theta_i \,.$$

Indeed, the operators θ_i and $\partial/\partial\theta_i$ are hermitian conjugates and the commutation relations (10.8) are identical to the commutation relations of fermion creation and annihilation operators:

$$a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = a_i a_j + a_j a_i = 0 \quad \text{and} \quad a_i^\dagger a_j + a_j a_i^\dagger = \delta_{ij} \,.$$

(*ii*) Note that the relations (10.8) exhibit a full symmetry between the hermitian conjugate operators θ_i and $\partial/\partial\theta_i$. Therefore, θ could also be associated with fermion annihilation and $\partial/\partial\theta$ with fermion creation.

Then, θ would become the empty state and 1 the occupied state. This remark becomes specially relevant when the parameter ω in the Hamiltonian (10.31) is negative. Then, the ground state is the vector θ.

In the more general framework of section 10.12, the vacuum would then correspond to the product of all generators.

One generally prefers identifying the ground state with the vacuum, and assign positive energies to particle excitations. An equivalent representation can be obtained by Grassmann Fourier transformation. Adding one generator η to the Grassmann algebra, one defines

$$\tilde{\psi}(\eta) = \int \mathrm{d}\theta \; \mathrm{e}^{\theta\eta}\, \psi(\theta).$$

Then, if $\psi(\theta) = \psi_0 + \theta\psi_1$,

$$\tilde{\psi}(\eta) = \psi_1 + \eta\psi_0$$

and θ and $\partial/\partial\theta$ are represented by $\partial/\partial\eta$ and η, respectively.

10.13 Grassmann path integral: one-state problem

We first construct a path integral representation of the kernel of the operator $U_0(t) = \mathrm{e}^{-tH_0}$, proportional to the density matrix at thermal equilibrium, in the case of the one-state problem. Since the density matrix then reduces to a 2×2 matrix, its calculation from a path integral may appear as an unnecessary complication. However, the path integral representation is useful because it can easily be generalized to an arbitrary number of available states. This justifies its introduction even to solve this elementary problem.

The method, in the case of a fermion Hamiltonian, follows, rather closely, the method of section 4.6, the main difference being that complex variables are replaced by Grassmann variables.

10.13.1 Grassmannian path integral

To construct a path integral, one needs the expansion of the kernel of the statistical operator (10.45) to first order for $t \to 0$:

$$\langle\theta|\, U_0(t) \left|\bar{\theta}\right\rangle = \exp\left[-\bar{\theta}\theta(1-\omega t) + O\left(t^2\right)\right]. \tag{10.50}$$

Using the semi-group property $U_0(t) = [U_0(t/n)]^n$ expressed in the form (10.41), one can then write the statistical operator at finite euclidean time as

$$\left\langle\theta'' \left|U_0(t'', t')\right| \bar{\theta}'\right\rangle = \lim_{n\to\infty} \int \left(\prod_{k=1}^{n-1} \mathrm{d}\theta_k \mathrm{d}\bar{\theta}_k\right) \exp\left[-\bar{\theta}_0\theta_0 - \mathcal{S}_\varepsilon(\theta, \bar{\theta})\right]$$

with

$$\mathcal{S}_\varepsilon(\theta, \bar{\theta}) = \sum_{k=1}^{n} \left[\bar{\theta}_{k-1}\left(\theta_k - \theta_{k-1}\right) - \omega\varepsilon\bar{\theta}_{k-1}\theta_k\right],$$

$\varepsilon = (t'' - t')/n$, and the definitions $\bar{\theta}_0 = \bar{\theta}'\,, \quad \theta_n = \theta''$.

The formal limit $n \to \infty$ yields a generalized path integral involving a summation over Grassmann paths $\{\theta(t), \bar{\theta}(t)\}$, which are generators of an infinite-dimensional Grassmann algebra.

The kernel representation of $U_0(t'', t') = U_0(t'' - t')$ is given by

$$\left\langle \theta'' \left| U_0(t'', t') \right| \bar{\theta}' \right\rangle = \int_{\bar{\theta}(t')=\bar{\theta}'}^{\theta(t'')=\theta''} \left[\mathrm{d}\theta(t) \mathrm{d}\bar{\theta}(t) \right] \exp\left[-\bar{\theta}(t')\theta(t') - \mathcal{S}_0(\theta, \bar{\theta}) \right] \tag{10.51}$$

with

$$\mathcal{S}_0(\theta, \bar{\theta}) = \int_{t'}^{t''} \mathrm{d}t \, \bar{\theta}(t) \left[\dot{\theta}(t) - \omega\theta(t) \right].$$

Notice that in the one-state problem, the integral is automatically Gaussian.

