# Statistical Physics: Mathematical Methods*

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November 19, 2023

*This text evolved from the one prepared by M. Lenz, E. Trizac and F. van Wijland.

# Contents

# 1 Tools

These notes summarize some mathematical tools that you have to master before starting the Statistical Mechanics Master 2 course. They are complemented by a series of Exercises listed in the second Section. In their preparation we have benefitted from the Preliminary Material prepared by Martin Lenz, Emmanuel Trizac and Fréderic van Wijland for the 2016-2020 Statistical Mechanics Lectures. The topics covered are standard and can also be found in many Lecture Notes and Books, see for example [1].

## 1.1 Definitions & limits

### 1.1.1 Polar coordinate system

The polar coordinate system is such that

$$\hat{e}_r = \cos\varphi\,\hat{e}_x + \sin\varphi\,\hat{e}_y \;, \qquad\qquad \hat{e}_\varphi = -\sin\varphi\,\hat{e}_x + \cos\varphi\,\hat{e}_y \;. \tag{1.1}$$

The Cartesian vectors $\hat{e}_x$ and $\hat{e}_y$ are orthogonal $\hat{e}_x \cdot \hat{e}_y = 0$ and have unit modulus $|\hat{e}_x|^2 = |\hat{e}_y|^2 = 1$. Consequently, $\hat{e}_r \cdot \hat{e}_\varphi = 0$ and $|\hat{e}_r|^2 = |\hat{e}_\varphi|^2 = 1$.

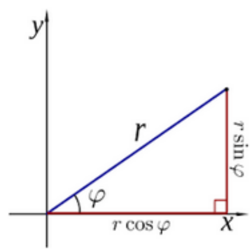



Figure 1.1: Polar coordinates notation convention.

### 1.1.2 Volume of a sphere in $n$ dimensions

Take an $n$-dimensional sphere with radius $R$. Its volume is

$$V_n(R) = \frac{\pi^{n/2}}{\Gamma(n/2+1)}\, R^n \equiv \Omega_n\, R^n \;. \tag{1.2}$$

$\Gamma(x)$ is the Gamma-function $\Gamma(x) = \int_0^\infty dy t^{x-1} e^{-y}$ which for integer argument $N$ equals $\Gamma(N) = (N-1)!$. $\Omega_n$ is the *angular* contribution, also the volume of a unit radius $n$-dimensional sphere.

### 1.1.3 Stirling's factorial approximation

Stirling formula gives an asymptotic expression for the factorial of a large number

$$N! \sim \sqrt{2\pi N}\left(\frac{N}{e}\right)^N , \tag{1.3}$$

where the symbol $\sim$ indicates that the ratio of the two expressions tends to 1 for $N \to \infty$. Taking the natural logarithm

$$\ln N! \sim N \ln N - N + \frac{1}{2}\ln N + \frac{1}{2}\ln(2\pi) = N \ln N - N + \mathcal{O}(\ln N) . \tag{1.4}$$

In Statistical Physics one usually works in the $N \gg 1$ limit in which one drops the correction proportional to $\ln N$ and smaller terms.

## 1.2 Probability theory

Let $P(x)$ be the *probability density* of a random variable $X$, so that $P(x)dx$ is the probability that $X$ takes values between $x$ and $x + dx$. $P(x) \geq 0$ for all $x$ and the normalisation implies $\int dx\, P(x) = 1$. Typically, one indicates with angular brackets, $\langle \dots \rangle$, the averages over $P(x)$, for example $\langle A \rangle = \int dx\, P(x)\, A(x)$, for a generic function $A(X)$. The normalisation reads $\langle 1 \rangle = 1$.

### 1.2.1 Scales

One usually characterises a *probability distribution function* (pdf) $P$ by some scale that could be its *average*, $\langle X \rangle = \int dx\, P(x)\, x$, or the *typical value* that the variable $X$ takes in a measurement, which is given by the maximum of $P$, $x_{\rm typ} = x$ such that $P(x_{\rm typ}) = \max_x P(x)$. For some distributions $\langle X \rangle$ and $x_{\rm typ}$ coincide while for other ones they do not.

### 1.2.2 Moments & cumulants

The $k$th *moment* of $P$ is the average of the $k$th power, $\langle X^k \rangle = \int dx\, P(x)\, x^k$.

Adding a *source* $h$ that couples linearly to the random variable $X$ one easily computes all moments. Indeed, by taking derivatives with respect to $h$:

$$\langle X^k \rangle = \frac{\partial^k}{\partial h^k} \int dx\, P(x)\, e^{hx}\Big|_{h=0} = \frac{\partial^k}{\partial h^k} \langle e^{hX} \rangle\Big|_{h=0} \equiv \frac{\partial^k}{\partial h^k} Z(h)\Big|_{h=0} , \tag{1.5}$$

where in the last equality we defined the *generating function* $Z(h) \equiv \langle e^{hX} \rangle$. The latter can also be written as

$$Z(h) = \sum_{n \geq 0} \frac{h^n}{n!} \langle X^n \rangle , \tag{1.6}$$

from the Taylor expansion of the exponential.

