Chapter 2
Gaussian Integrals

We must admit with humility that, while number is purely a product of our minds, space has a reality outside our minds, so that we cannot completely prescribe its properties a priori.
– Carl Friedrich Gauss.

In this chapter, we lay the mathematical foundations for the functional-integral formalism that we develop in later chapters. We start with introducing the Gaussian probability distribution together with the corresponding integrals over this distribution, called Gaussian integrals. These concepts are then generalized to higher dimensions, to the complex plane, and to what are called Grassmann variables. The multi-dimensional Gaussian integral is of great importance for the rest of this book. In Chap. 7, we show that it leads to an exact solution of noninteracting quantum gases, which then also forms the basis for a perturbative description of interacting quantum gases. The goal of this chapter is to highlight the practical use of several important mathematical results that are needed to understand the rest of the book. The chapter is not intended to be a full mathematical account of all the above-mentioned topics, meaning that proofs will often be omitted or replaced by illustrative examples. The more experienced reader who is already familiar with Gaussian integrals, complex analysis, and Grassmann algebras, can use this chapter for reference.

2.1 The Gaussian Integral over Real Variables

The Gaussian or normal probability distribution is the most common distribution in statistical physics. The main reason for this is that the probability distribution for the sum of N independent random variables, each with a finite variance, converges for large N to the Gaussian distribution. This is called the central limit theorem of probability theory. Famous physical examples of Gaussian distributions are the Maxwell distribution for the velocities of the atoms in a classical ideal gas, or the spatial distribution for an atom in the quantum-mechanical ground state of a harmonic trap. The Gaussian probability distribution is given by

$$P(x) = \sqrt{\frac{\alpha}{\pi}} \exp\left\{-\alpha x^2\right\}, \tag{2.1}$$

such that it is properly normalized to 1. This follows from

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}, \tag{2.2}$$

which is left as an exercise to the reader. The probability distribution of (2.1) has a maximum at $x = 0$, whereas in general the maximum could be at any arbitrary value x_0. Then, we have

$$P(x) = \sqrt{\frac{\alpha}{\pi}} \exp\left\{-\alpha(x - x_0)^2\right\}, \tag{2.3}$$

which corresponds, for example, to the probability distribution of the velocities in a thermal beam of atoms which is travelling at an average velocity x_0. The latter distribution has the property that the expectation value of the quantity x is equal to x_0, that is

$$\langle x \rangle \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\, x\, P(x) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x\, x\, \exp\left\{-\alpha(x - x_0)^2\right\} = x_0, \tag{2.4}$$

which is easily proven by performing the shift $x \rightarrow x + x_0$.

For our purposes, it is convenient to write the parameter α as $-G^{-1}/2 = -1/2G$, with $G < 0$. In the first instance, this looks overly complicated. However, it establishes a direct link with the notation used in later chapters for the Green's function in the functional-integral formalism. From now on, we also no longer explicitly denote the lower and upper limit of the integration when these are given by $-\infty$ and $+\infty$, respectively. With these changes, the Gaussian integral can be written as

$$\int \mathrm{d}x\, \exp\left\{\frac{1}{2} G^{-1} x^2\right\} = \sqrt{-2\pi G} = \sqrt{2\pi} \exp\left\{-\frac{1}{2}\log\left(-G^{-1}\right)\right\}. \tag{2.5}$$

2.1.1 Generating Function

By including a linear term Jx in the exponent, we introduce the generating function $Z(J)$ of the probability distribution. This is very useful because it allows us to calculate the expectation value of all the higher moments, i.e. the expectation values of x^n, by simply differentiating with respect to the current J. Specifically, we have for the Gaussian distribution

$$\begin{aligned} Z(J) &= \int \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left\{\frac{1}{2} G^{-1}(x - x_0)^2 + Jx\right\} \\ &= \int \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left\{\frac{1}{2} G^{-1}(x + GJ)^2 - \frac{1}{2} GJ^2 + Jx_0\right\} \\ &= \exp\left\{-\frac{1}{2} GJ^2 + Jx_0 - \frac{1}{2}\log\left(-G^{-1}\right)\right\}, \end{aligned} \tag{2.6}$$

where in the first step we performed the shift $x \to x + x_0$ before completing the square. Note that the additional factor $1/\sqrt{2\pi}$ conveniently cancels the factor $\sqrt{2\pi}$ coming from the Gaussian integral. The expectation value of x is now readily calculated from

$$\langle x \rangle = \frac{1}{Z(J)} \frac{\mathrm{d}}{\mathrm{d}J} Z(J) \bigg|_{J=0} = x_0, \tag{2.7}$$

and for $\langle x^2 \rangle$, we obtain

$$\langle x^2 \rangle = \frac{1}{Z(J)} \frac{\mathrm{d}^2}{\mathrm{d}J^2} Z(J) \bigg|_{J=0} = -G + x_0^2 = -G + \langle x \rangle^2. \tag{2.8}$$

Since we can always perform initially the shift $x \to x + x_0$, we consider from now on without loss of generality the case with $x_0 = 0$. A useful observation is that this leads to

$$\langle x^{2m+1} \rangle = 0, \tag{2.9}$$

where m is an integer. This is because the integrand of the integral

$$\int \mathrm{d}x\, x^{2m+1} \exp\left\{ \frac{1}{2} G^{-1} x^2 \right\}$$

is odd and the integral vanishes consequently. By repeatedly applying the derivative $\mathrm{d}/\mathrm{d}J$ an even number of times to the first line of (2.6) with $x_0 = 0$, we find that

$$\langle x^{2m} \rangle = \frac{1}{Z(J)} \frac{\mathrm{d}^{2m}}{\mathrm{d}J^{2m}} Z(J) \bigg|_{J=0}. \tag{2.10}$$