Generating function of fermion correlation functions. A generating function of fermion correlation functions with the weight $\mathrm{e}^{-\mathcal{S}_0}/\mathcal{Z}_0$ is provided by the more general integral obtained by adding to the action $\mathcal{S}_0$ linear terms corresponding to a coupling to external Grassmann sources $\bar{\eta}(t)$ and $\eta(t)$. We thus consider the more general path integral

$$\left\langle \theta'' \left| U_{\mathrm{G}}(t'', t'; \eta, \bar{\eta}) \right| \bar{\theta}' \right\rangle = \int_{\bar{\theta}(t')=\bar{\theta}'}^{\theta(t'')=\theta''} \left[\mathrm{d}\theta(t)\mathrm{d}\bar{\theta}(t)\right] \mathrm{e}^{-\bar{\theta}(t')\theta(t')}\, \mathrm{e}^{-\mathcal{S}_{\mathrm{G}}(\theta,\bar{\theta};\eta,\bar{\eta})} \tag{10.52}$$

with

$$\mathcal{S}_{\mathrm{G}}(\theta, \bar{\theta}; \eta, \bar{\eta}) = \mathcal{S}_0(\theta, \bar{\theta}) - \int_{t'}^{t''} \mathrm{d}t \left[\bar{\eta}(t)\theta(t) + \bar{\theta}(t)\eta(t)\right], \tag{10.53}$$

where now the four infinite sets $\{\theta(t)\}$, $\{\bar{\theta}(t)\}$, $\{\eta(t)\}$ and $\{\bar{\eta}(t)\}$ form a set of generators of the Grassmann algebra.

10.13.2 Calculation of the path integral

The integral (10.52) is Gaussian and can be calculated exactly. The 'saddle point equation' obtained by varying $\theta(t)$ yields

$$\dot{\bar{\theta}}(t) + \omega\bar{\theta}(t) + \bar{\eta}(t) = 0$$

and, thus, taking into account boundary conditions,

$$\bar{\theta}(t) = \bar{\theta}_{\mathrm{s}}(t) \equiv \mathrm{e}^{-\omega(t-t')}\,\bar{\theta}' - \int_{t'}^{t} \mathrm{e}^{-\omega(t-u)}\,\bar{\eta}(u)\mathrm{d}u\,.$$

In the same way, the variation of $\bar{\theta}(t)$ yields

$$\dot{\theta}(t) - \omega\theta(t) - \eta(t) = 0$$

and, thus,

$$\theta(t) = \theta_{\mathrm{s}}(t) \equiv \mathrm{e}^{-\omega(t''-t)}\,\theta'' - \int_{t}^{t''} \mathrm{e}^{-\omega(u-t)}\,\eta(u)\mathrm{d}u\,.$$

Translating $\theta(t)$ and $\bar{\theta}(t)$ by the solutions of the 'classical' equations: $\theta \mapsto \theta_{\mathrm{s}} + \theta$, $\bar{\theta} \mapsto \bar{\theta}_{\mathrm{s}} + \bar{\theta}$, one then obtains

$$\left\langle \theta'' \left| U_{\mathrm{G}}(t'', t'; \eta, \bar{\eta}) \right| \bar{\theta}' \right\rangle = \mathcal{N}(t', t'') \exp\left[-\bar{\theta}(t')\theta(t') - \mathcal{S}_{\mathrm{c}}(\theta'', \bar{\theta}'; \bar{\eta}, \eta)\right] \tag{10.54}$$

with

$$\bar{\theta}(t')\theta(t') = \bar{\theta}'\theta''\,\mathrm{e}^{-\omega(t''-t')} - \bar{\theta}' \int_{t'}^{t''} \mathrm{d}t\ \mathrm{e}^{-\omega(t-t')}\,\eta(t)$$

and

$$\begin{aligned} \mathcal{S}_{\mathrm{c}} &= -\int_{t'}^{t''} \bar{\eta}(t)\theta_{\mathrm{s}}(t)\mathrm{d}t \\ &= -\int_{t'}^{t''} \mathrm{d}t\,\bar{\eta}(t)\,\mathrm{e}^{-\omega(t''-t)}\,\theta'' + \int_{t'}^{t''} \mathrm{d}t \int_{t}^{t''} \mathrm{d}u\,\bar{\eta}(t)\,\mathrm{e}^{-\omega(u-t)}\,\eta(u)\,. \end{aligned}$$

To calculate the normalization

$$\mathcal{N}(t',t'') = \int_{\bar\theta(t')=0}^{\theta(t'')=0} [\mathrm{d}\theta(t)\mathrm{d}\bar\theta(t)] \exp\left[-\int_{t'}^{t''} \mathrm{d}t\,\bar\theta(t)\big(\dot\theta(t) - \omega\theta(t)\big)\right],$$

one again changes variables, setting

$$\bar\theta(t) = \mathrm{e}^{-\omega t}\,\bar\zeta(t)\,,\qquad \theta(t) = \mathrm{e}^{\omega t}\,\zeta(t).$$

The Jacobian equals 1. After this change, the dependence on ω has disappeared. One finds $\mathcal{N} = 1$ in the mixed representation evaluated for $\theta = \bar\theta = 0$. Thus $\mathcal{N} = 1$.

As in the boson case, correlation functions are obtained by differentiating expression (10.54) with respect to η and $\bar\eta$.