The function $W(h) \equiv \ln Z(h)$ is the generating function of the *cumulants* or *connected moments* of $P$

$$\langle X^k \rangle_c = \frac{\partial^k}{\partial h^k} W(h)\Big|_{h=0} . \tag{1.7}$$

Accordingly,

$$W(h) \equiv \ln Z(h) = \sum_{n \geq 1} \frac{h^n}{n!} \langle X^n \rangle_c . \tag{1.8}$$

*The moments are often called $m_k$ and the cumulants $\kappa_k$. Note that one is usually sloppy with the notation and does not distinguish between $X$ and $x$, typically using $x$ all over.*

### 1.2.3 Symmetries

One can often exploit symmetry properties to derive the result of an integral or a sum without the need to make the explicit calculation, and therefore with no effort. In the context of probability theory, the symmetry properties of the probability density $P$ under, for example, $x \mapsto -x$, are typically used to prove that even or odd moments vanish.

### 1.2.4 The central limit theorem

In probability theory, the central limit theorem (CLT) establishes that, in many situations of interest, when independent random variables are added, their properly normalised sum tends toward a normal (Gaussian) distributed variable (with a "bell curve") even if the elements in the sum are not normally distributed.

More precisely, for $X_i$ *independent identically distributed* *i.i.d.* random variables with *finite* average $\mu$ and variance $\sigma^2$, the variable $\chi$,

$$\chi = \frac{1}{N} \sum_{i=1}^{N} X_i , \tag{1.9}$$

is Gaussian distributed with average $\langle \chi \rangle = \mu$ and variance $\langle (\chi - \langle \chi \rangle)^2 \rangle = \sigma^2/N$.

Other "attractor distributions" of sums of random variables appear, for example, when the second moment of the elements $X_i$ is not finite or they are not *i.i.d.*

### 1.2.5 Gaussian integrals

We focus here on real variables. Extensions to complex variables are relatively easy to work out or can be found in textbooks.

*One variable*

The Gaussian integral is

$$I_1 \equiv \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \, e^{-\frac{(x-\mu)^2}{2\sigma^2}} = 1 . \tag{1.10}$$

It is the normalisation condition of the Gaussian probability density written in the *normal form*. It is then straightforward to show

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \, e^{-\frac{(x-\mu)^2}{2\sigma^2}} \, x = \mu \; , \qquad \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \, e^{-\frac{(x-\mu)^2}{2\sigma^2}} \, x^2 = \sigma^2 \; . \tag{1.11}$$

*The Hubbard-Stratonovich identify* or *Gaussian decoupling* is used to transform a quadratic dependence (on $\eta$) into a linear one, at the price of introducing a Gaussian integral over an auxiliary variable $x$:

$$e^{\frac{\eta^2}{2\sigma^2}} = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \, e^{-\frac{x^2}{2\sigma^2} + \frac{\eta x}{\sigma^2}} \; . \tag{1.12}$$

Another useful Gaussian identity is recovered from the previous one by setting $\eta = \pm i\sigma^2$:

$$\langle \, e^{\pm iX} \, \rangle = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \, e^{-\frac{x^2}{2\sigma^2}} \, e^{\pm ix} = e^{-\frac{\sigma^2}{2}} = e^{-\frac{\langle \, X^2 \, \rangle}{2}} \; . \tag{1.13}$$

*$N$ variables*

The $N$-dimensional integral

$$\mathcal{I}_N \equiv \left( \prod_{i=1}^{N} \int_{-\infty}^{\infty} dx_i \right) \, e^{-\frac{1}{2}\vec{x}^{\,t} A \vec{x} + \vec{x}^{\,t} \vec{\mu}} \tag{1.14}$$

with

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_N \end{pmatrix} \; , \qquad \vec{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \dots \\ \mu_N \end{pmatrix} \; , \qquad A = \begin{pmatrix} A_{11} & \dots & A_{1N} \\ A_{21} & \dots & A_{2N} \\ & \dots & \\ A_{N1} & \dots & A_{NN} \end{pmatrix} \; ,$$

and

$$-\frac{1}{2} \vec{x}^{\,t} A \vec{x} + \vec{x}^{\,t} \vec{\mu} \tag{1.15}$$

features the most generic quadratic form in the exponential. Note that $A$ plays here the role $\sigma^{-2}$ in the single variable case and that we have not introduced a normalisation (in the integration measure) such as the $\sqrt{2\pi\sigma^2}$ in $I_1$. For this reason we called $\mathcal{I}_N$ the $N$-dimensional integral in eq. (1.14) and we will construct the $I_N$ with the proper normalisation below. One can keep the symmetric part $(A + A^t)/2$ of the matrix $A$ only since the antisymmetric part $(A - A^t)/2$ yields a vanishing contribution once multiplied by the vector $\vec{x}$ and its transposed. Focusing now on a symmetric matrix, $A^t = A$, that we still call $A$ we can ensure that it is diagonalisable and all its eigenvalues are positive definite, $\lambda_i > 0$. One can then define $A^{1/2}$ as the matrix such that $A^{1/2}A^{1/2} = A$ and its eigenvalues are the square root of the ones of $A$. Writing $\vec{x}^{\,t} A \vec{x} = (\vec{x}^{\,t} A^{1/2})(A^{1/2}\vec{x}) = \vec{y}^{\,t}\,\vec{y}$, the integral $\mathcal{I}_N$ in (1.14) becomes