Explicitly calculating the right-hand side of (2.10), using the expression in the last line of (2.6), generates a large number of terms that vanish when we eventually take the limit $J \to 0$. To simplify the calculation, it is therefore convenient to realize that if we expand $Z(J)$ in powers of J only the terms proportional to J^{2m} contribute. In this manner, we find for $x_0 = 0$ that

$$\begin{aligned} \frac{1}{Z(J)} \frac{\mathrm{d}^{2m}}{\mathrm{d}J^{2m}} Z(J) \bigg|_{J=0} &= \frac{Z(0)}{Z(J)} \frac{\mathrm{d}^{2m}}{\mathrm{d}J^{2m}} \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{1}{2} G J^2 \right)^n \bigg|_{J=0} \\ &= \frac{(2m)!}{2^m m!} (-G)^m = (2m-1)!!(-G)^m, \end{aligned} \tag{2.11}$$

where $(2m-1)!! = (2m-1)(2m-3)(2m-5)\ldots 1$. Hence, we conclude that

$$\langle x^{2m} \rangle = (2m-1)!!(-G)^m. \tag{2.12}$$

It is important to realize that $(2m-1)!!$ is exactly the number of ways in which $2m$ numbers can be divided into m pairs. Thus, we have found that the expectation value of x^{2m} is equal to the sum of all possible ways in which $\langle x^{2m} \rangle$ can be factorized as

$\langle x^2 \rangle^m$. This last statement is the essence of the famous Wick's theorem that will turn out to be of great importance in later chapters.

2.1.2 Multi-Dimensional Gaussian Integral

The previous results can be immediately generalized to higher-dimensional integrals. Consider a diagonal $n \times n$ matrix $\mathbf{G}$,

$$\mathbf{G} = \begin{bmatrix} G_{11} & & & \\ & G_{22} & & \\ & & G_{33} & \\ & & & \ddots \end{bmatrix}, \tag{2.13}$$

with again $G_{jj} < 0$. Then, the inverse $\mathbf{G}^{-1}$ of $\mathbf{G}$ is clearly given by

$$\mathbf{G}^{-1} = \begin{bmatrix} \frac{1}{G_{11}} & & & \\ & \frac{1}{G_{22}} & & \\ & & \frac{1}{G_{33}} & \\ & & & \ddots \end{bmatrix}. \tag{2.14}$$

We want to evaluate the Gaussian integral

$$\int \left(\prod_{j=1}^{n} \mathrm{d}x_j \right) \exp\left\{ \frac{1}{2} \mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x} \right\} \equiv \int \mathrm{d}\mathbf{x} \exp\left\{ \frac{1}{2} \mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x} \right\}, \tag{2.15}$$

where $\mathbf{x}$ denotes the vector $(x_1, x_2, \ldots, x_n)$. Because the integral factorizes into a product of n one-dimensional integrals, we find that

$$\int \mathrm{d}\mathbf{x} \exp\left\{ \frac{1}{2} \mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x} \right\} = \frac{(2\pi)^{n/2}}{\sqrt{\prod_{j=1}^{n} (-G_{jj}^{-1})}} = \frac{(2\pi)^{n/2}}{\sqrt{\mathrm{Det}[-\mathbf{G}^{-1}]}}, \tag{2.16}$$

where $\mathrm{Det}[-\mathbf{G}^{-1}]$ denotes the determinant of the matrix $-\mathbf{G}^{-1}$. In the same way we find that (2.6) generalizes to

$$\begin{aligned} Z(\mathbf{J}) &= \int \frac{\mathrm{d}\mathbf{x}}{\sqrt{(2\pi)^n}} \exp\left\{ \frac{1}{2} \mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x} + \mathbf{J} \cdot \mathbf{x} \right\} \\ &= \exp\left\{ -\frac{1}{2} \mathbf{J} \cdot \mathbf{G} \cdot \mathbf{J} - \frac{1}{2} \mathrm{Tr}[\log(-\mathbf{G}^{-1})] \right\}, \end{aligned} \tag{2.17}$$

where we have taken again without loss of generality $\mathbf{x}_0 = \mathbf{0}$. Here $\mathrm{Tr}[\ldots]$ denotes the trace of a matrix, which is the sum of all diagonal elements. The n-th order correlation function $\langle x_{j_1} x_{j_2} \dots x_{j_n} \rangle$, given by the expectation value of the product of n coordinates x_j, is now easily calculated from

$$\langle x_{j_1} \dots x_{j_n} \dots \rangle = \frac{1}{Z(\mathbf{J})} \frac{\partial^n}{\partial J_{j_1} \dots \partial J_{j_n}} Z(\mathbf{J}) \bigg|_{\mathbf{J}=0} . \tag{2.18}$$

Example 2.1. Because $Z(\mathbf{J})$ depends quadratically on $\mathbf{J}$, it immediately follows that

$$\langle x_i \rangle = \frac{1}{Z(\mathbf{J})} \frac{\partial}{\partial J_i} Z(\mathbf{J}) \bigg|_{\mathbf{J}=0} = 0. \tag{2.19}$$

For the expectation value $\langle x_i x_j \rangle$, we find

$$\langle x_i x_j \rangle = \frac{1}{Z(\mathbf{J})} \frac{\partial^2}{\partial J_i \partial J_j} Z(\mathbf{J}) \bigg|_{\mathbf{J}=0} = -G_{ij}. \tag{2.20}$$

