2 Integrals over Grassmann variables

To construct a consistent quantum theory of *fermionic* fields, the field operators must fulfil the *anti-commutation* relations

$$\big\{\psi_\alpha(x), \psi^\dagger_\beta(y)\big\} = \delta^{(3)}(\vec{x}-\vec{y}\,)\,\delta_{\alpha\beta}\,, \tag{1}$$
$$\big\{\psi_\alpha(x), \psi_\beta(y)\big\} = \big\{\psi^\dagger_\alpha(x), \psi^\dagger_\beta(y)\big\} = 0\,,$$

at equal times $x^0 = y^0$. To construct a path-integral representation of such a theory, one uses *anti-commutating variables*, which are also called Grassmann numbers. They are introduced and explored in this section. We consider a set of n such numbers η_i, $i = 1\ldots n$, which fulfil the Grassmann algebra

$$\big\{\eta_i, \eta_j\big\} = 0\,, \tag{2}$$

implying that $\eta_i^2 = 0$, which makes the algebra extremely simple. The most general function of two Grassmann variables is

$$f(\eta_1, \eta_2) = f_{00} + f_{10}\,\eta_1 + f_{01}\,\eta_2 + f_{11}\,\eta_1\eta_2\,, \tag{3}$$

since $\eta_2\eta_1 = -\eta_1\eta_2$ and all higher-order terms vanish. The expansion coefficients are ordinary numbers. The Taylor expansion of Grassmann functions is thus always finite and exact. In the rest of this section, Latin letters refer to real or complex numbers, Greek letters denote the Grassmann variables.

Exercise 2.1. The Grassmann algebra can be implemented using anti-commutating matrices. Find a 2×2 matrix representation for the case of a single Grassman number.

Exercise 2.2. Argue that the class of matrices found above cannot be used to implement Grassmann algebra for the case of $n = 2$ and find a valid 4×4 matrix representation.
Hint: Consider the ansatz $\eta_1 = \theta_1 \otimes M_1$ and $\eta_2 = M_2 \otimes \theta_2$ where η_i are 2×2 matrices of the form found earlier and M_i are arbitrary 2×2 matrices to be identified.

Exercise 2.3. Equation (3) shows that the $n = 2$ algebra is four-dimensional. What is the dimension for general n?

The integral over a Grassmann function $f(\eta) = a + b\,\eta$ is defined as

$$\int \mathrm{d}\eta\, f(\eta) \equiv b\,. \tag{4}$$

Exercise 2.4. Show that, up to a normalization factor, this definition follows from the requirements of linearity and invariance of the integral under a shift $\eta \to \eta + \theta$.

One can also define the derivative of a Grassmann function as

$$\frac{\partial}{\partial\eta} f(\eta) = \frac{\partial}{\partial\eta}\,(a + b\,\eta) \equiv b\,, \tag{5}$$

which happens to be the same as the integral. For multiple integrals and derivatives one needs to adopt a sign convention. We define

$$\int \mathrm{d}\eta_2 \int \mathrm{d}\eta_1 \, \eta_1 \eta_2 \equiv \frac{\partial}{\partial \eta_2} \frac{\partial}{\partial \eta_1} \eta_1 \eta_2 \equiv +1 \,, \tag{6}$$

i.e. we perform the innermost integral (or derivative) first.

Exercise 2.5. Compute the Gaussian integrals

$$I(A) = \int \mathrm{d}\eta_n \int \mathrm{d}\eta_{n-1} \cdots \int \mathrm{d}\eta_1 \, e^{-\underline{\eta}^T A \underline{\eta}} \,, \tag{7}$$

where $\underline{\eta} = (\eta_1, \ldots, \eta_n)^T$ for $n = 2, 3, 4$. *Hints:* Taylor expand and note that only the terms proportional to $\eta_1 \eta_2 \ldots \eta_n$ contribute, which involve exactly one power of each variable. Note also that A can be chosen anti-symmetric.

Under a variable change $\theta = a\eta$, we have

$$1 = \int \mathrm{d}\theta \, \theta = \int \mathrm{d}(a\eta) \, a\eta \tag{8}$$

$$\Rightarrow \mathrm{d}(a\eta) = \frac{1}{a} \mathrm{d}\eta \,.$$

This is the opposite of the behaviour of regular (bosonic) integrals, where $\mathrm{d}(ax) = a \, \mathrm{d}x$. The Grassmann integral behaves like a derivative under variable transformations, which may not be surprising, since it is the same as the derivative.