10.13.3 Two-point function and partition function

From expression (10.54), one infers the functional $\operatorname{tr} U(\beta/2, -\beta/2; \eta, \bar{\eta})$, the trace being defined by equation (10.43):

$$\operatorname{tr} U_{\mathrm{G}}(\beta/2, -\beta/2; \eta, \bar{\eta}) = \int \mathrm{d}\bar{\theta}\, \mathrm{d}\theta\ \mathrm{e}^{-\bar{\theta}\theta} \left\langle \theta \left| U(\beta/2, -\beta/2; \eta, \bar{\eta}) \right| \bar{\theta} \right\rangle .$$

A simple evaluation of the Grassmann integrals yields

$$\operatorname{tr} U_{\mathrm{G}}(\beta/2, -\beta/2; \eta, \bar{\eta}) = \mathcal{Z}_0(\beta) \exp\left[-\int_{-\beta/2}^{\beta/2} \mathrm{d}u\, \mathrm{d}t\, \bar{\eta}(u) \Delta(t-u) \eta(t)\right],$$

where $\mathcal{Z}_0(\beta)$ is the partition function $\mathcal{Z}_0(\beta) = 1 + \mathrm{e}^{-\omega\beta}$ and

$$\Delta(t) = \tfrac{1}{2}\, \mathrm{e}^{-\omega t} \left[\operatorname{sgn}(t) + \tanh(\omega\beta/2)\right], \tag{10.55}$$

where $\operatorname{sgn}(t)$ is the sign function, $\operatorname{sgn}(t) = 1$ for $t > 0$, $\operatorname{sgn}(t) = -1$ for $t < 0$.

The function $\Delta(t)$ is the solution of the differential equation

$$\dot{\Delta}(t) + \omega\Delta(t) = \delta(t)$$

with, in contrast with the boson case (equations (3.37, 4.36)), anti-periodic boundary conditions:

$$\Delta(\beta/2) = -\Delta(-\beta/2).$$

In the limit $\beta \to \infty$, it reduces to

$$\Delta(t) = \tfrac{1}{2}\, \mathrm{e}^{-\omega t}\big(\mathrm{sgn}(t) + 1\big),$$

an expression identical to the one obtained in the case of holomorphic formalism (see equation (4.37)).

Despite the non-trivial way the trace is defined, the result obtained here is identical to the one given by a path integral with anti-periodic boundary conditions.

Thus,

$$\operatorname{tr} U_{\mathrm{G}}(\beta/2,-\beta/2;\eta,\bar\eta)=\int\left[\mathrm{d}\theta(t)\mathrm{d}\bar\theta(t)\right]\exp\left[-\mathcal{S}_{\mathrm{G}}(\theta,\bar\theta;\eta,\bar\eta)\right] \tag{10.56}$$

with $\theta(-\beta/2)=-\theta(\beta/2)$, $\bar\theta(-\beta/2)=-\bar\theta(\beta/2)$ and

$$\mathcal{S}_{\mathrm{G}}(\theta,\bar\theta;\eta,\bar\eta)=\int_{-\beta/2}^{\beta/2}\mathrm{d}t\,\left\{\bar\theta(t)\left[\dot\theta(t)-\omega\theta(t)\right]-\bar\eta(t)\theta(t)-\bar\theta(t)\eta(t)\right\}.$$

By contrast, the integral with periodic boundary conditions is obtained by integrating expression (10.54) with $\mathrm{e}^{\theta\bar\theta}$ and yields $\operatorname{tr}\mathrm{P}\,\mathrm{e}^{-\beta H}$ (*cf.* expression (10.39)).

The two-point correlation function calculated with the Gaussian measure $\mathrm{e}^{-\mathcal{S}_0}/\mathcal{Z}_0$ is obtained by differentiating $\operatorname{tr} U_{\mathrm{G}}(\beta/2,-\beta/2;\eta,\bar\eta)$ twice. One finds

$$\left\langle\bar\theta(t)\theta(u)\right\rangle=\Delta(t-u).$$

Since the integrand is Gaussian, all other correlation functions are obtained by using Wick's theorem (10.21), which here takes the form

$$\begin{aligned}&\left\langle \bar\theta(t_1)\theta(u_1)\ldots\bar\theta(t_p)\theta(u_p)\right\rangle\\ &\quad=\sum_{\substack{\text{permutations}\\ P \text{ of } \{1\ldots p\}}} \epsilon(P)\left\langle \bar\theta(t_1)\theta(u_{P_1})\right\rangle\left\langle \bar\theta(t_2)\theta(u_{P_2})\right\rangle\cdots\left\langle \bar\theta(t_p)\theta(u_{P_p})\right\rangle . \quad (10.57)\end{aligned}$$

Remark. The derivative of $\ln \mathcal{Z}_0$ with respect to ω is related to the two-point function (10.55) since

$$\frac{\mathrm{d}\ln \mathcal{Z}_0}{\mathrm{d}\omega}=\int_{-\beta/2}^{\beta/2}\mathrm{d}t\,\left\langle \bar\theta(t)\theta(t)\right\rangle=\beta\Delta(0)=\tfrac{1}{2}\beta[\mathrm{sgn}(0)+\tanh(\omega\beta/2)]$$

and, thus,

$$\mathcal{Z}_0(\beta)=\mathrm{e}^{\omega\beta(\mathrm{sgn}(0)+1)/2}+\mathrm{e}^{\omega\beta(\mathrm{sgn}(0)-1)/2}\,. \quad (10.58)$$

One faces a problem already encountered in the case of holomorphic path integrals.

The choice $\mathrm{sgn}(0) = -1$ corresponds to the normal order (10.31), but leads to the problem of non-commutation of time differentiation and path integration already encountered in the commutative case.

The choice $\mathrm{sgn}(0) = 0$ leads to the energy eigenvalues $\pm\omega/2$ and corresponds to the Hamiltonian $\omega[a^\dagger, a]/2$, which is the 'symmetrized' version of the operator (10.31). A way to ensure that the choice $\mathrm{sgn}(0) = 0$ yields the exact result, is to insert in the path integral the average of the normal and anti-normal ordered forms (see the discussion of section 4.7).