The above results were obtained for the specific case of a diagonal matrix. However, (2.17) is valid for any positive definite, symmetric matrix $-\mathbf{G}^{-1}$, where positive definite means that the matrix has only positive eigenvalues. First, note that $-\mathbf{G}^{-1}$ can always be assumed to be symmetric, because any antisymmetric part would give a vanishing contribution to the term $-\mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x}$. Then, a symmetric matrix can always be brought into diagonal form by a similarity transformation $\mathbf{S}$, which means that $\mathbf{S} \cdot \mathbf{G}^{-1} \cdot \mathbf{S}^{-1}$ is diagonal and $\mathbf{S}$ is orthonormal. Orthonormality implies that

$$|\mathrm{Det}[\mathbf{S}]| = 1, \tag{2.21}$$

such that the Jacobian of the coordinate transformation $\mathbf{x} = \mathbf{S}^{-1} \cdot \mathbf{x}'$ is equal to one. Applying the above considerations to (2.17), we have

$$\begin{aligned} Z(\mathbf{J}) &= \int \frac{d\mathbf{x}'}{\sqrt{(2\pi)^n}} \exp\left\{ \frac{1}{2} \mathbf{x}' \cdot \mathbf{S} \cdot \mathbf{G}^{-1} \cdot \mathbf{S}^{-1} \cdot \mathbf{x}' + \mathbf{J} \cdot \mathbf{S}^{-1} \cdot \mathbf{x}' \right\} \\ &= \exp\left\{ -\frac{1}{2} \mathbf{J} \cdot \mathbf{S}^{-1} \cdot \mathbf{S} \cdot \mathbf{G} \cdot \mathbf{S}^{-1} \cdot \mathbf{S} \cdot \mathbf{J} \right\} \frac{1}{\sqrt{\mathrm{Det}[-\mathbf{S} \cdot \mathbf{G}^{-1} \cdot \mathbf{S}^{-1}]}} \\ &= \exp\left\{ -\frac{1}{2} \mathbf{J} \cdot \mathbf{G} \cdot \mathbf{J} \right\} \frac{1}{\sqrt{\mathrm{Det}[-\mathbf{G}^{-1}]}}, \end{aligned} \tag{2.22}$$

where we also used the property that for an orthogonal matrix the inverse matrix and the transposed matrix are the same. Thus, we find that (2.17) is valid for any positive definite matrix $-\mathbf{G}^{-1}$.

2.2 Complex Analysis

In the following, we generalize the results of the previous paragraph to Gaussian integrals over n complex variables z_j. Before doing so, we first review some concepts from elementary complex analysis. The complex plane is a two-dimensional linear space, meaning that any number in the complex plane can be written as $x+\mathrm{i}y$, where x and y are real. Instead of using x and y as the independent variables to parametrize the complex plane, it is more convenient for our purposes to make a coordinate transformation that maps x and y onto the independent variables z and z^* in the following way

$$z = x+\mathrm{i}y \qquad \text{and} \qquad z^* = x-\mathrm{i}y. \tag{2.23}$$

Here, $|z|^2 = z^*z = x^2+y^2$ gives the square of the modulus of z, while the real and imaginary parts of z are given by $\mathrm{Re}[z] = (z+z^*)/2$ and $\mathrm{Im}[z] = (z-z^*)/2\mathrm{i}$. Instead of using the Cartesian coordinates x and y, it is also possible to introduce polar coordinates. In that case, complex numbers are written as

$$z = r\mathrm{e}^{\mathrm{i}\varphi}, \tag{2.24}$$

where $r = \sqrt{z^*z}$ is the complex modulus and $\varphi = \mathrm{Arg}[z]$ is the complex argument.

2.2.1 Differentiation and Contour Integrals

A general complex function $f(x,y)$ is a map from the complex plane to the complex plane and in general depends explicitly on both z and z^*. We write $f(x,y) = u(x,y) + \mathrm{i}v(x,y)$, where $u(x,y) = \mathrm{Re}[f(x,y)]$ and $v(x,y) = \mathrm{Im}[f(x,y)]$. In practise we will be dealing mostly with analytic functions, which turn out to depend only explicitly on $z = x+\mathrm{i}y$. Because such a function $f(x+\mathrm{i}y)$ or $f(z)$ only depends on z, we must have that $\mathrm{d}f/\mathrm{d}z = \partial f/\partial x = -\mathrm{i}\partial f/\partial y$ for an analytic function. Since

$$\frac{\partial f(x,y)}{\partial x} = \frac{\partial u(x,y)}{\partial x} + \mathrm{i}\frac{\partial v(x,y)}{\partial x} \tag{2.25}$$

and

$$-\mathrm{i}\frac{\partial f(x,y)}{\partial y} = -\mathrm{i}\frac{\partial u(x,y)}{\partial y} + \frac{\partial v(x,y)}{\partial y}, \tag{2.26}$$

we have that the functions u and v are not independent, but rather satisfy the following set of equations

$$\frac{\partial u(x,y)}{\partial x} = \frac{\partial v(x,y)}{\partial y} \qquad \text{and} \qquad \frac{\partial u(x,y)}{\partial y} = -\frac{\partial v(x,y)}{\partial x}. \tag{2.27}$$

These equations are known as the Cauchy-Riemann equations and satisfying them assures differentiability of the complex function.

