A midsummer's night homework
for a fruitful Statistical Physics course (and more) – iCFP M2

The purpose of this set of problems is to list a few prerequisites and calculations on which some of your previous-year fellows have stumbled. Of particular relevance are the ***remember*** recaps that conclude each exercise.

1 Vocabulary of probabilities

Let $P(x)dx$ be the probability that a random variable X takes a value between x and $x + dx$. The $n^{\rm th}$ moment of P is denoted by $m_n = \langle X^n \rangle = \int dx x^n P(x)$. The generating function of the moments of P is $Z(h) = \langle e^{hX} \rangle$. It owes its name to the fact that $\frac{d^n Z}{dh^n}\big|_{h=0} = \langle X^n \rangle$. One thus has that $Z(h) = \sum_{n\geq 0} \frac{h^n \langle X^n \rangle}{n!}$.

The function $W(h) = \ln Z(h)$ is the generating function of the cumulants (sometimes also called the connected moments) of P. By definition, the $n^{\rm th}$ cumulant κ_n of P is $\kappa_n = \frac{d^n W}{dh^n}\big|_{h=0}$. Notation wise, one often writes $\kappa_n = \langle X^n \rangle_c$, the index c referring to the cumulant. Hence $W(h) = \sum_{n\geq 1} \frac{h^n \langle X^n \rangle_c}{n!}$.

1.1 Determine the m_n's and κ_n's for $P(x) = e^{-|x|}/2$.

> Answer: $m_{2n} = 2n!$ and $\kappa_{2n} = \frac{2n!}{n}$ (because $Z(h) = \frac{1}{1-h^2}$ and thus $W(h) = -\ln(1-h^2)$). Odd moments and cumulants vanish.

1.2 For an arbitrary P, show that $\kappa_1 = m_1$, $\kappa_2 = m_2 - m_1^2$.

> Answer: Starting from $Z = 1 + hm_1 + \frac{h^2}{2}m_2 + \frac{h^3}{3!}m_3 + \frac{h^4}{4!}m_4 + \mathcal{O}(h^5)$, we have $W(h) = \ln Z(h) = m_1 h + \frac{h^2}{2}(-m_1^2 + m_2) + \frac{h^3}{3!}(2m_1^3 - 3m_1 m_2 + m_3) + \frac{h^4}{4!}(-6m_1^4 + 12m_1^2 m_2 - 3m_2^2 - 4m_1 m_3 + m_4)$, so that, by straight identification, $\kappa_1 = m_1$, $\kappa_2 = m_2 - m_1^2$, $\kappa_3 = 2m_1^3 - 3m_1 m_2 + m_3$ and $\kappa_4 = -6m_1^4 + 12m_1^2 m_2 - 3m_2^2 - 4m_1 m_3 + m_4$.

1.3 Find similar relationships for κ_3 in terms of m_3, m_2 and m_1, and for κ_4 in terms of m_4, m_3, m_2 and m_1.

1.4 Show that for an even P, the relationship between κ_4 and the moments m_n $(n \leq 4)$ simplifies into $\kappa_4 = m_4 - 3\,m_2^2$.

> Answer: This is a direct consequence of having $m_1 = 0$. We also have $m_3 = 0$ here (but this is useless for our purpose).

Remember the definitions of moments, cumulants, and the relations hidden above, that can be rewritten as

$$\begin{aligned}
\langle X^2 \rangle_c &= \left\langle\, (X - \langle X \rangle)^2 \,\right\rangle \\
\langle X^3 \rangle_c &= \left\langle\, (X - \langle X \rangle\,)^3 \,\right\rangle \\
\langle X^4 \rangle_c &= \left\langle\, (X - \langle X \rangle)^4 \,\right\rangle - 3\left\langle\, (X - \langle X \rangle)^2 \,\right\rangle^2
\end{aligned}$$

Note that the first two lines, together with the fact that $\langle X \rangle_c = \langle X \rangle$, might lead to believe that the cumulants are trivially connected to centered moments (i.e. those of the shifted variable $X - \langle X \rangle$). It is not the case, as the third line illustrates.

2 Fourier transforms and series

Let f_n be a function defined on an N-site lattice, $n = 1, \dots, N$ (N is assumed to be even) with lattice spacing a ($L = Na$ is the total length of the lattice). We define $\widetilde{f}_q = \sum_{n=1}^{N} e^{iqna} f_n$.

2.1 Show that if $q = \frac{2\pi k}{Na}$, $k = -N/2+1, \dots, N/2$ then $f_n = \frac{1}{N} \sum_q \widetilde{f}_q \, e^{-iqna}$.

> Answer: Start from the answer $\sum_q e^{-iqna} \widetilde{f}_q = \sum_q e^{-iqna} \sum_m e^{iqma} f_m = \sum_m f_m N \delta_{n,m} = N f_n$.

It should be appreciated that Fourier Transformation can be defined up to an arbitrary normalization factor A through

$$\widetilde{f}_q = \frac{1}{A} \sum_{n=1}^{N} e^{iqna} f_n \qquad \text{and} \qquad f_n = \frac{A}{N} \sum_q \widetilde{f}_q \, e^{-iqna},$$

and this is reflected in the variety of conventions found in the literature.

2.2 We denote $x = na$. We take the $N \to \infty$ and $a \to 0$ limits, with $L = Na$ fixed. To this end, it is convenient to adopt the convention $A = 1/a$. This is the limit of a continuous but finite interval. Express $\widetilde{f}_q$ as an integral involving $f(x)$. How does one obtain $f(x)$ if $\widetilde{f}_q$ is given?

> Answer: Start from the definition $\widetilde{f}_q = a \sum_{n=1}^{N} e^{iqna} f_n$ and convert the summation $\sum_n$ into and integral $\int_0^L \frac{dx}{a}$, which leads to $\widetilde{f}_q = \int_0^L dx f(x) e^{iqx}$. Things work also backwards, as $f_n = \frac{1}{Na} \sum_q \widetilde{f}_q e^{-iqna}$ converts into $f(x) = \frac{1}{L} \sum_q \widetilde{f}_q e^{-iqx}$, but now $q = \frac{2k\pi}{L}$ with $k \in \mathbb{Z}$.

2.3 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 $A = 1$).

2.4 Let $f(\tau)$ be a periodic function with period β, then prove that $f(\tau) = \sum_{n \in \mathbb{Z}} \widetilde{f}_{\omega_n} e^{-i\omega_n \tau}$ where $\omega_n = \frac{2\pi n}{\beta}$ and where $\widetilde{f}_{\omega_n}$ will be given in terms of f.