$$\mathcal{I}_N = \left( \prod_{i=1}^{N} \int_{-\infty}^{\infty} dy_i \right) \; J \; e^{-\frac{1}{2}\vec{y}^{\,t}\vec{y} + \vec{y}^{\,t}(A^{-1/2}\vec{\mu})} \tag{1.16}$$

where $J = \det(A^{1/2})^{-1} = (\det A)^{-1/2}$ is the Jacobian of the change of variables. Calling $\vec{\mu}' = A^{-1/2}\vec{\mu}$ one has the product of $N$ integrals of the type $\mathcal{I}_1$; thus

$$\mathcal{I}_N = (2\pi)^{N/2} \; (\det A)^{-1/2} \; e^{\frac{1}{2}\vec{\mu}^{\,t} A^{-1}\vec{\mu}} \tag{1.17}$$

It should be now clear how to write the normalised multi-variate Gaussian integral $I_N$.

Several more compact notations for the multiple integrals $\prod_{i=1}^{N} \int dx_i \dots$ are used in the literature. For example, $\int dx_1 \dots dx_N \dots$ or $\int \prod_{i=1}^{N} dx_i \dots$.

*A scalar field in one dimension*

Finally, the functional Gaussian integral is the continuum limit of the $N$-dimensional one

$$\vec{x} \equiv (x_1, \dots, x_N) \to \phi(x) \; , \tag{1.18}$$

which one can interpret as the $1, \dots, N$ indices becoming the argument $x \in \mathbb{R}$ and the $x_1, \dots, x_N$ variables the field $\phi(x)$. Then

$$\mathcal{I} = \int \mathcal{D}\phi \; e^{-\frac{1}{2}\int dx \int dy \; \phi(x) A(x,y) \phi(y) + \int dx \; \phi(x)\mu(x)} \; . \tag{1.19}$$

The *functional integral* runs over all functions $\phi(x)$ with the spatial point $x$ living on the real axis. The *integral measure* represents $\mathcal{D}\phi = \prod_x d\phi(x)$ (think of real space approximated by a one-dimensional lattice, or a chain, with sites $x$ labeled by the lattice site $i = 1, \dots, N$). The sum over $ij$ in the first term in the exponential of the $N$-dimensional integral $\mathcal{I}_N$ became the double integral $\int dx \int dy$, while the single sum in the second term is now just one integral $\int dx$. The first and the second terms in the exponential are quadratic and linear in the field, respectively. In analogy with the $\mathcal{I}_N$ case one has

$$\mathcal{I} = (\det A)^{-1/2} \; e^{\frac{1}{2}\int dx \int dy \; \mu(x) \, A^{-1}(x,y) \, \mu(y)} \tag{1.20}$$

where we ignore the proportionality constant which depends on the definition of the path-integral measure $\mathcal{D}\phi$ (factors $2\pi$). The actual value of this constant is not important since it does not depend on the relevant parameters. The functional inverse $A^{-1}$ appearing in (1.20) is defined by

$$\int dy \; A^{-1}(x,y) A(y,z) = \delta(x - z) \tag{1.21}$$

and $\det A$ is a functional determinant.

The extension of these identities to vector $N$ dimensional integrals, scalar fields defined in $d$-dimensional space, etc. are straightforward.

### 1.2.6 Novikov's thm (integration by parts)

Take a random variable $X$ with a Gaussian distribution with mean $\mu$ and variance $\sigma^2$. The next identity follows from a simple integration by parts

$$\left\langle \frac{(X-\mu)}{\sigma^2} f(X) \right\rangle = \int \frac{dx}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \frac{(x-\mu)}{\sigma^2} f(x) = -\int \frac{dx}{\sqrt{2\pi\sigma^2}} \frac{d}{dx}\left(e^{-\frac{(x-\mu)^2}{2\sigma^2}}\right) f(x)$$

$$\Longrightarrow \langle (X-\mu) f(X) \rangle = \sigma^2 \int \frac{dx}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \frac{df(x)}{dx} = \sigma^2 \left\langle \frac{df(X)}{dX} \right\rangle , \qquad (1.22)$$

for any generic function $f(X)$ decaying to zero at $\pm\infty$ sufficiently fast so as to neglect the border contributions.

The generalisation of the latter to $N$-dimensional vectors reads

$$\langle (X_i-\mu_i) f(\vec{X}) \rangle = \sum_{j=1}^{N} \langle (X_i-\mu_i)(X_j-\mu_j) \rangle \left\langle \frac{\partial f(\vec{X})}{\partial X_j} \right\rangle \qquad (1.23)$$

since $\langle (X_i-\mu_i)(X_j-\mu_j) \rangle = (A^{-1})_{ij}$.