Example 2.2. To explicitly demonstrate the use of the Cauchy-Riemann equations, we test for two simple complex functions whether or not they are analytic functions. First, consider the complex function $f(x,y) = x + \mathrm{i}y = z$, i.e. $u(x,y) = x$ and $v(x,y) = y$. Clearly it satisfies the Cauchy-Riemann equations, since $\partial u/\partial x = 1 = \partial v/\partial y$ and $\partial u/\partial y = 0 = -\partial v/\partial x$. However, the complex conjugate $f(x,y) = x - \mathrm{i}y = z^*$ is not analytic, because it does not satisfy the Cauchy-Riemann equations. Indeed, we have $\partial u/\partial x = 1 \neq -1 = \partial v/\partial y$. This illustrates the above statement that functions depending explicitly on z^* are not analytic.

Besides being able to take the derivative of a complex function we also want to be able to integrate it. In principle, the integral of a general complex function between two points in the complex plane depends on the specific path taken. However, if the function $f(z)$ satisfies the Cauchy-Riemann equations in all points enclosed by two different paths connecting z_i and z_f, then the integral $\int_{z_\mathrm{i}}^{z_\mathrm{f}} \mathrm{d}z f(z)$ gives the same result for each of the two paths. This leads directly to the Cauchy-Goursat theorem, stating that for any function f which is analytic on a closed contour C and at all points inside the contour, the integral along the contour vanishes, i.e.

$$\oint_C \mathrm{d}z\, f(z) = 0. \tag{2.28}$$

We will not prove this theorem here, but we give a simple demonstration in Example 2.3. With the Cauchy-Goursat theorem, it is then possible to prove the important Cauchy integral formula

$$f(z_0) = \frac{1}{2\pi\mathrm{i}} \oint_C \mathrm{d}z \frac{f(z)}{z - z_0}, \tag{2.29}$$

where the integration over the contour C is in a counterclockwise fashion. This will always be the convention for contour integration from now on.

Example 2.3. Consider the function $f(z) = z$, and let the contour C be the circle centered at $z = 0$ with radius R. The circle is parameterized by $z = R\mathrm{e}^{\mathrm{i}\phi}$, where φ runs counterclockwise from 0 to 2π. Hence, $\mathrm{d}z = \mathrm{i}R\mathrm{e}^{\mathrm{i}\varphi}\mathrm{d}\varphi$ and we find

$$\oint_C \mathrm{d}z\, z = \int_0^{2\pi} \mathrm{d}\varphi\; \mathrm{i}R^2 \mathrm{e}^{2\mathrm{i}\varphi} = \frac{R^2}{2}\mathrm{e}^{2\mathrm{i}\varphi}\Big|_0^{2\pi} = 0. \tag{2.30}$$

This illustrates the Cauchy-Goursat theorem. Consider in (2.29) the function $f(z) = 1$ and take for the contour C the circle based at z_0 with radius R. We obtain

$$\frac{1}{2\pi i}\oint_C dz\,\frac{f(z)}{z-z_0} = \frac{1}{2\pi i}\int_0^{2\pi} d\varphi\,\frac{iRe^{i\varphi}}{Re^{i\varphi}} = 1 = f(z_0). \tag{2.31}$$

This illustrates the Cauchy integral formula.

The Cauchy integral formula can be used to express the derivatives of a complex function in terms of a contour integral. By differentiating both sides of (2.29) n times with respect to z_0, we obtain

$$\frac{d^n}{dz_0^n} f(z_0) = \frac{n!}{2\pi i}\oint_C dz \frac{f(z)}{(z-z_0)^{n+1}}. \tag{2.32}$$

2.2.2 Laurent Series and the Residue Theorem

For a function $f(x)$ that depends on the real variable x, it is possible to make a Taylor series expansion around the nonsingular point x_0, i.e.

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x-x_0)^n, \tag{2.33}$$

where $f^{(n)}(x) = d^n f(x)/dx^n$ and where we assumed that the sum on the right-hand side converges. A similar expansion holds for complex functions that are analytic throughout the interior of a circle centered at z_0 with radius R. In that case, the function can be written as

$$f(z) = \sum_{n=0}^{\infty} \frac{f^{(n)}(z_0)}{n!}(z-z_0)^n. \tag{2.34}$$

Now, suppose that we have a function that is singular at a single point z_0 that lies within a circle centered at z_0 and with radius R_1, as is illustrated in Fig. 2.1. We call S the region enclosed by the circle excluding the singular point z_0. For each point z that lies within S, the function $f(z)$ is given by

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z-z_0)^n, \tag{2.35}$$

where the coefficients are given by

$$a_n = \frac{1}{2\pi i}\oint_C dz\,\frac{f(z)}{(z-z_0)^{n+1}}, \tag{2.36}$$

and C is any contour that encloses z_0 and lies within S. This series expansion is also known as the Laurent series expansion. The coefficient a_{-1}, which is the integral of

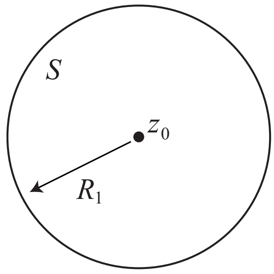

Fig. 2.1 Laurent series expansion. The region S is enclosed by a circle with radius R_1 that is centered at z_0, but excludes the point z_0 itself.