> Answer: We use directly the results pertaining to a continuous but finite interval above to get $\widetilde{f}_{\omega_n} = \beta^{-1} \int_0^\beta f(\tau) \, e^{i\omega_n \tau} \, d\tau$. The integral can be computed on any interval of length β.

2.5 Solve the Schrödinger equation for a free particle with Hamiltonian $\widehat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ in a one dimensional box of size L ($x \in [0, L]$) first with periodic boundary conditions, second when the system is bounded by impenetrable walls. For each case, find the eigenvalues ε and the eigenfunctions $\psi_\varepsilon(x)$. It will be convenient to write $\varepsilon = \frac{\hbar^2 k^2}{2m}$. Be very precise as to which range of values k may cover.

> Answer: For periodic boundary conditions we find that $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ with $k = 2\pi n/L$ and $n \in \mathbb{Z}$, with $\psi_{\varepsilon_k} = \frac{1}{\sqrt{L}} e^{ikx}$ where the factor $\sqrt{L}$ stems from normalization. For impenetrable boundary conditions, the above relation for ε remains true, but a slight change of method is required. We can directly solve the differential equation, with the requirement that ψ vanishes at $x = 0$ and $x = L$. We find that $k = n\pi/L$ with $n \in \mathbb{N}^*$ and $\psi_{\varepsilon_k} = \sqrt{\frac{2}{L}} \sin kx$.

Focus on circulant matrices. Consider a real matrix M such that its elements $M_{k\ell} = m_{k-\ell}$ are a periodic function of $k - \ell$ only ($0 \le k, \ell \le N-1$, and $m_{-1} = m_{N-1}$, $m_0 = m_N$ *etc.*):

$$M = \begin{pmatrix} m_0 & m_1 & m_2 & \dots & m_{N-1} \\ m_{N-1} & m_0 & m_1 & \dots & m_{N-2} \\ m_{N-2} & m_{N-1} & m_0 & \dots & m_{N-3} \\ \vdots & & & \ddots & \vdots \\ m_1 & m_2 & m_3 & \dots & m_0 \end{pmatrix}$$

Such a situation arises in problems that are invariant by translation (with cyclic boundary conditions). The matrix M can be diagonalized by discrete Fourier transform. Indeed, we first define

$$\widetilde{M}(q) = \sum_\ell M_{k\ell} \, e^{iq(k-\ell)} \qquad \text{with} \qquad q = \frac{2\pi}{N} n, \quad n = 1, 2, \dots N.$$

A key point is that $\widetilde{M}(q)$ exists and is independent of k because the summation does not depend on k. The above equation can be rewritten $\sum_\ell M_{k\ell} \, e^{-iq\ell} = \widetilde{M}(q) e^{-iqk}$, meaning that **the $\widetilde{M}(q)$ are the N eigenvalues of M.**

The corresponding eigenvectors indexed by the values of q are $(e^{-iq}, e^{-2iq} \dots e^{-Niq})^T$. Hence, $Tr(M) = \sum_q \widetilde{M}(q)$, that will be used during the lectures. The above treatment also shows that $\widetilde{M}(q)\widetilde{M^{-1}}(q) = 1$. Another interesting byproduct is that since the $\widetilde{M^{-1}}(q)$ are available, the matrix M^{-1} is known explicitly as well, and reads

$$M^{-1}_{k\ell} = \frac{1}{N} \sum_q \frac{1}{\widetilde{M}(q)} e^{-iq(k-\ell)}.$$

The reason for this simplicity is that both M and M^{-1} are actually defined from a mere one-argument function $m(x)$.

Remember that in the vectorial case, one defines Fourier transformation in d dimensions through

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

One may choose $A = 1$. Integrations over $\boldsymbol{q}$ then go hand in hand with $(2\pi)^d$ factors, as above and below. A useful relation is $\int e^{-i\boldsymbol{q}\cdot\boldsymbol{x}} \frac{d\boldsymbol{q}}{(2\pi)^d} = \delta^{(d)}(\boldsymbol{x})$ and it does not hurt to keep in mind Plancherel-Parseval relation for two complex functions f and g

$$\boxed{\int_{\mathbb{R}^d} f(\boldsymbol{x})\, g(\boldsymbol{x})\, d\boldsymbol{x} = \int_{\mathbb{R}^d} \widetilde{f}(\boldsymbol{q})\; \widetilde{g}(-\boldsymbol{q})\, \frac{d\boldsymbol{q}}{(2\pi)^d}}.$$

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

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

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 $q = 2\pi n/L$, where $n \in \mathbb{Z}$.
- If f is defined on an N-site lattice with constant a, then $q = 2\pi n/(Na)$, where $n = 0, 1, \dots N-1$ (or, if N is even, $n = -N/2+1, \dots, N/2-1, N/2$. 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 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 $\boldsymbol{q}$ vectors should be restricted.

3 Gaussian integration

Let $\boldsymbol{x} = (x_1, \dots, x_n)$ and $\boldsymbol{h} = (h_1, \dots, h_n)$ be n-component vectors. We define $Z(\boldsymbol{h}) = \int d\boldsymbol{x} e^{-\frac{1}{2}x_i\Gamma_{ij}x_j + h_i x_i}$, where Γ is for the moment a positive definite $n \times n$ matrix. We use the notation $\frac{1}{2}x_i\Gamma_{ij}x_j - h_i x_i$ for $\frac{1}{2}\boldsymbol{x}\cdot(\Gamma\boldsymbol{x}) - \boldsymbol{h}\cdot\boldsymbol{x}$ (*i.e.*, we implicitly sum over repeated indices). We also define $P(\boldsymbol{x}) = \frac{1}{Z(\boldsymbol{0})} e^{-\frac{1}{2}\boldsymbol{x}\cdot(\Gamma\boldsymbol{x})}$ and the angular brackets mean $\langle \dots \rangle = \int d\boldsymbol{x} \dots P(\boldsymbol{x})$.

3.1 Verify that $\langle e^{\boldsymbol{h}\cdot\boldsymbol{x}} \rangle = \frac{Z(\boldsymbol{h})}{Z(\boldsymbol{0})}$.

3.2 What is the reason for which one can restrict the analysis to a symmetric matrix Γ? This property will be assumed in the rest of the exercise.