10.14 Grassmann path integrals: generalization

The preceding formalism can be generalized to a Grassmann algebra with an arbitrary number of generators θ_i, as the calculation of the partition function in the second quantization formalism of section 10.12 requires.

10.14.1 General Hamiltonian

A general Hamiltonian is represented by a differential operator $H(\boldsymbol{\theta}, \partial/\partial\boldsymbol{\theta}; t)$ acting on functions of θ_i's. A Hamiltonian written in normal form with all differentiations on the right, can also be represented by the kernel (section 10.9)

$$\left\langle \boldsymbol{\theta} \left| H \right| \bar{\boldsymbol{\theta}} \right\rangle = H(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}; t)\mathcal{I}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}).$$

An important restriction is that the matrix elements of the Hamiltonian must belong to the commutative subalgebra $\mathfrak{A}^+$ (equation (10.44)).

A Hamiltonian does not necessarily conserve the number of fermions. Fermion number conservation implies that in each monomial contributing to the kernel, the number of θ and $\bar{\theta}$ factors is equal.

The generalized form of equation (10.50) is

$$\left\langle \boldsymbol{\theta} \left| U(t+\varepsilon, t) \right| \bar{\boldsymbol{\theta}} \right\rangle = \exp\left[-\sum_i \theta_i \bar{\theta}_i - \varepsilon\, H(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}; t) + O\left(\varepsilon^2\right) \right].$$

Following the method of section 10.13.1, one then derives a path integral representation for $U(t'', t')$ at finite euclidean time difference. One obtains

$$\left\langle \boldsymbol{\theta}'' \left| U(t'', t') \right| \bar{\boldsymbol{\theta}}' \right\rangle = \int_{\bar{\boldsymbol{\theta}}(t')=\bar{\boldsymbol{\theta}}'}^{\boldsymbol{\theta}(t'')=\boldsymbol{\theta}''} \left[\mathrm{d}\boldsymbol{\theta}(t) \mathrm{d}\bar{\boldsymbol{\theta}}(t) \right] \mathrm{e}^{-\bar{\boldsymbol{\theta}}(t')\cdot\boldsymbol{\theta}(t')} \exp\left[-\mathcal{S}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) \right] \tag{10.59}$$

with

$$\mathcal{S}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) = \int_{t'}^{t''} \mathrm{d}t \, \left\{ \bar{\boldsymbol{\theta}}(t) \cdot \dot{\boldsymbol{\theta}}(t) + H\left[\boldsymbol{\theta}(t), \bar{\boldsymbol{\theta}}(t); t \right] \right\}. \tag{10.60}$$

Partition function. In the case of a time-independent Hamiltonian, the corresponding partition function then reads

$$\mathcal{Z}(\beta) = \operatorname{tr} U(\beta/2, -\beta/2) = \int \left[\mathrm{d}\boldsymbol{\theta}(t)\mathrm{d}\bar{\boldsymbol{\theta}}(t)\right] \exp\left[-\mathcal{S}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}})\right], \tag{10.61}$$

where the path integral has to be calculated with anti-periodic boundary conditions:

$$\boldsymbol{\theta}(-\beta/2) = -\boldsymbol{\theta}(\beta/2), \quad \bar{\boldsymbol{\theta}}(-\beta/2) = -\bar{\boldsymbol{\theta}}(\beta/2).$$

This follows, for example, from the representation (10.56) and perturbation theory in the form of equation (10.64). The trace of the right hand side involves only $\operatorname{tr} U_{\mathrm{G}}$, which can be calculated from the path integral with anti-periodic boundary conditions (equation (10.56)).

Fermion systems with pair interactions. We now specialize the expressions of section 10.14 to the many-fermion systems described in sections 10.11, 10.12. The partition function $\mathcal{Z}(\beta,\mu)$ is then given by a Grassmann path integral of the form (10.61) where the action is

$$\mathcal{S}(\boldsymbol{\theta},\bar{\boldsymbol{\theta}}) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[\bar{\boldsymbol{\theta}}(t)\cdot\left(\dot{\boldsymbol{\theta}}(t)+\mu\boldsymbol{\theta}(t)\right) + H\left(\boldsymbol{\theta}(t),\bar{\boldsymbol{\theta}}(t)\right)\right], \tag{10.62}$$

$$H(\boldsymbol{\theta},\bar{\boldsymbol{\theta}}) = \sum_i \theta_i\omega_i\bar{\theta}_i + \tfrac{1}{2}\sum_{i_1,i_2,j_1,j_2} \theta_{i_1}\theta_{i_2}H^{(2)}_{i_1 i_2,j_1 j_2}\bar{\theta}_{j_1}\bar{\theta}_{j_2}\,,$$

a form analogous to the boson expression (4.60).

10.14.2 Equation of state

Differentiating the path integral (10.61), one verifies that the equation state can be written as

$$\langle \mathbf{N} \rangle = \frac{1}{\beta} \frac{\partial \ln \mathcal{Z}}{\partial \mu} = \frac{1}{\beta} \sum_i \int_{-\beta/2}^{\beta/2} \mathrm{d}t \, \left\langle \theta_i(t) \bar{\theta}_i(t) \right\rangle = \sum_i \left\langle \theta_i(0) \bar{\theta}_i(0) \right\rangle ,$$

where in the second expression the expectation value is calculated with the weight $\mathrm{e}^{-\mathcal{S}}/\mathcal{Z}$ and time translation invariance has been used.