$f(z)$ along the contour C, is called the residue of f at the singular point z_0

$$a_{-1} = \frac{1}{2\pi \mathrm{i}} \oint_C f(z)\mathrm{d}z \equiv \mathrm{Res}[f(z_0)]. \tag{2.37}$$

For our purpose, analytic functions that have the following expansion in terms of a Laurent series are most relevant

$$f(z) = \sum_{n=-m}^{\infty} a_n (z - z_0)^n, \tag{2.38}$$

and the singularity at $z = z_0$ is called a pole of order m. For the residue, this leads to

$$\mathrm{Res}[f(z_0)] = \frac{1}{(m-1)!} \lim_{z \to z_0} \frac{\mathrm{d}^{m-1}}{\mathrm{d}z^{m-1}} \left((z - z_0)^m f(z)\right). \tag{2.39}$$

The concept of the residue allows for a generalization of Cauchy's integral formula of (2.29) to any contour enclosing a finite number of finite-order poles. This leads to the residue theorem, that is

$$\oint_C \mathrm{d}z\, f(z) = 2\pi \mathrm{i} \sum_j \mathrm{Res}[f(z_j)]. \tag{2.40}$$

Example 2.4. The function $f(z) = 1/((1 - \mathrm{i}z)(1 + \mathrm{i}z))$ is not analytic in $z = \pm \mathrm{i}$. To find the Laurent series expansion of $f(z)$ at $z = \mathrm{i}$, we start by writing

$$\frac{1}{1 + \mathrm{i}z} = -\mathrm{i}(z - \mathrm{i})^{-1}. \tag{2.41}$$

Moreover, the Taylor series of the term $1/(1 - \mathrm{i}z)$ is given by,

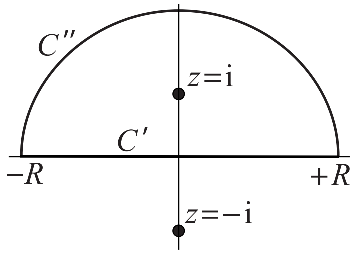

Fig. 2.2 Illustration of the contour $C = C' + C''$ used in Example 2.5.

$$\frac{1}{1-\mathrm{i}z} = \sum_{n=0}^{\infty} \frac{1}{2^{(n+1)}} \mathrm{i}^n (z-\mathrm{i})^n. \tag{2.42}$$

Multiplying the two terms gives the Laurent series of the function $f(z)$,

$$\begin{aligned} f(z) &= -\sum_{n=0}^{\infty} \left(\frac{\mathrm{i}}{2}\right)^{n+1} (z-\mathrm{i})^{n-1} \\ &= \sum_{n=-1}^{\infty} a_n (z-\mathrm{i})^n, \end{aligned} \tag{2.43}$$

where $a_n = -(\mathrm{i}/2)^{n+2}$. This shows that the residue is equal to $a_{-1} = -\mathrm{i}/2$.

Example 2.5. Suppose we want to calculate the following integral along the real axis

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \frac{1}{1+x^2}.$$

This is a standard integral whose answer is known to be $\arctan x|_{-\infty}^{+\infty} = \pi$. Now we show how we can also obtain this result by making use of the residue theorem. We start by extending the function $f(x) = 1/(1+x^2)$ on the real axis to the function $f(z)$ in the complex plane, such that

$$f(z) = \frac{1}{(z+\mathrm{i})(z-\mathrm{i})}. \tag{2.44}$$

This function has poles in the complex plane at $z = \pm\mathrm{i}$. To be able to apply the residue theorem, we use the contour C shown in Fig. 2.2. It is the union of the line C', which is the part of the real axis from $-R$ to $+R$, and C'', which is the semicircle in the upper half-plane centered at zero with radius R. Our original integral can be obtained by taking the limit $R \to \infty$ and subtracting the integral along the path C''. Due to the residue theorem, we have that

$$\oint_C \mathrm{d}z \, f(z) = 2\pi\mathrm{i} \, \mathrm{Res}[f(z=\mathrm{i})] = \pi. \tag{2.45}$$

The contour integral along the semicircle C'' vanishes in the limit $R \to \infty$, since

$$\lim_{R\to\infty} \int_{C''} \mathrm{d}z \, \frac{1}{1+z^2} = \lim_{R\to\infty} \int_0^{\pi} \mathrm{d}\varphi \, \frac{\mathrm{i}}{R\mathrm{e}^{\mathrm{i}\varphi}} = 0. \tag{2.46}$$

As a result, we see that we retrieve the original answer, as desired.

2.3 Gaussian Integrals over Complex Variables

In this section, we generalize the results that we obtained for the Gaussian integral along the real axis in (2.5) to integrations over the complex plane. We assume that the complex number G^{-1} has a real part that is less than zero. We find

$$\begin{aligned} \int \mathrm{d}z^*\mathrm{d}z \, \exp\left\{G^{-1}z^*z\right\} &\equiv \int \frac{\partial(z^*,z)}{\partial(x,y)} \mathrm{d}x \, \mathrm{d}y \, \exp\left\{G^{-1}(x^2+y^2)\right\} \\ &= \int \mathrm{d}x \, \mathrm{d}y \, 2\mathrm{i} \exp\left\{G^{-1}x^2\right\} \exp\left\{G^{-1}y^2\right\} \\ &= -2\pi\mathrm{i}G, \end{aligned} \tag{2.47}$$

where the integral is over the full complex plane. The coordinate transformation of (2.23) that maps x and y onto z^* and z, also defines the measure $\mathrm{d}z^*\mathrm{d}z$ through the relation

$$\mathrm{d}z^*\mathrm{d}z \equiv \frac{\partial(z^*,z)}{\partial(x,y)} \mathrm{d}x \, \mathrm{d}y = 2\mathrm{i} \, \mathrm{d}x \, \mathrm{d}y, \tag{2.48}$$

where in the last step we explicitly calculated the Jacobian of the coordinate transformation. Just like in the real case, we can add a linear term $z^*J + J^*z$ to the exponent of the Gaussian integral and define the generating function

$$\begin{aligned} Z(J,J^*) &= \int \frac{\mathrm{d}z^*\mathrm{d}z}{2\pi\mathrm{i}} \, \exp\left\{G^{-1}z^*z + z^*J + J^*z\right\} \\ &= \exp\left\{-J^*GJ - \log\left(-G^{-1}\right)\right\}, \end{aligned} \tag{2.49}$$

which is shown by completing the square. As before, we can calculate all moments with this generating function, such that we have for example

$$\langle zz^* \rangle = \frac{1}{Z(J,J^*)} \frac{\mathrm{d}^2}{\mathrm{d}J^*\mathrm{d}J} Z(J,J^*) \bigg|_{J^*=J=0} = -G. \tag{2.50}$$