> Answer: Because only the symmetric part of Γ enters the final expressions: $\boldsymbol{x}\cdot(\Gamma\boldsymbol{x}) = \boldsymbol{x}\cdot(\Gamma + \Gamma^T)\boldsymbol{x}/2 + \boldsymbol{x}\cdot(\Gamma - \Gamma^T)\boldsymbol{x}/2 = \boldsymbol{x}\cdot(\Gamma + \Gamma^T)\boldsymbol{x}/2$.

3.3 Prove that $\frac{1}{2}\boldsymbol{x}\cdot(\Gamma\boldsymbol{x}) - \boldsymbol{h}\cdot\boldsymbol{x} = \frac{1}{2}(\boldsymbol{x} - \Gamma^{-1}\boldsymbol{h})\cdot[\Gamma(\boldsymbol{x} - \Gamma^{-1}\boldsymbol{h})] - \frac{1}{2}(\Gamma^{-1}\boldsymbol{h})\cdot[\Gamma(\Gamma^{-1}\boldsymbol{h})]$. Show then that$\langle \boldsymbol{x} \rangle = \Gamma^{-1}\boldsymbol{h}$. Prove also that $\langle e^{\boldsymbol{h}\cdot\boldsymbol{x}} \rangle = e^{\frac{1}{2}\boldsymbol{h}\cdot(\Gamma^{-1}\boldsymbol{h})}$.

Answer: The first equality can be found by expanding the right-hand side. Then, we write $\langle e^{\boldsymbol{h}\cdot\boldsymbol{x}}\rangle = Z(\mathbf{0})^{-1}\int d\boldsymbol{x}\, e^{-\frac{1}{2}\boldsymbol{x}\cdot(\Gamma\boldsymbol{x})+\boldsymbol{h}\cdot\boldsymbol{x}}$, which we cast in the form $\langle e^{\boldsymbol{h}\cdot\boldsymbol{x}}\rangle = e^{\frac{1}{2}\boldsymbol{h}\cdot(\Gamma^{-1}\boldsymbol{h})}Z(\mathbf{0})^{-1}\int d\boldsymbol{x}\, e^{-\frac{1}{2}\mathbf{y}\cdot(\Gamma\mathbf{y})}$, where $\mathbf{y} = \boldsymbol{x} - \Gamma^{-1}\boldsymbol{h}$. Changing the integration variable from $\boldsymbol{x}$ to $\mathbf{y}$ is just a translation (with unit Jacobian) and thus $\langle e^{\boldsymbol{h}\cdot\boldsymbol{x}}\rangle = e^{\frac{1}{2}\boldsymbol{h}\cdot(\Gamma^{-1}\boldsymbol{h})}$, by definition of $Z(\mathbf{0})$. As a byproduct, we get $\langle\boldsymbol{x}\rangle = \Gamma^{-1}\boldsymbol{h}$.

3.4 In order to establish that $Z(\mathbf{0}) = \frac{(2\pi)^{n/2}}{\sqrt{\det\Gamma}}$, we introduce the eigenvalues $\lambda_1,\dots,\lambda_n$ of Γ. We define the diagonal matrix $D = \begin{pmatrix}\lambda_1 & & \\ & \ddots & \\ & & \lambda_n\end{pmatrix}$, and we denote by Q the matrix such that $\Gamma = QDQ^T$. By changing variables from $\boldsymbol{x}$ to $\mathbf{y} = Q^{-1}\boldsymbol{x}$, find the announced expression for $Z(\mathbf{0})$.

Answer: Given Γ has been assumed symmetric we know that not only Q exists but it also verifies $Q^T = Q^{-1}$. This ensures in particular that the Jacobian of the change of variable from $\boldsymbol{x}$ to $\mathbf{y}$ is unity, as $|\det Q| = 1$. As a result $Z(\mathbf{0}) = \int d\mathbf{y} e^{-\frac{1}{2}y_i P_{ij} y_j} = \prod_i\left(\int dy_i e^{-\frac{1}{2}y_i\lambda_i y_i}\right) = \prod_i\left(\sqrt{\frac{2\pi}{\lambda_i}}\right) = \frac{(2\pi)^{n/2}}{\sqrt{\det\Gamma}}$

3.5 Let $G_{ij} = \langle x_i x_j\rangle$. Prove that $G_{ij} = \left.\dfrac{\partial^2 \ln Z(\boldsymbol{h})}{\partial h_i\partial h_j}\right|_{\boldsymbol{h}=\mathbf{0}}$.

3.6 Show then that $G = \Gamma^{-1}$.

Answer: Once we know that $G_{ij} = \left.\frac{\partial^2 \ln Z(\boldsymbol{h})}{\partial h_i\partial h_j}\right|_{\boldsymbol{h}=\mathbf{0}}$, or, equivalently, that $G_{ij} = \left.\frac{\partial^2 \ln Z(\boldsymbol{h})/Z(\mathbf{0})}{\partial h_i\partial h_j}\right|_{\boldsymbol{h}=\mathbf{0}}$, we use that $\ln Z(\boldsymbol{h})/Z(\mathbf{0}) = \frac{1}{2}\boldsymbol{h}\cdot(\Gamma^{-1}\boldsymbol{h})$, which we differentiate with respect to h_i and then h_j.

3.7 *More difficult; skip if short on time.* Show that $G_{ij} = -2\frac{\partial\ln Z(\mathbf{0})}{\partial\Gamma_{ij}}$. Using that $\frac{\partial\det\Gamma}{\partial\Gamma_{ij}} = \det\Gamma(\Gamma^{-1})_{ji}$, get to the same conclusion that $G = \Gamma^{-1}$.

Answer: To prove that $\frac{\partial\det\Gamma}{\partial\Gamma_{ij}} = \det\Gamma(\Gamma^{-1})_{ji}$ for a given pair (i,j), we introduce E, an $n\times n$ matrix whose elements are all zero, except for the (i,j) one, $E_{ij} = \varepsilon$. By definition, $\frac{\partial\det\Gamma}{\partial\Gamma_{ij}} = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(\det(\Gamma+E) - \det\Gamma)$. We use that $\det(I + \Gamma^{-1}E) = 1 + \mathrm{Tr}(\Gamma^{-1}E) + \mathcal{O}(\varepsilon^2) = 1 + \varepsilon(\Gamma^{-1})_{ji} + \mathcal{O}(\varepsilon^2)$ to conclude.

3.8 *Skip if short on time, but stare at the result a little while.* Prove that $\langle x_1x_2x_3x_4\rangle = G_{12}G_{34} + G_{13}G_{24} + G_{14}G_{23}$.