### 1.2.7 Wick's theorem

Take a Gaussian variable $X$ with mean $\langle x \rangle = \mu$ and variance $\sigma^2 = \langle X^2 \rangle - \langle X \rangle^2$. Its probability density is

$$P(x) = (2\pi\sigma^2)^{-1/2} e^{-(x-\mu)^2/(2\sigma^2)} . \qquad (1.24)$$

All moments $\langle X^k \rangle$ can be computed with (1.5). One finds

$$\langle e^{hX} \rangle = e^{\frac{h^2\sigma^2}{2} + h\mu} \qquad (1.25)$$

and then

$$\langle X^k \rangle = \frac{\partial^k}{\partial h^k} e^{\frac{h^2\sigma^2}{2} + \mu h} \Big|_{h=0} \qquad (1.26)$$

from where

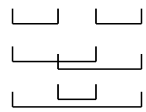
$$\langle X \rangle = \mu , \qquad \langle X^2 \rangle = \sigma^2 + \mu^2 ,$$
$$\langle X^3 \rangle = 3\sigma^2\mu + \mu^3 , \qquad \langle X^4 \rangle = 3\sigma^4 + 6\sigma^2\mu^2 + \mu^4$$

*etc.* One recognises the structure of Wick's theorem: given $k$ factors $X$ one organises them in pairs leaving the averages $\mu$ aside.

We note that keeping the average of the Gaussian variable different from zero is annoying. It is therefore convenient to translate it, $X - \mu \mapsto X$, or, equivalently, change variables to $Y = X - \mu$. By working with the new variable one sets, effectively, the average to zero.

The simplest way of seeing Wick's theorem in action is by drawing examples with the contractions. For example, for $\langle X^4 \rangle$:

$$\langle\, X^4 \,\rangle = \langle\; X \;\, X \;\, X \;\, X \;\rangle$$



$$\langle\, X^4 \,\rangle = 3 \,\langle\, X^2 \,\rangle^2 \tag{1.27}$$

If, instead of computing moments one focuses on cumulants, one has to focus on $W(h) = \ln Z(h) = \mu + \frac{h^2\sigma^2}{2}$ and its derivatives with respect to $h$:

$$\langle\, X \,\rangle_c = 0 \;, \qquad \langle\, X^2 \,\rangle_c = \sigma^2 \;, \qquad \langle\, X^k \,\rangle_c = 0 \;\; \forall\, k \geq 3 \;, \tag{1.28}$$

and the cumulant expansion stops at order 2 (included) for a Gaussian variable.

The generalisation to $N$ Gaussian variables is immediate. Equation (1.25) becomes

$$\langle\, e^{\vec{h}\,\vec{x}} \,\rangle = e^{\frac{1}{2}\vec{h}A^{-1}\vec{h}+\vec{h}\vec{\mu}} \tag{1.29}$$

and the generalization of (1.26) leads to

$$\langle\, x_i \,\rangle = \mu_i \;, \qquad \langle\, x_i x_j \,\rangle = {A^{-1}}_{ij} + \mu_i\mu_j \;, \tag{1.30}$$

*etc.* In other words, wherever there is $\sigma^2$ in the single variable case we replace it by ${A^{-1}}_{ij}$ with the corresponding indices, and $\mu$ by $\mu_i$.

The generalisation to a field theory necessitates the introduction of functional derivatives that we describe below. For completeness we present the result for a scalar field in $d$ dimensions:

$$\langle\, \phi(\vec{x}) \,\rangle = \mu(\vec{x}) \;, \qquad \langle\, \phi(\vec{x})\phi(\vec{y}) \,\rangle = A^{-1}(\vec{x},\vec{y}) + \mu(\vec{x})\mu(\vec{y}) \;, \tag{1.31}$$

*etc.*

### 1.2.8 Jensen's inequality

Jensen's inequality relates the value of a convex function of an integral to the integral of the convex function. In its simplest form the inequality states that the convex transformation of a mean is less than or equal to the mean applied after convex transformation; it is a simple corollary that the opposite is true of concave transformations.

In probability theory, the Jensen's inequality implies that, for $X$ a random variable and $f$ a convex function, then

$$f(\langle\, X \,\rangle) \leq \langle\, f(X) \,\rangle \;. \tag{1.1}$$

We recall that a function is convex function iff $\forall x_1, x_2$ and $t \in [0,1]$:

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2) \; . \tag{1.2}$$

## 1.3 Functional analysis

A functional $F[h]$ is a function of a scalar function $h : \vec{x} \to h(\vec{x})$. The variation of a functional $F$ when one changes the function $h$ by an infinitesimal amount allows one to define the functional derivative. More precisely, one defines $\delta F \equiv F[h+\delta h] - F[h]$. Next, and one tries to write this infinitesimal increment as $\delta F = \int d^dx \;\alpha(\vec{x})\delta h(\vec{x}) + \frac{1}{2}\int d^dx d^dy \;\beta(\vec{x},\vec{y})\,\delta h(\vec{x})\delta h(\vec{y}) + \ldots$. The successive functional derivatives of $F$ with respect to $h$ evaluated at the spatial point $\vec{x}$, $\vec{x}$ and $\vec{y}$, *etc.* are then defined as

$$\frac{\delta F}{\delta h(\vec{x})} = \alpha(\vec{x}) \; , \qquad \frac{\delta^2 F}{\delta h(\vec{x})\delta h(\vec{y})} = \beta(\vec{x},\vec{y}) \tag{1.3}$$