Next, consider the diagonal $n \times n$ matrix $\mathbf{G}^{-1}$, i.e.

$$\mathbf{G}^{-1} = \begin{bmatrix} \frac{1}{G_{11}} & & & \\ & \frac{1}{G_{22}} & & \\ & & \frac{1}{G_{33}} & \\ & & & \ddots \end{bmatrix}. \tag{2.51}$$

We want to evaluate the Gaussian integral

$$\int \left(\prod_{j=1}^{n} \frac{\mathrm{d}z_j^* \, \mathrm{d}z_j}{2\pi \mathrm{i}} \right) \exp\left\{ \mathbf{z}^* \cdot \mathbf{G}^{-1} \cdot \mathbf{z} \right\} \equiv \int \frac{\mathrm{d}\mathbf{z}^* \mathrm{d}\mathbf{z}}{(2\pi \mathrm{i})^n} \exp\left\{ \mathbf{z}^* \cdot \mathbf{G}^{-1} \cdot \mathbf{z} \right\}, \tag{2.52}$$

where $\mathbf{z}$ is the complex vector $(z_1, \ldots, z_n)$. As before, the integral factorizes and we find that

$$\int \frac{\mathrm{d}\mathbf{z}^* \mathrm{d}\mathbf{z}}{(2\pi \mathrm{i})^n} \exp\left\{ \mathbf{z}^* \cdot \mathbf{G}^{-1} \cdot \mathbf{z} \right\} = \frac{1}{\prod_{j=1}^{n} (-G_{jj}^{-1})} = \frac{1}{\mathrm{Det}[-\mathbf{G}^{-1}]}. \tag{2.53}$$

Now, we can also generalize (2.49) to

$$\begin{aligned} Z(\mathbf{J}, \mathbf{J}^*) &= \int \frac{\mathrm{d}\mathbf{z}^* \mathrm{d}\mathbf{z}}{(2\pi \mathrm{i})^n} \exp\left\{ \mathbf{z}^* \cdot \mathbf{G}^{-1} \cdot \mathbf{z} + \mathbf{z}^* \cdot \mathbf{J} + \mathbf{J}^* \cdot \mathbf{z} \right\} \\ &= \exp\left\{ -\mathbf{J}^* \cdot \mathbf{G} \cdot \mathbf{J} - \mathrm{Tr}[\log(-\mathbf{G}^{-1})] \right\}. \end{aligned} \tag{2.54}$$

The above results were obtained for the specific case of a diagonal matrix. However, (2.54) is true for all positive definite hermitian matrices $-\mathbf{G}^{-1}$, because these can be diagonalized by a unitary transformation $\mathbf{U}$ with $|\mathrm{Det}[\mathbf{U}]| = 1$.

2.4 Grassmann Variables

To complete our discussion of Gaussian integrals we introduce another set of numbers, namely the set of anticommuting complex numbers or Grassmann numbers. These turn out to be very useful in setting up the functional-integral formalism for fermionic quantum gases. The reason for this is that, as we see later, fermionic behavior is mathematically expressed by anticommuting creation and annihilation operators. To illustrate this we note that if a fermionic creation operator anticommutes with itself then its square gives zero, which expresses the Pauli principle that two fermions cannot be created in the same quantum state. In order to consider eigenvalues of such anticommuting operators we need anticommuting numbers, i.e. the Grassmann numbers.

A Grassmann algebra is a set of Grassmann variables, which are called the generators of the algebra. They span a complex linear space by making linear combinations of them with complex coefficients. The simplest example that we can think of is the set $\{1, \phi\}$. By definition, we have for a Grassmann variable ϕ that its anticommutator vanishes, i.e. $[\phi, \phi]_+ = \phi\phi + \phi\phi = 0$. We can think of the elements

1 and ϕ as basis vectors of a linear space. However, in order to find a matrix representation of the algebra, it is actually more convenient to think of the elements also as operators. For instance, since we have that $1 \cdot 1 = 1$ and $1 \cdot \phi = \phi$, we see that 1 can be viewed as an operator on the Grassmann algebra that sends both 1 and ϕ to themselves. The element ϕ then sends the basis vector 1 to ϕ, while the other basis vector ϕ is mapped onto 0. In terms of matrices, the above mappings of basis vectors are readily found in matrix form as

$$1 \sim \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \phi \sim \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}. \tag{2.55}$$

Note that the above matrices automatically satisfy all rules imposed on the algebra. Furthermore, since $\phi^2 = 0$, the most general function of ϕ is simply $F(\phi) = f_1 + f_2\phi$.