Answer: Since $\langle x_1x_2x_3x_4\rangle = Z(\mathbf{0})^{-1}\left.\frac{\partial^4 Z(\boldsymbol{h})}{\partial h_{i_1}\partial h_{i_2}\partial h_{i_3}\partial h_{i_4}}\right|_{\boldsymbol{h}=\mathbf{0}}$, we also have that

$$\langle x_1x_2x_3x_4\rangle = \left.\frac{\partial^4 e^{\frac{1}{2}\boldsymbol{h}\cdot(\Gamma^{-1}\boldsymbol{h})}}{\partial h_{i_1}\partial h_{i_2}\partial h_{i_3}\partial h_{i_4}}\right|_{\boldsymbol{h}=\mathbf{0}}.$$

This is a tedious but straightforward derivation.

Using the same method as above, one can show that an arbitrary average $\langle x_{i_1}\dots x_{i_{2m}}\rangle$ can be written in terms of the elements of G. This result is known as Wick's theorem. The idea goes as as follows. Consider first a pairing of the indices $\{i_1,\dots,i_{2n}\}$, namely a (non ordered) set of n pairs made of the $2n$ original indices, which we write $\{(j_1,j_2),(j_3,j_4),\dots,(j_{2n-1},j_{2n})\}$. Take now the product of all the $G_{j_1,j_2}\dots G_{j_{2n-1},j_{2n}}$. One obtains $\langle x_{i_1}\dots x_{i_{2m}}\rangle$ as the summation over all possible pairings $\{(j_1,j_2),(j_3,j_4),\dots,(j_{2n-1},j_{2n})\}$ of $G_{j_1,j_2}\dots G_{j_{2n-1},j_{2n}}$. There are altogether $(2n-1)!! = (2n-1)(2n-3)\dots 1$ such pairings, and thus as many terms in the summation. For instance with $n = 3$ (6 indices), one can form $5\times 3 = 15$ pairings.

The following manipulations will be reviewed during the lectures and tutorials. They are not, strictly speaking, prerequisites. We now turn to a direct application in terms of fields living in continuum space. Below, $\mathcal{D}m$ is then a shorthand for $dm_1dm_2...dm_N$, for a scalar field m defined on a N-site lattice, taking furthermore the limit $N\to\infty$. The resulting object is called a functional integral *and to tame such a* *construction, be discrete and think of $\mathcal{D}m$ as referring to a finite but large product $dm_1dm_2...dm_N$. When dealing with a vectorial field $\mathbf{m}$ as in the remainder, the product defining $\mathcal{D}\boldsymbol{m}$ should be considered for all n components of $\boldsymbol{m}$. Beware also that from now on, $\boldsymbol{x}$ no longer is a Gaussian vector, but simply a position in space that now plays a role similar to the index $i = 1, \ldots, N$ in the lattice case.*

3.9 Let $Z[\boldsymbol{h}] = \int \mathcal{D}\boldsymbol{m}\, e^{-H[\boldsymbol{m}]+\int d\boldsymbol{x} \boldsymbol{h}(\boldsymbol{x})\cdot\boldsymbol{m}(\boldsymbol{x})}$, where $H[\boldsymbol{m}] = \int_{L^d} d\boldsymbol{x} \left(\frac{1}{2}\partial_\mu m_i \partial_\mu m_i + \frac{t}{2} m_i m_i\right)$ and periodic boundary conditions in space are assumed (space integrals run over a cubic volume L^d). One should keep in mind that in the discrete formulation on a lattice, we are back to a Gaussian problem of the same type as above, with an appropriate choice for the matrix Γ. Hence, "$\boldsymbol{m}$" can be viewed as a (infinite) collection of vectorial correlated Gaussian variables, each of them being $\boldsymbol{m}(\boldsymbol{x})$, where $\boldsymbol{x}$ is a continuous coordinate. The index $\mu = 1, \ldots, d$ refers to a space direction while $i = 1, \ldots, n$ refers to a component of $\boldsymbol{m}$ and summation over repeated indices is implied as earlier. Verify that with $\Gamma_{i,i'}(\boldsymbol{x}, \boldsymbol{x}') = \delta_{i,i'}\delta^{(d)}(\boldsymbol{x}-\boldsymbol{x}')(-\Delta_{\boldsymbol{x}}+t)$ we then have $H = \frac{1}{2}\int_{L^d} d\boldsymbol{x}\, d\boldsymbol{x}' \sum_{i,i'} m_i(\boldsymbol{x})\, \Gamma_{i,i'}(\boldsymbol{x}, \boldsymbol{x}')\, m_{i'}(\boldsymbol{x}')$. Our goal is next to compute the correlation function $G_{i,i'}(\boldsymbol{x}, \boldsymbol{x}') = \langle m_i(\boldsymbol{x})\, m_{i'}(\boldsymbol{x}')\rangle$, and related quantities.

3.10 Going to Fourier space, show that $\widetilde{\Gamma}_{i,i'}(\boldsymbol{q}, \boldsymbol{q}') = \delta_{i,i'}\,(2\pi)^d\,\delta^{(d)}(\boldsymbol{q}+\boldsymbol{q}')\,(\boldsymbol{q}^2+t)$.

Answer: We Fourier transform Γ with respect to $\boldsymbol{x}$ and $\boldsymbol{x}'$ to get the desired expression

$$\begin{aligned}\widetilde{\Gamma}_{i,i'}(\boldsymbol{q}, \boldsymbol{q}') &= \delta_{i,i'}\int d\boldsymbol{x} d\boldsymbol{x}' \delta^{(d)}(\boldsymbol{x}-\boldsymbol{x}')\,(-\Delta_{\boldsymbol{x}}+t)\; e^{i\boldsymbol{q}\cdot\boldsymbol{x}}\, e^{i\boldsymbol{q}'\cdot\boldsymbol{x}'} = \delta_{i,i'}\int d\boldsymbol{x}(q^2+t)\, e^{i(\boldsymbol{q}+\boldsymbol{q}')\cdot\boldsymbol{x}} \\ &= \delta_{i,i'}\,(\boldsymbol{q}^2+t)\,(2\pi)^d\,\delta^{(d)}(\boldsymbol{q}+\boldsymbol{q}').\end{aligned}$$