In the case of independent particles, expectation values involve only the Gaussian two-point function (10.55). One recovers the standard expression (with the choice $\operatorname{sgn}(0) = -1$)

$$\langle \mathbf{N} \rangle = \sum_i \frac{1}{\mathrm{e}^{\beta(\omega_i - \mu)} + 1} = \operatorname{tr} \frac{1}{\mathrm{e}^{\beta(H^{(1)} - \mu)} + 1} , \qquad (10.63)$$

where $H^{(1)}$ is the one-particle Hamiltonian.

At low temperature, that is for $\beta \to \infty$,

$$\langle \mathbf{N} \rangle \sim \sum_i \theta(\mu - \omega_i),$$

where $\theta(s)$ is the step function. The chemical potential can be identified with the Fermi energy: at zero temperature, all states below the Fermi energy are occupied; all states above the Fermi energy are empty.

At low temperature, when interactions between fermions are added, only states with energies close to the Fermi energy are relevant.

10.14.3 Perturbative expansion

We have shown in section 10.4 how to calculate Gaussian integrals and expectation values of polynomials. The same method can be used here to calculate the path integral (10.61) perturbatively.

Expressing a Hamiltonian as the sum of a quadratic term and an interaction,

$$H(\boldsymbol{\theta},\bar{\boldsymbol{\theta}}) = -\sum_i \omega_i \bar{\theta}_i \theta_i + H_{\mathrm{I}}(\boldsymbol{\theta},\bar{\boldsymbol{\theta}}),$$

one expands the integral in powers of H_{I} and calculates the successive terms, for example, using Wick's theorem (10.57).

One verifies that the perturbative expansion of general matrix elements has the formal representation

$$\begin{aligned}&\left\langle \boldsymbol{\theta}'' \left| U(t'',t') \right| \bar{\boldsymbol{\theta}}' \right\rangle \\ &\quad = \exp\left[-\int \mathrm{d}t\, H_{\mathrm{I}}(\partial/\partial\bar{\eta}, -\partial/\partial\eta)\right] \left\langle \boldsymbol{\theta}'' \left| U_{\mathrm{G}}(\eta;t'',t') \right| \bar{\boldsymbol{\theta}}' \right\rangle\Big|_{\eta=\bar{\eta}=0}, \quad (10.64)\end{aligned}$$

where U_{G} is the product of integrals (10.52) corresponding to the different pairs of generators $\theta_i, \bar{\theta}_i$.

Ambiguities. In perturbative calculations, problems due to operator ordering appear here also, as in the case of the holomorphic path integral. Indeed, perturbative calculations involve $\mathrm{sgn}(0)$. The ansatz consistent with the normal-order construction, is again to set $\mathrm{sgn}(0_-)=-1$, but generates some difficulties. It is more convenient to substitute to $H(\boldsymbol{\theta},\bar{\boldsymbol{\theta}})$ the equivalent expression consistent with $\mathrm{sgn}(0)=0$.

10.14.4 The evolution operator

With the conventions of section 10.13, for a finite number of fermions and a normal-ordered Hamiltonian of the form $h(\boldsymbol{\theta}, \partial/\partial\boldsymbol{\theta})$, the evolution operator is given by the path integral

$$\langle \boldsymbol{\theta}'' |\, U(t'', t') \,| \bar{\boldsymbol{\theta}}' \rangle = \int \left[\prod_\alpha \mathrm{d}\theta_\alpha(t) \mathrm{d}\bar{\theta}_\alpha(t) \right] \exp i\mathcal{A}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}), \tag{10.65a}$$

$$\mathcal{A}(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) = \int_{t'}^{t''} \mathrm{d}t \left\{ i\bar{\boldsymbol{\theta}}(t) \cdot \dot{\boldsymbol{\theta}}(t) - h\left[\boldsymbol{\theta}(t), \bar{\boldsymbol{\theta}}(t) \right] \right\} + i\bar{\boldsymbol{\theta}}(t') \cdot \boldsymbol{\theta}(t'), \tag{10.65b}$$

real time continuation of the representation (10.60). We recall that hermiticity is equivalent to $\mathcal{A} = \bar{\mathcal{A}}$.

In the case of a free Hamiltonian

$$h(\theta,\bar\theta)=\omega\theta\bar\theta=-\omega\bar\theta\theta\,,$$

if ω is negative the one-particle state has an energy lower than the vacuum or ground state (see also the discussion at the end of section 10.12.3). This simply means that the two states have been misidentified; they have to be interchanged. A simple transformation deals with the problem. We set

$$v(t)=\bar\theta(t),\quad \bar v(t)=\theta(t)\,.$$

Then, after an integration by parts of the term $iv(t)\dot{\bar v}(t)$,

$$\mathcal{A}(v,\bar v)=\int_{t'}^{t''}\mathrm{d}t\,[i\bar v(t)\dot v(t)+|\omega|\bar v(t)v(t)]-i\bar v(t'')\cdot v(t''),$$

which now corresponds to one-particle states with positive energy. In addition, in the boundary term t' has been replaced by t''.