*etc.* In particular

$$\frac{\delta \phi(\vec{x})}{\delta \phi(\vec{y})} = \delta^d(\vec{x}-\vec{y}) \; . \tag{1.4}$$

These definitions are such that all usual properties of partial derivatives apply: the variation of a sum of functionals is the sum of the variations (linearity), the variation of a product of two functionals is the variation of the first times the second one plus the first one times the variation of the second one (product rule) and the chain rule

$$\frac{\delta F[\phi(\vec{y})]}{\delta \phi(\vec{x})} = F'[\phi(\vec{y})]\,\frac{\delta \phi(\vec{y})}{\delta \phi(\vec{x})} = F'[\phi(\vec{y})]\,\delta(\vec{x}-\vec{y}) \; . \tag{1.5}$$

Most Hamiltonians or Ginzburg-Landau free-energies can be written as the space integral of a density which is a functional of $\phi(\vec{x})$ and $\vec{\nabla}\phi(\vec{x})$:

$$F[\phi] = \int d^dx \; f[\phi(\vec{x}), \vec{\nabla}\phi(\vec{x})] \; . \tag{1.6}$$

Its variation with respect to $\phi$ reads

$$\begin{aligned}
\frac{\delta F[\phi]}{\delta\phi(\vec{x})} &= \frac{\delta}{\delta\phi(\vec{x})} \int d^d y \; f[\phi(\vec{y}), \vec{\nabla}\phi(\vec{y})] = \int d^d y \; \frac{\delta}{\delta\phi(\vec{x})} f[\phi(\vec{y}), \vec{\nabla}\phi(\vec{y})] \\
&= \int d^d y \; \left\{ \frac{\partial f}{\partial \phi} \frac{\delta\phi(\vec{y})}{\delta\phi(\vec{x})} + \frac{\partial f}{\partial \vec{\nabla}\phi} \cdot \frac{\delta\vec{\nabla}\phi(\vec{y})}{\delta\phi(\vec{x})} \right\} \\
&= \int d^d y \; \left\{ \frac{\partial f}{\partial \phi} \, \delta^d(\vec{x}-\vec{y}) + \frac{\partial f}{\partial \vec{\nabla}\phi} \cdot \vec{\nabla}_{\vec{y}} \, \frac{\delta\phi(\vec{y})}{\delta\phi(\vec{x})} \right\} \\
&= \int d^d y \; \left\{ \frac{\partial f}{\partial \phi} \, \delta^d(\vec{x}-\vec{y}) + \frac{\partial f}{\partial \vec{\nabla}\phi} \cdot \vec{\nabla}_{\vec{y}} \, \delta^d(\vec{x}-\vec{y}) \right\} \\
&= \int d^d y \; \left\{ \frac{\partial f}{\partial \phi} \, \delta^d(\vec{x}-\vec{y}) - \left( \vec{\nabla}_{\vec{y}} \cdot \frac{\partial f}{\partial \vec{\nabla}\phi} \right) \, \delta^d(\vec{x}-\vec{y}) \right\} \\
&= \frac{\partial f}{\partial \phi}(\vec{x}) - \vec{\nabla}_{\vec{x}} \cdot \frac{\partial f}{\partial \vec{\nabla}\phi}(\vec{x}) \; . \qquad (1.7)
\end{aligned}$$

One either assumes that $\phi(\vec{x})$ vanishes at the boundaries of its domain of definition or it satisfies periodic boundary conditions.

The generalization to vectorial or tensorial cases is straightforward.

## 1.4 Fourier transforms and series

### 1.4.1 Discrete Fourier transforms

The discrete Fourier transform is the linear and invertible transformation of a sequence of $N$ complex numbers $\{f_n\} = f_1, f_2, \dots, f_N$ into another sequence of complex numbers, $\{\widetilde{f}_k\} = \widetilde{f}_1, \widetilde{f}_2 \dots, \widetilde{f}_N$. It is defined by

$$\mathcal{F}_k(\{f_n\}) = \widetilde{f}_k = \frac{1}{A} \sum_{n=1}^{N} f_n \; e^{-i\frac{2\pi}{N}kn} \qquad (1.8)$$

with inverse

$$f_n = \mathcal{F}_n^{-1}(\{\widetilde{f}_k\}) = \frac{A}{N} \sum_{k=1}^{N} \widetilde{f}_k \; e^{i\frac{2\pi}{N}kn} \; . \qquad (1.9)$$

The normalisation factor $A$ is arbitrary and, in this discrete formulation is usually set to $A = 1$. The freedom to choose $A$ is reflected in the variety of conventions found in the literature.