3.11 Note that Γ is an operator and not a matrix anymore. Let $G = \Gamma^{-1}$. The equation defining the components of G is $\sum_{i'}\int d\boldsymbol{x}'\, \Gamma_{i,i'}(\boldsymbol{x}, \boldsymbol{x}')\; G_{i',i''}(\boldsymbol{x}', \boldsymbol{x}'') = \delta_{i,i''}\,\delta^{(d)}(\boldsymbol{x}''-\boldsymbol{x})$. Deduce from this result that $\widetilde{G}_{i,i'}(\boldsymbol{q}, \boldsymbol{q}') = (2\pi)^d\,\delta^{(d)}(\boldsymbol{q}+\boldsymbol{q}')\,\delta_{i,i'}\,(\boldsymbol{q}^2+t)^{-1}$. This is telling us that the correlation function reads

$$G_{i,i'}(\boldsymbol{x}, \boldsymbol{x}') = \left\langle m_i(\boldsymbol{x}) m_{i'}(\boldsymbol{x}')\right\rangle = \delta_{i,i'}\int \frac{d\boldsymbol{q}}{(2\pi)^d}\,\frac{e^{i\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{x}')}}{\boldsymbol{q}^2+t}. \tag{1}$$

Answer: We start from Plancherel-Parseval relation:

$$\int d\boldsymbol{x}'\, \Gamma_{i,i'}(\boldsymbol{x}, \boldsymbol{x}')\; G_{i',i''}(\boldsymbol{x}', \boldsymbol{x}'') = \int \frac{d\boldsymbol{q}'}{(2\pi)^d}\, \Gamma_{i,i'}(\boldsymbol{x}, -\boldsymbol{q}')\; G_{i',i''}(\boldsymbol{q}', \boldsymbol{x}'')$$

being somewhat cavalier with notation (the arguments of the functions tell us if we deal with an object in real space, in Fourier space, or mixed as on the rhs). We subsequently Fourier transform

$$\sum_{i'}\int \frac{d\boldsymbol{q}'}{(2\pi)^d}\, \Gamma_{i,i'}(\boldsymbol{x}, -\boldsymbol{q}')\; G_{i',i''}(\boldsymbol{q}', \boldsymbol{x}'') = \delta_{i,i''}\,\delta^{(d)}(\boldsymbol{x}''-\boldsymbol{x})$$

with respect to $\boldsymbol{x}$ and $\boldsymbol{x}''$:

$$\sum_{i'}\int \frac{d\boldsymbol{q}'}{(2\pi)^d}\, \widetilde{\Gamma}_{i,i'}(\boldsymbol{q}, -\boldsymbol{q}')\, \widetilde{G}_{i',i''}(\boldsymbol{q}', \boldsymbol{q}'') = \delta_{i,i''}\,(2\pi)^d\,\delta^{(d)}(\boldsymbol{q}+\boldsymbol{q}'').$$

Inserting the above expression for $\widetilde{\Gamma}_{i,i'}(\boldsymbol{q}, \boldsymbol{q}')$ yields $\widetilde{G}_{i,i'}(\boldsymbol{q}, \boldsymbol{q}') = (2\pi)^d\delta^{(d)}(\boldsymbol{q}+\boldsymbol{q}')\delta_{i,i'}/(\boldsymbol{q}^2+t)$.
Thus,

$$\begin{aligned}G_{i,i'}(\boldsymbol{x}, \boldsymbol{x}') &= \left\langle m_i(\boldsymbol{x}) m_{i'}(\boldsymbol{x}')\right\rangle = \int \frac{d\boldsymbol{q}}{(2\pi)^d}\,\frac{d\boldsymbol{q}'}{(2\pi)^d}\,(2\pi)^d\,\delta^{(d)}(\boldsymbol{q}+\boldsymbol{q}')\,\delta_{i,i'}\,\frac{1}{\boldsymbol{q}^2+t}\,e^{i\boldsymbol{q}\cdot\boldsymbol{x}+\boldsymbol{q}'\cdot\boldsymbol{x}'} \\ &= \delta_{i,i'}\int \frac{d\boldsymbol{q}}{(2\pi)^d}\,\frac{e^{i\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{x}')}}{\boldsymbol{q}^2+t}.\end{aligned}$$

Note that the function $\boldsymbol{x} \mapsto \int \frac{d\boldsymbol{q}}{(2\pi)^d}\frac{\exp(i\boldsymbol{q}\cdot\boldsymbol{x})}{\boldsymbol{q}^2+t}$ is not defined at $\boldsymbol{x} = \boldsymbol{0}$ (except in $d = 1$) due to a large $\boldsymbol{q}$ divergence. In condensed-matter physics, this divergence is an artifact of the continuum space limit from which we started. At large $\boldsymbol{q}$, or equivalently at short distances, the continuum expression is simply not valid. For instance, magnetization is carried by ions living on an underlying lattice structure. In polymer or liquid-crystal physics, the short-distance cut-off signalling the breakdown of the continuum limit is played by the elementary monomer size or by the molecular size, respectively. Hence, if the short distance behavior is needed, one must return to a description going beyond the continuum limit valid only at scales large with respect to the microscopic ones.

3.12 Show that in the absence of an external magnetic field, $\langle \boldsymbol{m}(\boldsymbol{x}) \cdot \boldsymbol{m}(\mathbf{y})\rangle = n \int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{e^{i\boldsymbol{q}\cdot(\boldsymbol{x}-\mathbf{y})}}{q^2+t}$.

Answer: Comes straightforwardly from $\langle \boldsymbol{m}(\boldsymbol{x}) \cdot \boldsymbol{m}(\mathbf{y})\rangle = \sum_i G_{i,i}(\boldsymbol{x},\mathbf{y})$.

3.13 What is the effect of having a non vanishing external field $\boldsymbol{h}(\boldsymbol{x})$ (no calculations asked)? Compute then $\langle \boldsymbol{m}(\boldsymbol{x})\rangle$ as a function of $\widetilde{\boldsymbol{h}}(\boldsymbol{q})$. What happens if $\boldsymbol{h}$ is uniform?