Exercises

Exercise 10.1

One site electron problem. Electrons living on one site are still characterized by the two possible values of their spin. A site thus can be empty, occupied by one electron with spin up or down, or two electrons with spin up and down.

One denotes below by θ_+, θ_- the Grassmann variables associated with spin up and down electrons, respectively. Hermiticity is then defined with respect to the Grassmann scalar product.

Write, in normal-ordered form, the most general hermitian Hamiltonian invariant under spin reversal and conserving total electron number. One then considers the Hamiltonian

$$H = \omega \left(\theta_+ \frac{\partial}{\partial \theta_+} + \theta_- \frac{\partial}{\partial \theta_-} \right) + v\, \theta_- \theta_+ \frac{\partial}{\partial \theta_+} \frac{\partial}{\partial \theta_-} \,, \quad \omega > 0 \,, \quad v \in \mathbb{R} \,. \tag{10.66}$$

What are its symmetries? Determine its spectrum. Infer the partition function at temperature $1/\beta$. Show that the situation $v < -2\omega$ has a natural interpretation if the role of creation and annihilation operators is interchanged.

Solution. In addition to the terms appearing in (10.66), one possible additional term is

$$\theta_+ \frac{\partial}{\partial \theta_-} + \theta_- \frac{\partial}{\partial \theta_+} \,.$$

It is eliminated if one demands separate conservation of up and down electron numbers.

The four eigenvectors are $1, \theta_+, \theta_-, \theta_-\theta_+$ and the corresponding eigenvalues are $E_0 = 0$, $E_1 = E_2 = \omega$, $E_3 = 2\omega + v$, respectively. The partition function thus is

$$\mathcal{Z}(\beta) = 1 + 2\,\mathrm{e}^{-\omega\beta} + \mathrm{e}^{-(2\omega+v)\beta} \,.$$

When $2\omega + v$ is negative, the ground state is no longer the empty state but, instead, the doubly-occupied state. The description in terms of electron excitations is no longer convenient. The excitations now correspond to remove electrons. A formal way to implement this idea is to introduce the operators

$$\zeta_- = \frac{\partial}{\partial\theta_+}\,,\ \zeta_+ = \frac{\partial}{\partial\theta_-}\,,\ \theta_+ = \frac{\partial}{\partial\zeta_-}\,,\ \theta_- = \frac{\partial}{\partial\zeta_+}\,.$$

This transformation is consistent with the commutation relations and hermitian conjugation. The Hamiltonian can then be rewritten as

$$H = E_0 - (\omega + v)\left(\zeta_+\frac{\partial}{\partial\zeta_+} + \zeta_-\frac{\partial}{\partial\zeta_-}\right) + v\zeta_-\zeta_+\frac{\partial}{\partial\zeta_+}\frac{\partial}{\partial\zeta_-}\,,\ E_0 = 2\omega + v\,,$$

where $2\omega + v < 0$ implies $-\omega - v > \omega > 0$.

Exercise 10.2

Write the path integral representation of the corresponding partition function. Expand and calculate it up to second order in v (the one-component Gaussian two-point function is given by equation (10.55)).

Solution.

$$\mathcal{Z}(\beta) = \int [\mathrm{d}\theta(t)\mathrm{d}\bar{\theta}(t)] \exp\left[-\mathcal{S}(\theta, \bar{\theta})\right],$$

where the action takes the form (10.62):

$$\mathcal{S}(\theta, \bar{\theta}) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[\sum_{\pm} \bar{\theta}_{\pm}(t)\dot{\theta}_{\pm}(t) + H\big(\theta(t), \bar{\theta}(t)\big)\right],$$

$$H(\theta, \bar{\theta}) = \omega \sum_{\pm} \theta_{\pm}\bar{\theta}_{\pm} + v\,\theta_{-}\theta_{+}\bar{\theta}_{+}\bar{\theta}_{-}\,,$$

and the boundary conditions are anti-periodic:

$$\theta_{\pm}(-\beta/2) = -\theta_{\pm}(\beta/2),\ \bar{\theta}_{\pm}(-\beta/2) = -\bar{\theta}_{\pm}(\beta/2).$$

The perturbative expansion takes the form

$$\mathcal{Z}(\beta)/\mathcal{Z}_0(\beta) = 1 - v\int_{-\beta/2}^{\beta/2} \mathrm{d}t \left\langle \theta_-(t)\theta_+(t)\bar{\theta}_+(t)\bar{\theta}_-(t)\right\rangle$$

$$+ \tfrac{1}{2}v^2 \int_{-\beta/2}^{\beta/2} \mathrm{d}t\,\mathrm{d}u \left\langle \theta_-(t)\theta_+(t)\bar{\theta}_+(t)\bar{\theta}_-(t)\theta_-(u)\theta_+(u)\bar{\theta}_+(u)\bar{\theta}_-(u)\right\rangle + O(v^3),$$

where $\mathcal{Z}_0$ is the square of the partition function (10.58) and the Gaussian expectation values $\langle\bullet\rangle$ over θ_+ and θ_- factorize. One finds

$$\begin{aligned}\mathcal{Z}(\beta)/\mathcal{Z}_0(\beta) &= 1 - v\beta\Delta^2(0) + \tfrac{1}{2}v^2\beta\int_{-\beta/2}^{\beta/2} \mathrm{d}t\,\bigl(\Delta^2(0) - \Delta(t)\Delta(-t)\bigr)^2 \\ &\quad + O(v^3) \\ &= 1 - \tfrac{1}{4}v\beta\bigl(\operatorname{sgn}(0) + \tanh(\omega\beta/2)\bigr)^2 \\ &\quad + \tfrac{1}{32}v^2\beta^2\bigl(1 + 2\operatorname{sgn}(0)\tanh(\omega\beta/2) + \operatorname{sgn}^2(0)\bigr)^2 + O(v^3).\end{aligned}$$