The previous discussion is easily generalized to the set $\{1, \phi, \phi^*, \phi^*\phi\}$ of two such Grassmann variables, where ϕ and ϕ^* are independent variables. The two Grassmann variables anticommute with each other, giving

$$[\phi, \phi^*]_+ = \phi\phi^* + \phi^*\phi = 0. \tag{2.56}$$

As before, we also have that $\phi^2 = \phi^{*2} = 0$, such that the above set is complete. The complex conjugation in this algebra is defined by

$$(\phi)^* = \phi^*, \qquad (\phi^*)^* = \phi, \qquad (\phi^*\phi)^* = (\phi)^*(\phi^*)^* = \phi^*\phi, \tag{2.57}$$

and the most general function on this algebra yields

$$A(\phi^*, \phi) = a_{11} + a_{12}\phi + a_{21}\phi^* + a_{22}\phi^*\phi\ . \tag{2.58}$$

It is natural to define differentiation of Grassmann variables by

$$\frac{\partial}{\partial \phi} A(\phi^*, \phi) = a_{12} - a_{22}\phi^*, \tag{2.59}$$

where the minus sign occurs because we need to permute ϕ^* and ϕ before we can differentiate with respect to ϕ. The differentiation of (2.59) is called a left differentiation. Similarly, we have

$$\frac{\partial}{\partial \phi^*} A(\phi^*, \phi) = a_{21} + a_{22}\phi, \tag{2.60}$$

where this time the minus sign is absent, because now we do not have to permute the Grassmann variables. Furthermore, we find

$$\frac{\partial^2}{\partial \phi^* \partial \phi} A(\phi^*, \phi) = -\frac{\partial^2}{\partial \phi \partial \phi^*} A(\phi^*, \phi) = -a_{22}\ . \tag{2.61}$$

Next, we introduce integration over the Grassmann variables. Note that since $\phi^2 = 0$, we only have two possible integrals to consider, namely $\int d\phi\ 1$ and $\int d\phi\ \phi$. We define these by

$$\int d\phi\ 1 = 0 \tag{2.62}$$

and

$$\int d\phi\ \phi = 1\ . \tag{2.63}$$

This means that integration is equivalent to differentiation. The main reason for the above definitions is that we want the integration to obey the rules of partial integration. In particular, this implies that

$$\int d\phi\ \frac{\partial F(\phi)}{\partial \phi} = 0\ , \tag{2.64}$$

for any function $F(\phi) = f_1 + f_2\phi$. Obviously, this condition requires that $\int d\phi\ 1 = 0$. The result for $\int d\phi\ \phi$ then turns out to be merely a question of normalization. The most general quadratic integral for the present Grassmann algebra thus yields

$$\int d\phi^* d\phi\ A(\phi^*, \phi) = \int d\phi^* d\phi\ (a_{11} + a_{12}\phi + a_{21}\phi^* + a_{22}\phi^*\phi) = -a_{22}\ . \tag{2.65}$$

All the above definitions are then readily further generalized to the Grassmann algebra generated by the Grassmann variables ϕ_j and ϕ_j^* with $j = 1, 2, \ldots, n$. It is left as an exercise to show that with the above definitions, the Gaussian integral over $2n$ Grassmann variables leads to

$$\int \left(\prod_j d\phi_j^* d\phi_j \right)\ \exp\left\{ \sum_{j,j'} \phi_j^* G^{-1}_{j,j'} \phi_{j'} \right\} = \mathrm{Det}[-\mathbf{G^{-1}}] = e^{\mathrm{Tr}[\log(-\mathbf{G^{-1}})]}\ . \tag{2.66}$$

Note the difference with the result from (2.54), namely

$$\int \left(\prod_j \frac{d\phi_j^* d\phi_j}{2\pi i} \right)\ \exp\left\{ \sum_{j,j'} \phi_j^* G^{-1}_{j,j'} \phi_{j'} \right\} = \frac{1}{\mathrm{Det}[-\mathbf{G^{-1}}]} = e^{-\mathrm{Tr}[\log(-\mathbf{G^{-1}})]}\ , \tag{2.67}$$

which is valid for ordinary complex variables. These last two results will be used extensively throughout the rest of the book.

2.5 Problems

Exercise 2.1. Prove the Gaussian integral in (2.2). To do so, consider

$$\left(\int dx\ e^{-\alpha x^2} \right)^2 = \int dx\ dy\ e^{-\alpha(x^2+y^2)}, \tag{2.68}$$

and make use of the fact that the integrand is invariant under rotations, so that you can use polar coordinates to perform the integration.

Exercise 2.2. Consider a Gaussian probability distribution with nonzero average $\langle x\rangle = x_0$. Calculate $\langle x^3\rangle$ and $\langle x^4\rangle$ by transforming to the variable $x' = x - x_0$ that has a Gaussian probability distribution centered around zero, such that you can use (2.9) and (2.12). Also calculate $\langle x^3\rangle$ and $\langle x^4\rangle$ by making use of the generating function from (2.6), namely

$$Z(J) = \exp\left\{-\frac{1}{2}GJ^2 + x_0 J - \frac{1}{2}\log\left(-G^{-1}\right)\right\}. \tag{2.69}$$

Exercise 2.3. Observe that partial integration of the Gaussian integral leads to the following identity,

$$\int \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left\{\frac{1}{2}G^{-1}x^2\right\} = -\int \frac{\mathrm{d}x}{\sqrt{2\pi}} G^{-1}x^2 \exp\left\{\frac{1}{2}G^{-1}x^2\right\}. \tag{2.70}$$

Prove now equation (2.12) by making repeated use of partial integration.

Exercise 2.4. Prove that

$$\oint_C \mathrm{d}z \frac{1}{(z-z_0)^{n+1}} = 2\pi \mathrm{i}\delta_{n,0} \tag{2.71}$$

by taking the contour C to be a circle with radius R around z_0, such that $z = z_0 + R\mathrm{e}^{\mathrm{i}\varphi}$ and the contour integral becomes an integral over φ.