These definitions can be applied to temporal, equally delayed, measurements, with $t_N = N\tau$ the total duration of the measurement, and $\tau$ the delay between subsequent ones. A generic discrete instant is then denoted $t_n = n\tau$. The Fourier transform indices

$k$ order the angular frequencies, $\omega_k = 2\pi k/(\tau N) = 2\pi k/t_N$ and the expression in the exponential can be rewritten as $i\frac{2\pi}{N}kn = i\omega_k t_n$.

$f_n$ could also be a complex function defined on an $N$-site lattice with spacing $a$ and total linear length $L = Na$. In this case, the dimension full variables are $x_n = na$ and $q_k = 2\pi k/(aN) = 2\pi k/L$. The expression in the exponential becomes $i\frac{2\pi}{N}kn = iq_k x_n$.

Some interesting limits are the following. For concreteness, we focus on the spatial notation, with $x_n = na$.

– Let us take $N \to \infty$ and $a \to 0$ with $L = Na$ fixed. This is the limit of a continuous but finite interval. The space points $x_n$ tend to the real variable $x$.

We can now express $\widetilde{f}_k$ as an integral involving $f(x)$. The most convenient convention to use is $A = 1/a$. Starting from the definition $\widetilde{f}_k = a\sum_{n=1}^{N} e^{i2\pi k/N\, n}\, f_n = a\sum_{n=1}^{N} e^{iq_k x_n}\, f_n$ with $q_k = 2\pi k/L$, we then convert the summation $a\sum_{n=1}^{N}$ into an integral $\int_0^L dx$, and we arrive at $\widetilde{f}_{q_k} = \int_0^L dx\, f(x)\, e^{iq_k x}$. Note that $q_k$ takes discrete values indexed by $k$.

One can also proceed backwards, $f_n = \frac{1}{Na}\sum_{k=1}^{N} \widetilde{f}_k\, e^{-i\frac{2\pi}{N}kn}$ converts into $f(x) = \frac{1}{L}\sum_{k=1}^{\infty} \widetilde{f}_k\, e^{-iq_k x}$ with $q_k = \frac{2k\pi}{L}$ and $k \in \mathbb{N}$.

– Let $f(\tau)$ be a periodic function of a continuous variable $\tau$ (we interpret it as a time) with period $\beta$. Using the results pertaining to a continuous but finite interval discussed in the previous item, $\widetilde{f}_{\omega_k} = \beta^{-1}\int_0^\beta d\tau\, f(\tau)\, e^{i\omega_k \tau}$. The integral can be computed on any interval of length $\beta$.

– We now consider $N \to \infty$ with $L/N = a$ fixed. This is the limit of an infinite lattice. Show that in this limit $f_n = a\int_{-\pi/a}^{+\pi/a} \frac{dq}{2\pi}\, \widetilde{f}_q\, e^{-iqna}$ (we are back to the convention $A = 1$).

### 1.4.2 Continuous real $d$-dimensional space

In the vectorial $d$-dimensional infinite volume case one defines

$$\widetilde{f}(\vec{q}) = \frac{1}{A}\int_{\mathbb{R}^d} d^dx\; f(\vec{x})\, e^{i\vec{q}\cdot\vec{x}} \qquad \text{and} \qquad f(\vec{r}) = A\int_{\mathbb{R}^d} \frac{d^dq}{(2\pi)^d}\; \widetilde{f}(\vec{q})\, e^{-i\vec{q}\cdot\vec{x}} \; .$$

One may choose $A = 1$. Integrations over $\vec{q}$ then go hand in hand with $(2\pi)^d$ factors. A useful relation is

$$\int_{\mathbb{R}^d} \frac{d^dq}{(2\pi)^d}\; e^{-i\vec{q}\cdot\vec{x}} = \delta^{(d)}(\vec{x}) \tag{1.10}$$

The so-called Plancherel-Parseval relation for two complex functions $f$ and $g$ is

$$\int_{\mathbb{R}^d} d^dx\; f(\vec{x})\, g(\vec{x}) = \int_{\mathbb{R}^d} \frac{d^dq}{(2\pi)^d}\; \widetilde{f}(\vec{q})\; \widetilde{g}(-\vec{q}) \; . \tag{1.11}$$

In quantum mechanics, one tends to like a symmetric $f \leftrightarrow \widetilde{f}$ connection, which requires choosing $A = (2\pi)^{d/2}$. A similar goal may be achieved, say in 1 dimension, by working with ordinary frequency rather than with angular frequency:

$$\widetilde{f}(\nu) = \int_{\mathbb{R}} f(x)\, e^{2i\pi\nu x}\, dx \qquad \text{and} \qquad f(x) = \int_{\mathbb{R}} \widetilde{f}(\nu)\, e^{-2i\pi\nu x}\, d\nu.$$

In so doing, $2\pi$ factors appear in the exponentials, but not elsewhere. Indeed, $\int d\nu\; e^{-2i\pi\nu x} = \delta(x)$ and the Plancherel-Parseval relation reads

$$\int dx\; f(x)g(x) = \int d\nu\; \widetilde{f}(\nu)\widetilde{g}(-\nu) \tag{1.12}$$

Taking now $g(x) = f^*(x)$:

$$\int dx\; \left|f(x)\right|^2 = \int d\nu\; \left|\widetilde{f}(\nu)\right|^2 \quad \text{since} \quad \left[\widetilde{f}(\nu)\right]^* = \widetilde{f}^*(-\nu)\;. \tag{1.13}$$

Finally, attention should be paid to the domain of definition of the function $f(x)$ to be Fourier-analyzed. For $d = 1$:

– If $x \in \mathbb{R}$, then $q \in \mathbb{R}$.