Setting $\epsilon = \mathrm{sgn}(0)$, one concludes

$$\begin{aligned} E_0 &= -(1+\epsilon)\omega + \tfrac{1}{4}(1+\epsilon)^2 v\,, \\ E_1 = E_2 &= -\epsilon\omega - \tfrac{1}{4}(1-\epsilon^2) v\,, \\ E_3 &= (1-\epsilon)\omega + \tfrac{1}{4}(1-\epsilon)^2 v\,. \end{aligned}$$

For $\mathrm{sgn}(0) = -1$, one recovers the spectrum of the initial Hamiltonian. To obtain the same result with the convention $\mathrm{sgn}(0) = 0$, one must substitute $\omega \mapsto \omega' = \omega + v/2$ and shift the empty state energy by $E_0 = -\omega' + v/4$.

Exercise 10.3

One now adds the term

$$\gamma\left(\theta_-\theta_+ + \frac{\partial}{\partial\theta_+}\frac{\partial}{\partial\theta_-}\right)$$

with γ real, to the Hamiltonian, which becomes

$$H = \omega\left(\theta_+ \frac{\partial}{\partial\theta_+} + \theta_- \frac{\partial}{\partial\theta_-}\right) + v\,\theta_-\theta_+ \frac{\partial}{\partial\theta_+}\frac{\partial}{\partial\theta_-} + \gamma\left(\theta_-\theta_+ + \frac{\partial}{\partial\theta_+}\frac{\partial}{\partial\theta_-}\right). \tag{10.67}$$

This model describes the interaction with a medium that can absorb and emit electron pairs with equal probability. Determine the eigenvectors and spectrum of the total Hamiltonian.

Solution. The new interaction mixes only the spinless states 1 and $\theta_-\theta_+$. The energies of the other states are unchanged. In the $1, \theta_-\theta_+$ subspace the Hamiltonian reads

$$\begin{pmatrix} 0 & \gamma \\ \gamma & 2\omega + v \end{pmatrix}$$

with eigenvalues

$$\omega + v/2 \pm \sqrt{(\omega + v/2)^2 + \gamma^2}\,. \tag{10.68}$$

The ground state energy thus is $\omega + v/2 - \sqrt{(\omega + v/2)^2 + \gamma^2}$ and the partition function is given by

$$\mathcal{Z}(\beta) = 2\,\mathrm{e}^{-\omega\beta}\left(1 + \mathrm{e}^{-\beta v/2}\cosh\sqrt{(\omega + v/2)^2 + \gamma^2}\right) . \tag{10.69}$$

Exercise 10.4

In what follows one sets $v = 0$ and $\rho = \sqrt{\omega^2 + \gamma^2}$, $\omega = \rho\cos\varphi$, $\gamma = \rho\sin\varphi$. Show that the spectrum then has an interpretation in terms of two independent quasi-particles by setting

$$\theta_+ = a\eta_+ + b\frac{\partial}{\partial\eta_-}\,, \quad \theta_- = d\eta_- + c\frac{\partial}{\partial\eta_+}\,, \quad a, b, c, d \in \mathbb{R}\,,$$

where η_+, η_- are two generators of a Grassmann algebra, and the corresponding operators $\eta_\pm$ and $\partial/\partial\eta_\pm$ are hermitian conjugate in the same way as $\theta_\pm$ and $\partial/\partial\theta_\pm$.

First, express $\partial/\partial\theta_\pm$ in terms of the η type operators. Then, show that the consistency of these transformations with the commutation relations (10.8) imply three conditions on the coefficients a, b, c, d that express that a, b, c, d are the four entries of an orthogonal matrix. Finally determine the coefficients to reduce the Hamiltonian to the form

$$H = E_0 + \Omega\left(\eta_+ \frac{\partial}{\partial\eta_+} + \eta_- \frac{\partial}{\partial\eta_-}\right), \quad \Omega > 0\,.$$

Solution. The form of the Hamiltonian is obtained for the choice

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \cos(\varphi/2) & \sin(\varphi/2) \\ -\sin(\varphi/2) & \cos(\varphi/2) \end{pmatrix},$$

and $E_0 = \omega - \rho$, $\Omega = \rho$.

Exercise 10.5

Write the corresponding path integral representation of the partition function and perform the change of variables

$$\theta_+ = a\eta_+ + b\bar{\eta}_- \,, \quad \theta_- = d\eta_- + c\bar{\eta}_+ \,,$$
$$\bar{\theta}_+ = a\bar{\eta}_+ + b\eta_- \,, \quad \bar{\theta}_- = d\bar{\eta}_- + c\eta_+ \,,$$

using the values found in the preceding exercise. Show that the resulting path integral is consistent with the spectrum.