Exercise 2.5. Contour integration
Using contour integration, show
(a) that the following one-dimensional integral yields

$$\int \mathrm{d}q \, \frac{1}{E^+ - q^2/m} \mathrm{e}^{\mathrm{i}qx/\hbar} = -\mathrm{i}\pi\sqrt{\frac{m}{E}} \exp\left\{\frac{\mathrm{i}|x|\sqrt{mE}}{\hbar}\right\}, \tag{2.72}$$

where $E^+ = E + \mathrm{i}\eta$ with η an infinitesimally small positive number, and
(b) that the following three-dimensional integral yields

$$\int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{\alpha^2 + \gamma\mathbf{k}^2} = \frac{1}{4\pi\gamma}\frac{\mathrm{e}^{-r/\xi}}{r}, \tag{2.73}$$

where $\xi = \sqrt{\gamma}/\alpha$ is also called the correlation length. Hint: use spherical coordinates $\mathrm{d}\mathbf{k} = k^2\sin(\vartheta)\,\mathrm{d}k\,\mathrm{d}\vartheta\,\mathrm{d}\varphi$, such that $\mathbf{k}\cdot\mathbf{r} = kr\cos(\vartheta)$, and perform the integrations over the angles first.

Exercise 2.6. Find a matrix representation of the Grassmann algebra generated by ϕ and ϕ^*. Note that we need at least 4×4 matrices.

Exercise 2.7. Prove (2.66). To this end, it is instructive to first show that

$$\int \mathrm{d}\phi_1^* \,\mathrm{d}\phi_1 \,\mathrm{d}\phi_2^* \,\mathrm{d}\phi_2 \,\exp\{-\alpha_{11}\phi_1^*\phi_1 - \alpha_{12}\phi_1^*\phi_2 - \alpha_{21}\phi_2^*\phi_1 - \alpha_{22}\phi_2^*\phi_2\} = \alpha_{11}\alpha_{22} - \alpha_{21}\alpha_{12}, \tag{2.74}$$

before considering the general case of an integral over $2n$ Grassmann variables.

Exercise 2.8. Hubbard-Stratonovich Transformation
Consider the following integral Z over the complex variables ϕ_j^* and ϕ_j,

$$Z = \int \left(\prod_{j=1}^{n} \frac{\mathrm{d}\phi_j^* \mathrm{d}\phi_j}{2\pi \mathrm{i}}\right) \exp\left\{\sum_{j,j'=1}^{n} \left(\phi_j^* G_{0;j,j'}^{-1}\phi_{j'} - \frac{V_{j,j'}}{2}\phi_j^*\phi_{j'}^*\phi_{j'}\phi_j\right)\right\}, \tag{2.75}$$

where $\mathbf{G}_0^{-1}$ and $\mathbf{V}$ are invertible matrices with only negative eigenvalues, i.e.

$$\sum_{j''} V_{j,j''}V_{j'',j'}^{-1} = \sum_{j''} G_{0;j,j''}^{-1} G_{0;j'',j'} = \delta_{j,j'}. \tag{2.76}$$

Note that we cannot calculate the integral exactly, because it is not Gaussian, due to the quartic term in the exponential. However, we are going to perform a trick to transform the quartic term away.
(a) Show that the integral Z can be written as

$$Z = \int \left(\prod_{j=1}^{n} \frac{\mathrm{d}\phi_j^* \,\mathrm{d}\phi_j}{2\pi \mathrm{i}}\right)\left(\prod_{j=1}^{n} \frac{\mathrm{d}\eta_j}{\sqrt{2\pi}}\right) \exp\left\{\frac{1}{2}\mathrm{Tr}[\log(-\mathbf{V})]\right\} \tag{2.77}$$
$$\times \exp\left\{\sum_{j,j'}\left(\phi_j^* G_{0;j,j'}^{-1}\phi_{j'} + \frac{1}{2}\eta_j V_{j,j'}\eta_{j'} - \eta_j V_{j,j'}\phi_{j'}^*\phi_{j'}\right)\right\},$$

where η is a real variable. Note that there is no longer a quartic term, since we have transformed it away. This is the essence of the Hubbard-Stratonovich transformation, which we use many times when treating interacting quantum gases.
Hint: use the following identity

$$\int \left(\prod_{j=1}^{n} \frac{\mathrm{d}\eta_j}{\sqrt{2\pi}}\right) \exp\left\{\frac{1}{2}\sum_{j,j'}\left(\eta_j - \phi_j^*\phi_j\right)V_{j,j'}\left(\eta_{j'} - \phi_{j'}^*\phi_{j'}\right)\right\} = \mathrm{e}^{-\mathrm{Tr}[\log(-\mathbf{V})]/2}.$$

(b) Show that Z can be written in the following way

$$Z = \mathrm{e}^{\mathrm{Tr}[\log(-\mathbf{V})]/2} \int \left(\prod_{j=1}^{n} \frac{\mathrm{d}\eta_j}{\sqrt{2\pi}}\right) \exp\left\{\frac{1}{2}\sum_{j,j'}\eta_j V_{j,j'}\eta_{j'} - \mathrm{Tr}\left[\log\left(-\mathbf{G}_0^{-1} + \mathbf{\Sigma}\right)\right]\right\},$$

where we introduced the matrix $\Sigma_{j,j'} = \sum_{j''}\eta_{j''}V_{j'',j'}\delta_{j,j'}$.

Additional Reading

- S. Hassani, *Mathematical Physics, A Modern Introduction to Its Foundations*, (Springer-Verlag, Berlin, 1999).
- A mathematically concise textbook on many-particle systems is J. W. Negele and H. Orland *Quantum Many-Particle Systems*, (Westview Press, Boulder, 1998).
- For a thorough mathematical treatment of complex functions, S. Lang *Complex Analysis*, (Springer, Berlin, 1999).