Answer: Not much changes, as long as we work with the "shifted" field $\boldsymbol{m} - \langle \boldsymbol{m}\rangle$, with mean value subtracted. For computing this mean value, we use the discrete result of question 3 above ($\langle \boldsymbol{x}\rangle = \Gamma^{-1}\boldsymbol{h}$), but we have to pay some attention in mapping discrete sums with integrals. The counterpart of $\Gamma_{ij} m_i m_j$ (implicit summation over repeated indices as always) is $\int d\boldsymbol{x} d\boldsymbol{x}' m(\boldsymbol{x}) m(\boldsymbol{x}') \dots$ and we can proceed, writing

$$\langle m_i(\boldsymbol{x})\rangle = \sum_{i'} \int d\boldsymbol{x}' G_{i,i'}(\boldsymbol{x},\boldsymbol{x}')\, h_{i'}(\boldsymbol{x}') = \int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{e^{i\boldsymbol{q}\cdot\boldsymbol{x}}}{\boldsymbol{q}^2+t} \widetilde{h}_i(-\boldsymbol{q}).$$

This simplifies into $\langle \boldsymbol{m}\rangle = \boldsymbol{h}/t$ when $\boldsymbol{h}$ is uniform. This can be recovered directly from the simpler description where all gradient terms in our Hamiltonian are dropped, restricting ourselves to $\boldsymbol{x}$-independent fields $\boldsymbol{m}$. We then have $H = Vt\boldsymbol{m}^2/2 - V\boldsymbol{h}\cdot\boldsymbol{m}$ where V is the system's volume, which drops out from the calculation of the mean value.

3.14 If $\boldsymbol{j}$ is an n-component constant vector and $\boldsymbol{h} = \boldsymbol{0}$, show that

$$\langle e^{\boldsymbol{j}\cdot\boldsymbol{m}(\boldsymbol{x})}\rangle = e^{\boldsymbol{j}^2 G(\boldsymbol{0})/2},$$

where G is given by Eq. (2) below. The latter is not always well defined ; this depends on space dimension. For instance, a divergent $G(\boldsymbol{0})$ would be an artifact of our continuous space description.

Answer: We have shown that for a Gaussian discrete vectorial variable $\boldsymbol{X}$, of $\boldsymbol{0}$-mean, $\langle \exp(\boldsymbol{H}\cdot\boldsymbol{X})\rangle = \exp(H_i G_{ij} H_j/2)$ where G_{ij} is the correlation function $\langle X_i X_j\rangle$. This result is generalized here to the continuous case:

$$\langle e^{\boldsymbol{j}\cdot\boldsymbol{m}(\boldsymbol{x})}\rangle = \langle e^{\int \boldsymbol{H}(\boldsymbol{x}')\cdot\boldsymbol{m}(\boldsymbol{x}')\, d\boldsymbol{x}'}\rangle = e^{\frac{1}{2}\int d\mathbf{y} d\mathbf{y}' H_i(\mathbf{y}) G_{ij}(\mathbf{y},\mathbf{y}') H_j(\mathbf{y}')} = e^{\frac{1}{2}\int d\mathbf{y} d\mathbf{y}' H_i \langle m_i(\mathbf{y}) m_j(\mathbf{y}')\rangle H_j},$$

with $H_i(\mathbf{y}) = j_i\, \delta^{(d)}(\mathbf{y}-\boldsymbol{x})$. This simplifies into $\langle e^{\boldsymbol{j}\cdot\boldsymbol{m}(\boldsymbol{x})}\rangle = e^{\frac{1}{2}\boldsymbol{j}^2 G(\boldsymbol{0})}$ where $G(\boldsymbol{0}) = \int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{1}{q^2+t}$. We have already discussed in the correction of question 11 that in practice this Fourier integral, which is based on the use of a continuum limit, is not always appropriate ($G(\boldsymbol{0})$ diverges for $d \geq 2$). Instead, one must resort to an expression in which the Fourier transform lives on a lattice. Spatial derivatives become finite differences. On a cubic lattice, this has the effect of replacing $\boldsymbol{q}^2$ with $a^{-2}\left(2 - \frac{2}{d}\sum_{\mu=1}^{d} \cos(q_\mu a)\right)$ (whose $a \to 0$ limit is indeed $\boldsymbol{q}^2$), and $\int \frac{d\boldsymbol{q}}{(2\pi)^d}$ becomes $\sum_{\boldsymbol{q}}$ with the $\boldsymbol{q}$ components being now quantized as in question 1 of section 2.
To be specific, we discuss the case $d = 1$ and for $n = 1$, where there is actually no short-distance singularity so that the discrete and continuous descriptions should match if appropriately compared. Instead of $H[m] = \int dx\, \left[(\partial_x m)^2 + t\, m^2\right]/2$, one would have here

$$H[m] = a^{-1}\sum_x \left\{ \frac{1}{2}\left[m(x+a) - m(x)\right]^2 + a^2\, \frac{t}{2}\, m^2(x) \right\}$$

with $x = ja$ and $j = 0, \dots, N-1$ is a site index; then one finds $G(x) = \frac{a}{N}\sum_q \frac{e^{iqx}}{ta^2+2-2\cos qa}$ with $q = \frac{2k\pi}{Na}$, $k = -N/2{+}1, \dots, N/2$. In the large N limit, we arrive at $G(x) = a^2 \int_{-\pi/a}^{\pi/a} \frac{dq}{2\pi} \frac{e^{iqx}}{ta^2+2-2\cos qa}$ and $G(0) = [t(4{+}ta^2)]^{-1/2}$. It is also possible to determine the difference $G(x) - G(0)$ as $t \to 0^+$ on a finite lattice: $\lim_{t\to 0^+}(G(x=ja) - G(0)) = -a\frac{j(N-j)}{2N}$ where $j = 0, \dots, N-1$.
In the next exercise, we will compute a related $G(x)$, that given by Eq. (2) for $d = 1$, associated to the Hamiltonian $\int dx\, \left[(\partial_x m)^2 + t\, m^2\right]/2$, which yields $1/(2\sqrt{t})$ when evaluated at $x = 0$. This is fully compatible with our $[t(4 + ta^2)]^{-1/2}$ result above for $G(0)$, taking $a \to 0$..

3.15 Under the same condition, show that

$$\langle e^{\boldsymbol{j}\cdot[\boldsymbol{m}(\boldsymbol{x})-\boldsymbol{m}(\boldsymbol{x}')]}\rangle = e^{\left[j^2 G(0) - j^2 G(\boldsymbol{x}-\boldsymbol{x}')\right]}.$$