– If $f$ is periodic of period $L$, then $q = 2\pi k/L$, where $k \in \mathbb{Z}$.

– If $f$ is defined on an $N$-site lattice with constant $a$, then $q_k = 2\pi k/(Na)$, where $k = 0, 1, \ldots N-1$ (or, if $N$ is even, $k = -N/2+1, \ldots, N/2-1, N/2$). If $N \to \infty$ (infinite lattice) at fixed $a$, $0 \le q \le 2\pi/a$ or equivalently $-\pi/a \le q \le \pi/a$. If $N \to \infty$ and $Na = L$ is fixed, the $q_k$ remain discrete and we are back to a periodic function results with period $L$. Finally, beyond the one-dimensional case, more complex lattices are met, leading to non-trivial so-called *Brillouin zones* in Fourier space, where $\vec{q}$ vectors should be restricted.

## 1.5 The saddle-point method

Imagine one has to compute the following integral

$$I \equiv \int_a^b dx\; e^{-Nf(x)}\;, \tag{1.1}$$

with $f(x)$ a positive definite function in the interval $[a, b]$, in the limit $N \to \infty$. It is clear that due to the rapid exponential decay of the integrand, the integral will be dominated by the minimum of the function $f$ in the interval. Assuming there is only one absolute minimum, $x_0 \in [a, b]$, one then Taylor expands $f(x)$ upto second order

$$f(x) = f(x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + \mathcal{O}((x - x_0)^3) \tag{1.2}$$

and, dropping the $\mathcal{O}((x-x_0)^3)$ corrections obtains

$$I \sim e^{-Nf(x_0)} \int_a^b dx\, e^{-N\frac{1}{2}f''(x_0)(x-x_0)^2} = e^{-Nf(x_0)}\, [Nf''(x_0)]^{-1/2} \int_{y_a}^{y_b} dy\, e^{-\frac{1}{2}(y-y_0)^2} \;, \quad (1.3)$$

where we implicitly assumed $f''(x_0) \geq 0$. In the transformed variables $y_0 \equiv \sqrt{Nf''(x_0)}x_0$ and similarly for $y_a$ and $y_b$. The Gaussian integral is just an error function and one can finds its numerical value in Tables. This is the saddle point method also called the *method of steepest descent* or *Laplace's method*.

One readily proves

$$I \equiv \int_a^b dx\, e^{-Nf(x)}\, g(x) \sim e^{-Nf(x_0)}\, [Nf''(x_0)]^{-1/2}\, g(x_0) \;, \quad (1.4)$$

f there are more than one minima in $[a,b]$ one should, in principle, sum the contribution from each. However, one will be the dominant one. Interesting phenomena occurs when on varying a parameter minimum rises above the other. Then the asymptotic expression for the integral changes in a non-analytic way. In statistical physics, this is the mechanism for a first order phase transition.

In cases in which there is no absolute minimum within the integration interval, the integral is dominated by its lower bound. The first derivative of $f$ may not vanish there and the Taylor expansion reads $f(x) = f(a) + f'(a)(x-a) + \mathcal{O}((x-a)^2)$. Applying this expansion to first order to the example,

$$\begin{aligned} I &\sim e^{-Nf(a)} \int_a^b dx\, e^{-Nf'(a)(x-a)} = e^{-Nf(a)}\, [Nf'(a)]^{-1}\, [e^{-Nf'(a)(b-a)} - 1] \\ &\sim -e^{-Nf(a)}\, [Nf'(a)]^{-1} \;. \end{aligned} \quad (1.5)$$

where we further ssumed $f'(a) > 0$ One has to check whether the contribution of higher order terms is actually negligible.

This argument can be extended to multidimensional integrals.

# 2 Exercises

## 2.1 Definitions & limits

### 2.1.1 Stirling's factorial approximation

(a) Plot $\ln N!$ and its approximation in Eq. (1.3) for various $N$ and compare.

## 2.2 Probability theory

### 2.2.1 Scales

(a) Show that $\langle X \rangle = x_{\rm typ}$ for a Gaussian pdf.

(b) Find a well-know pdf for which $\langle X \rangle \neq x_{\rm typ}$.

(c) Which is the most common situation, $\langle X \rangle = x_{\rm typ}$ or $\langle X \rangle \neq x_{\rm typ}$?