Exercise 2.6. For a general variable transformation $\xi_i = B_{ij} \eta_j$, prove that

$$\mathrm{d}\xi_n \ldots \mathrm{d}\xi_1 = (\det B)^{-1} \mathrm{d}\eta_n \ldots \mathrm{d}\eta_1 \,. \tag{9}$$

Hint: proceed as in eq. (8), using $\eta_{i_1} \ldots \eta_{i_n} = \epsilon_{i_1 \ldots i_n} \eta_1 \ldots \eta_n$.

To work with the complex-valued Dirac field, one introduces complex Grassmann variables

$$\eta \equiv \frac{1}{\sqrt{2}} \left(\eta_1 + i\eta_2 \right) \,, \quad \eta^* \equiv \frac{1}{\sqrt{2}} \left(\eta_1 - i\eta_2 \right) \,. \tag{10}$$

One can treat η and η^* as independent variables and define

$$\int \mathrm{d}\eta^* \mathrm{d}\eta \, \eta \, \eta^* \equiv 1 \,. \tag{11}$$

Exercise 2.7. Derive the following identities for Gaussian integrals with complex Grassmann variables:

$$\left(\prod_{i=1}^{n} \int \mathrm{d}\eta_i^* \int \mathrm{d}\eta_i \right) e^{-\underline{\eta}^\dagger A \underline{\eta}} = \det A \,, \tag{12}$$

$$\left(\prod_{i=1}^{n}\int \mathrm{d}\eta_i^* \int \mathrm{d}\eta_i\right) e^{-\underline{\eta}^\dagger A\,\underline{\eta}+\underline{\eta}^\dagger\underline{\theta}+\underline{\theta}^\dagger\underline{\eta}} = \det A\; e^{\underline{\theta}^\dagger A^{-1}\underline{\theta}}\,, \tag{13}$$

for a Hermitian matrix A. *Hint:* Derive eq. (12) by performing a change of variables which diagonalizes A, and complete the square to obtain eq. (13).

Except for the normalization, the only difference to regular (bosonic) Gaussian integrals is the appearance of $\det A$ instead of $(\det A)^{-1}$. As in the bosonic case, all moments can be obtained by taking derivatives of eq. (13) with respect to θ_i and θ_j^*.

Exercise 2.8. Use this technique to compute the integrals

$$\left(\prod_{k=1}^{n}\int \mathrm{d}\eta_k^* \int \mathrm{d}\eta_k\right) e^{-\underline{\eta}^\dagger A\,\underline{\eta}}\,\eta_i\eta_j^*\;, \tag{14}$$

$$\left(\prod_{k=1}^{n}\int \mathrm{d}\eta_k^* \int \mathrm{d}\eta_k\right) e^{-\underline{\eta}^\dagger A\,\underline{\eta}}\,\eta_i\eta_j^*\eta_l\eta_m^*\;. \tag{15}$$

Wick's theorem for Grassmann integrals has thus exactly the same form as in the bosonic case, but one needs to keep track of the minus signs which arise when variables are reordered.

Exercise 2.9. Dual numbers are a special case of Grassman algebra with $n = 1$. They are very useful for being able to compute the derivative of an arbitrary computer code, using a technique known as automatic differentiation. This finds extensive use in machine learning, where the derivative of a loss function with respect to the parameters of a neural network is needed during the training process for implementing the so-called back-propagation algorithm. It also finds many applications in physics for computing Jacobians or gradients of complicated integrands. The core idea of auto-differentiation is to take an existing function defined over real numbers, and change the type of its arguments to dual real numbers, represented with $\bar{x} = c_0 + c_1\varepsilon$. Then the implementation of every elementary operation is defined by the Taylor expansion of the operation truncated to order $\mathcal{O}(\varepsilon)$. For instance, the function redefinition:

`f(x:Float)=x**2` $\rightarrow$ `f(x:Dual<Float>)=x**2`

with $\bar{x}^2$ implemented as $c_0^2 + 2c_0\varepsilon$ allows one to directly obtain the numerical evaluation of the derivative $f'(x)$ by reading the ε coefficient of $f(x+\varepsilon)$. The power of this approach only becomes apparent when realising that this construction satisfies the composition rule and that most complicated functions implemented on a computer are composites of elementary ops.

Compute the derivative of the function $f(x) = x\sin(x)$ using dual numbers and writing it as $f(x) = g_\times(x, s(x))$ with $g_\times(x, y) = xy$ and $s(x) = \sin(x)$.

Exercise 2.10. Find what is the shape of dual numbers necessary to keep track of up to the second derivative in a variable x and up to the first derivative in another variable y. Notice that this more general case of dual numbers is no longer isomorphic to a Grassmann algebra.