Solution. After the change of variables, one finds a path integral corresponding to the Hamiltonian

$$H = \Omega \left(\eta_+ \frac{\partial}{\partial \eta_+} + \eta_- \frac{\partial}{\partial \eta_-} \right),$$

up to an additive constant.

Exercise 10.6

Spin group: fermion representation. One now considers the three operators

$$\tau_1 = \frac{1}{2}\left(\theta_+ \frac{\partial}{\partial\theta_-} + \theta_- \frac{\partial}{\partial\theta_+}\right), \ \tau_2 = \frac{i}{2}\left(\theta_- \frac{\partial}{\partial\theta_+} - \theta_+ \frac{\partial}{\partial\theta_-}\right),$$
$$\tau_3 = \frac{1}{2}\left(\theta_+ \frac{\partial}{\partial\theta_+} - \theta_- \frac{\partial}{\partial\theta_-}\right).$$

In what follows, one sets $\hbar = 1$.

Verify that the operators are hermitian. Calculate the products $\tau_i\tau_j$ and $\boldsymbol{\tau}^2 = \sum_i \tau_i^2$. Infer the commutators $[\tau_i, \tau_j]$. Find the eigenvectors and eigenvalues of τ_3 and $\boldsymbol{\tau}^2$. Calculate the commutators of τ_i with the Hamiltonian (10.66) and the interaction (10.67). Comment.

Solution. The operators are generators of the Lie algebra of the spin group

$SU(2)$:

$$\tau_i \tau_j = \tfrac{1}{3}\boldsymbol{\tau}^2 \delta_{ij} + \tfrac{1}{2} i \epsilon_{ijk} \tau_k \,,$$
$$\boldsymbol{\tau}^2 = \frac{3}{4}\left(\theta_+ \frac{\partial}{\partial \theta_+} + \theta_- \frac{\partial}{\partial \theta_-} - 2\theta_+ \frac{\partial}{\partial \theta_+} \theta_- \frac{\partial}{\partial \theta_-}\right).$$

The eigenvectors of τ_3 are $1, \theta_+, \theta_-, \theta_+\theta_-$ with eigenvalues $0, 1/2, -1/2, 0$, respectively, that is the spin components of the corresponding states. The corresponding eigenvalues of $\boldsymbol{\tau}^2$ are $0, 3/4, 3/4, 0$, as expected for spin $1/2$ particles. Finally, $\theta_+ \partial/\partial\theta_+$ and $\theta_- \partial/\partial\theta_-$ commute, and introducing

$$h = \theta_+ \frac{\partial}{\partial \theta_+} + \theta_- \frac{\partial}{\partial \theta_-} \,,$$

one verifies

$$\tau_i h = h \tau_i = \tau_i \,.$$

The commutation of the Hamiltonian (10.66) with the generators of the $SU(2)$ group follows from these relations and the commutations of the τ_i's with $\boldsymbol{\tau}^2$. One verifies that the interaction (10.67) is also $SU(2)$ invariant, which explains the form of the spectrum.

Exercise 10.7

Spin group: alternative representation. One now considers the operators

$$\tau_1 = \frac{1}{2}\left(\theta_+\theta_- + \frac{\partial}{\partial\theta_-}\frac{\partial}{\partial\theta_+}\right), \ \tau_2 = \frac{1}{2i}\left(\theta_+\theta_- - \frac{\partial}{\partial\theta_-}\frac{\partial}{\partial\theta_+}\right),$$
$$\tau_3 = \frac{1}{2}\left(\frac{\partial}{\partial\theta_+}\theta_+ - \theta_-\frac{\partial}{\partial\theta_-}\right) = \frac{1}{2}\left(1 - \theta_+\frac{\partial}{\partial\theta_+} - \theta_-\frac{\partial}{\partial\theta_-}\right).$$

The questions are the same as above. In addition, show that the Hamiltonian (10.67) can be expressed in terms of the $\boldsymbol{\tau}$ matrices. Recover the spectrum (10.68).

Solution. One finds, for example,

$$\boldsymbol{\tau}^2 = \frac{3}{4}\left(1 - \theta_+\frac{\partial}{\partial\theta_+} - \theta_-\frac{\partial}{\partial\theta_-} + 2\theta_+\frac{\partial}{\partial\theta_+}\theta_-\frac{\partial}{\partial\theta_-}\right).$$

The eigenvectors of τ_3 are $1, \theta_+, \theta_-, \theta_+\theta_-$ with eigenvalues $\frac{1}{2}, 0, 0, -\frac{1}{2}$, respectively, that is the spin components of the corresponding states. The corresponding eigenvalues of $\boldsymbol{\tau}^2$ are $\frac{3}{4}, 0, 0, \frac{3}{4}$.

Finally, the complete Hamiltonian can be written as

$$H = \omega - (2\omega + v)\tau_3 + \tfrac{2}{3}v\boldsymbol{\tau}^2 - 2\gamma\tau_1 \,.$$

After a rotation in the $(1, 3)$ plane, one can rewrite it as

$$H = \omega + \tfrac{2}{3}v\boldsymbol{\tau}^2 + 2\sqrt{\gamma^2 + (\omega + v/2)^2}\,\tau_3 \,,$$

which shows that the spectrum is

$$\omega + v/2 \pm \sqrt{\gamma^2 + (\omega + v/2)^2},\ \omega\,,\ \omega\,.$$