### 2.2.2 Moments & cumulants

(a) Take an exponential probability density $P(x) = \frac{1}{2}\, e^{-|x|}$. Calculate the momenta $\langle X^k \rangle$ and cumulants $\langle X^k \rangle_c$.

(b) For an arbitrary $P$ find a few generic relations between cumulants and momenta.

(c) Take a random variable $X$ with a Lévy distribution $P(x) = \sqrt{c/(2\pi)}\, e^{-c/2x}/x^{3/2}$ with $c$ a constant fixed by normalisation. Compare the tail ($x \gg 1$) of this probability density to the one of the conventional Poisson or Gaussian variables. What do you observe? Compute the generic momentum $\langle X^k \rangle$ of such a Lévy variable. Are these finite? For which $k$?

### 2.2.3 Symmetries

(a) Show that the odd moments of a symmetric pdf $P$ with support on the interval $[-a, a]$ vanish.

(b) Show that the even moments of a anti-symmetric pdf $P$ with support on the interval $[-a, a]$ vanish.

(c) Use symmetry arguments to show the first identity in (1.11).

### 2.2.4 Gaussian integrals

1. Take two correlated Gaussian random variables $X$ and $Y$. We know the five correlations $\langle X \rangle = 0$, $\langle Y \rangle = 0$, $\langle X^2 \rangle = 3$, $\langle XY \rangle = 1$, $\langle Y^2 \rangle = 2$.

   (a) Calculate the averages $\langle X^4 \rangle$, $\langle X^3 Y \rangle$, $\langle X^2 Y^2 \rangle$, $\langle XY^3 \rangle$, $\langle Y^4 \rangle$.

   (b) Which is the Gaussian distribution that yields these averages?

### 2.2.5 The central limit theorem

(a) Plot the probability distribution of $\chi = N^{-1} \sum_{i=1}^{N} X_i$, with $X_i$ *i.i.d.* Gaussian random variables with mean $\mu$ and variance $\sigma^2$, for $N = 1, 2, 3, 4, 5, 10, 100$. Conclude.

(b) Repeat for $X_i$ *i.i.d.* Lévy random variables. Is the sum $\chi$ converging to a Gaussian random variable? Discuss.

## 2.3 Functional derivatives

Let $q(t)$ be a function of time $t$ and $S[q]$ be a functional of $q$. The functional derivative of $S$ with respect to $q(t_0)$ is defined such that when $q \to q+\delta q$ (meaning that the trajectory $q(t)$ is perturbed by $\delta q(t)$), the functional changes from $S$ to $S + \delta S$, with

$$\delta S = \int dt' \, \frac{\delta S}{\delta q(t')} \; \delta q(t') \,, \tag{2.6}$$

to first order in $\delta q$. This relation defines the functional derivative $\delta S/\delta q(t')$, which is a functional of $q$ and a function of $t'$.

1. What is $\frac{\delta q(t_1)}{\delta q(t_2)}$?

2. If $S$ can be written in the form $S[q] = \int_0^\infty dt\, L(q(t), \dot{q}(t))$, where $L$ is a function of $q(t)$ and $\dot{q}(t)$, prove that $\frac{\delta S}{\delta q(t_0)} = \frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}$ where everything is evaluated at $t = t_0$. In mechanics, $L$ is a Lagrangian while $S$ is an action.

3. If now $S[\phi]$ is a functional of a field $\phi$ living in $d$-dimensional space, such that $S[\phi] = \int d^d x\, \mathcal{L}(\phi, \partial_\mu \phi)$, (where $\mu = 1, \ldots, d$ refers to space directions), explain why $\frac{\delta S}{\delta \phi(\vec{x}_0)} = \frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi}$ (at $\vec{x}_0$).

4. Let $S[\phi] = \int dx\, \left(\frac{1}{2}\left(\frac{d\phi}{dx}\right)^2 + \frac{r}{2}\phi^2\right)$. Determine $\frac{\delta S}{\delta \phi(x_1)}$ and then $\frac{\delta^2 S}{\delta \phi(x_2)\delta \phi(x_1)}$.

**Remember** the connection between functional derivatives and Euler-Lagrange equations. Besides, our first order expansion Eq. (2.6) can be pushed one order higher:

$$\delta S \;=\; S[q+\delta q] - S[q] \;=\; \int \frac{\delta S}{\delta q(t')}\, \delta q(t')\, dt' \;+\; \frac{1}{2}\int \left.\frac{\delta^2 S}{\delta q(t')\delta q(t'')}\right|_q \delta q(t')\; \delta q(t'')\; dt'\, dt''.$$

Side comment: functional derivatives and functional integrals have nothing to do with each other, in the sense that our introductory discussion does not involve any functional integration, but simple integration instead.

## 2.4 Saddle-point

1. Use Laplace's method to prove Stirling's approximation of $N!$. Hint: start from $N! = \Gamma(N+1) = \int_0^\infty dx\, e^{-x} x^N$.

**Acknowledgements.** We thank S. Wei for pointing out some typos in a previous version of this file.

# References

[1] N. Dupuis, *Notes on the many-body problem* Ch. 1 *Functional integrals* (2019).