Answer: We could proceed as in the previous question by defining an *ad hoc* field

$$\boldsymbol{h}(\mathbf{y}) \;=\; \boldsymbol{j}\left(\delta^{(d)}(\mathbf{y}-\boldsymbol{x}) - \delta^{(d)}(\mathbf{y}-\boldsymbol{x}')\right)$$

and by writing that $\langle e^{\boldsymbol{j}\cdot[\boldsymbol{m}(\boldsymbol{x})-\boldsymbol{m}(\boldsymbol{x}')]}\rangle = e^{\frac{1}{2}\int d\mathbf{y}d\mathbf{y}' h_i(\mathbf{y})G_{ij}(\mathbf{y},\mathbf{y}')h_j(\mathbf{y}')}$. An alternative is to note that $\boldsymbol{m}(\boldsymbol{x}) - \boldsymbol{m}(\boldsymbol{x}')$ is yet another Gaussian variable (not a collection thereof, but a mere n-dimensional such vector) and to invoke the cumulant property

$$\left\langle e^{\boldsymbol{j}\cdot[\boldsymbol{m}(\boldsymbol{x})-\boldsymbol{m}(\boldsymbol{x}')]}\right\rangle \;=\; e^{j_\ell\, K_{\ell p}\, j_p\,/2}$$

where $K_{\ell p} = \left\langle[m_\ell(\boldsymbol{x}) - m_\ell(\boldsymbol{x}')][m_p(\boldsymbol{x}) - m_p(\boldsymbol{x}')]\right\rangle \;=\; \delta_{\ell p}\;[2G(\mathbf{0}) - 2G(\boldsymbol{x}-\boldsymbol{x}')]$ with $G(\boldsymbol{x}-\boldsymbol{x}')$ defined as in the rhs of Eq. (1), but without the $\delta_{i,i'}$ (see Eq. (2) below). Hence

$$\left\langle e^{\boldsymbol{j}\cdot[\boldsymbol{m}(\boldsymbol{x})-\boldsymbol{m}(\boldsymbol{x}')]}\right\rangle \;=\; e^{\left[j^2G(0) - j^2 G(\boldsymbol{x}-\boldsymbol{x}')\right]}.$$

We note that for $|\boldsymbol{x}-\boldsymbol{x}'| \to \infty$, the above result reduces to $e^{j^2G(0)} = \langle e^{\boldsymbol{j}\cdot\boldsymbol{m}(\boldsymbol{x})}\rangle^2$, as it should.

Two technical side comments. To show the Wick theorem, one can use repeatedly the identity, valid for Gaussian variables and any function f:

$$\langle x_i\, f(\boldsymbol{x})\rangle \;=\; \sum_j \langle x_i x_j\rangle \left\langle \frac{\partial f}{\partial x_j}\right\rangle.$$

In addition, the key result $\langle x_i x_j\rangle = (\Gamma^{-1})_{ij}$ can be recovered by the following trick, arguably the most expedient. We start by endowing our Gaussian vector $\boldsymbol{x}$ with a mean, denoted $\boldsymbol{a}$:

$$a_\ell \;=\; \mathcal{N}\int d\boldsymbol{x}\, x_\ell\, \exp\left(-\frac{1}{2}\Gamma_{ij}(x_i - a_i)(x_j - a_j)\right),$$

where $\mathcal{N}$ is the normalization factor, independent of $\boldsymbol{a}$. Taking the derivative wrt a_k, we get

$$\delta_{k\ell} \;=\; \mathcal{N}\int d\boldsymbol{x}\, x_\ell\, \Gamma_{km}(x_m - a_m)\exp\left(-\frac{1}{2}\Gamma_{ij}(x_i - a_i)(x_j - a_j)\right).$$

Taking now $\boldsymbol{a} = 0$, this yields $\delta_{k\ell} = \Gamma_{km}\langle x_m x_\ell\rangle$, or equivalently $\langle x_m x_\ell\rangle = (\Gamma^{-1})_{m\ell}$.

Remember that for a Gaussian distribution with probability density $P(x_1, \ldots x_n) \propto \exp(-\Gamma_{ij}\, x_i x_j/2)$, it is the matrix inverse of Γ that gives the covariances as $\langle x_i x_j\rangle \;=\; (\Gamma^{-1})_{ij}$. Two other properties are also often useful. First the cumulant generating relation

$$\frac{\int_{\mathbb{R}^n} dx_1 \ldots dx_n \exp\left(-\frac{1}{2}\Gamma_{ij}\, x_i x_j \;+\; h_i x_i\right)}{\int_{\mathbb{R}^n} dx_1 \ldots dx_n \exp\left(-\frac{1}{2}\Gamma_{ij}\, x_i x_j\right)} \;=\; \exp\left[\frac{1}{2}\, h_i\, (\Gamma^{-1})_{ij}\, h_j\right].$$

Second, Wick's theorem according to which higher order mean values follow from tracking all possible pairing of the corresponding indices:

$$\langle x_1x_2x_3x_4\rangle \;=\; \langle x_1x_2\rangle\langle x_3x_4\rangle + \langle x_1x_3\rangle\langle x_2x_4\rangle + \langle x_1x_4\rangle\langle x_2x_3\rangle.$$

This implies in particular that $\langle x_i^4\rangle \;=\; 3\langle x_i^2\rangle^2$. When dealing with a Gaussian vector (or variable) of non-vanishing mean, one has first to shift $\boldsymbol{x}$ by its mean value to use the above results. This means in particular that $\langle x_i x_j\rangle - \langle x_i\rangle\langle x_j\rangle \;=\; (\Gamma^{-1})_{ij}$. Note finally that the cumulant property implies that the cumulant generating function stops at order 2, a distinctive feature of Gaussian variables:

$$\boxed{\left\langle e^{hX}\right\rangle \;=\; e^{h\langle X\rangle + \frac{h^2}{2}\,\langle X^2\rangle_c}},$$

where $\langle X^2\rangle_c$ is the variance (second cumulant).
Important. When dealing with Gaussian fields (infinite collection of variables), and in case of doubt, it is always possible to go back to the discrete formulation with a Gaussian vector having a large number of components.
Finally, correlation functions of the type

$$G(\boldsymbol{x}) \;=\; \int \frac{d\boldsymbol{q}}{(2\pi)^d}\,\frac{e^{i\boldsymbol{q}\cdot\boldsymbol{x}}}{\boldsymbol{q}^2 + t} \tag{2}$$

are often met in statistical physics, since they arise within a Gaussian description. Computing such an integral is feasible with the residue theorem, in dimension $d = 1$ (see next exercise) and $d = 3$ where it yields

$$G(\boldsymbol{r}) \;=\; \frac{1}{4\pi r}\, e^{-r\sqrt{t}}.$$

In other space dimensions, the result is more involved. It is in particular wrong to write $G(\boldsymbol{r})$, as sometimes found, as $e^{-r\sqrt{t}}/r^{d-2}$, up to some constant. Such an expression does not even give the right large r behavior.

4 Green's functions

You may have encountered Green's function when trying to solve a linear problem involving a field created by some sources (for instance, in the case of the Poisson equation $-\Delta\phi = \frac{\rho}{\varepsilon_0}$ where the charge density ρ is given, and you try to compute the electrostatic potential ϕ). The connection with the previous section is the following. Take a Gaussian variable $\boldsymbol{x}$ with an energy function $\frac{1}{2}\boldsymbol{x}\cdot(\Gamma\boldsymbol{x}) - \boldsymbol{h}\cdot\boldsymbol{x}$. If the external field $\boldsymbol{h}$ is zero, then of course $\langle\boldsymbol{x}\rangle$ vanishes as well. However, if $\boldsymbol{h}\neq\boldsymbol{0}$, then $\langle\boldsymbol{x}\rangle$ takes a nonzero value. It is not hard to realize that $\Gamma\langle\boldsymbol{x}\rangle = \boldsymbol{h}$: this is a linear problem with a source $\boldsymbol{h}$ driving a nonzero response $\langle\boldsymbol{x}\rangle$. Finding the response involves inverting Γ: $\langle\boldsymbol{x}\rangle = G\,\boldsymbol{h}$, where $G = \Gamma^{-1}$ is the Green's function. It is always good to have a small mental library of common Green's functions. If $\Gamma(\boldsymbol{x},\boldsymbol{x}')$ is an operator, the fact that $G(\boldsymbol{x},\boldsymbol{x}')$ is its Green's function means that $\int d\mathbf{y}\,\Gamma(\boldsymbol{x},\mathbf{y})\,G(\mathbf{y},\boldsymbol{x}') = \delta^{(d)}(\boldsymbol{x}-\boldsymbol{x}')$. The Green's function G can be a distribution.

4.1 We seek for G when $\Gamma(\boldsymbol{x},\mathbf{y}) = \delta^{(d)}(\boldsymbol{x}-\mathbf{y})(-\Delta_{\boldsymbol{x}}+r)$. Such a Γ appears in a number of contexts, from particle physics to condensed or soft matter. In the present case, we have that $(-\Delta_{\boldsymbol{x}}+r)G(\boldsymbol{x},\mathbf{y}) = \delta^{(d)}(\boldsymbol{x}-\mathbf{y})$. This differential equation admits a solution that is translation invariant, $G(\boldsymbol{x}-\mathbf{y})$. Find a Fourier representation of G.

> Answer: We Fourier-transform the differential equation to get $G(\boldsymbol{x}-\mathbf{y}) = \int \frac{d\boldsymbol{q}}{(2\pi)^d}\frac{e^{i\boldsymbol{q}\cdot(\boldsymbol{x}-\mathbf{y})}}{q^2+r}$.

4.2 Compute the explicit form of $G(x-y)$ in the $d=1$ case in real space, for $r>0$ and then for vanishing r.

> Answer: We find (*e.g.*, using a contour integral) $G(x-y) = \frac{e^{-\sqrt{r}|x-y|}}{2\sqrt{r}}$ for $r>0$ and $G(x-y) = -\frac{1}{2}|x-y|$ for $r=0$. The latter corresponds to the one-dimensional Coulomb potential (think e.g. of the potential created by an infinite uniformly charged plate, which is linear in the distance x to the plate.

4.3 Let $\Gamma(t,t') = \delta(t-t')\frac{d}{dt'}$. Find $G(t,t')$.

> Answer: $G(t,t') = \Theta(t-t')$ is the Heaviside step function.

We finish with two more examples that connect with other areas of physics. First, $\Gamma(x,t;x',t') = \delta(t-t')\delta(x-x')\left[\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right]$. This yields the heat equation, that admits the diffusion kernel

$$G(\boldsymbol{x},t;\boldsymbol{x}',t') \;=\; \Theta(t-t')\frac{e^{-\frac{(\boldsymbol{x}-\boldsymbol{x}'))^2}{4D(t-t')}}}{\sqrt{4\pi D(t-t')}^{d}}$$

as a Green's function. The step function makes causality explicit.

Second, we consider $\Gamma(x,t;x',t') = \delta(t-t')\delta(x-x')\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right]$, the Green's function of which turns out to be problematic. Such a kernel Γ shows up in the Lorentz gauge, where Maxwell's equations read $\Box\vec{A} = \mu_0\vec{j}$ and $\Box\phi = \rho/\varepsilon_0$; $\Box$ is the three dimensional generalization of the wave operator $\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}$. The question is tricky, since Γ is strictly speaking not invertible. Depending on the subspace of functions one is working with, it does admit different Green's function (advanced, retarded, Feynman).

5 Legendre transform

Let $Z(\boldsymbol{h}) = \int d\boldsymbol{x}e^{-H(\boldsymbol{x})+\boldsymbol{x}\cdot\boldsymbol{h}}$ be a function of a vector $\boldsymbol{h}$ that can be interpreted as the canonical partition function of a system characterized by the $\boldsymbol{x}$ degrees of freedom in some external field $\boldsymbol{h}$. We use a continuum notation for $\boldsymbol{x}$, but these could also be discrete variables like Ising spins. The (opposite and dimensionless) free energy is $W(\boldsymbol{h}) = \ln Z(\boldsymbol{h})$. Here, unlike in section 3, we do not assume H to be quadratic.

5.1 Angular brackets $\langle\ldots\rangle$ denote an average with respect to $\dfrac{e^{-H(\boldsymbol{x})+\boldsymbol{x}\cdot\boldsymbol{h}}}{Z(h)}$. Show that $\langle x_i\rangle = \left.\dfrac{\partial W}{\partial h_i}\right|$.

5.2 Show that $G_{ij} = \langle x_i x_j\rangle - \langle x_i\rangle\langle x_j\rangle = \left.\dfrac{\partial^2 W}{\partial h_i\partial h_j}\right|$.

5.3 Let $\xi_i(\boldsymbol{h}) = \frac{\partial W}{\partial h_i}$. We denote by $h_i(\boldsymbol{\xi})$ the inverse function giving $\boldsymbol{h}$ as a function of $\boldsymbol{\xi}$ and we define $\Gamma(\boldsymbol{\xi}) = \boldsymbol{\xi}\cdot\boldsymbol{h} - W(\boldsymbol{h})$ but what we really mean is $\Gamma(\boldsymbol{\xi}) = \boldsymbol{\xi}\cdot\boldsymbol{h}(\boldsymbol{\xi}) - W(\boldsymbol{h}(\boldsymbol{\xi}))$. This Γ depends on $\boldsymbol{\xi}$ only. It is the Legendre transform of $-W$ (see the comment below for the sign convention). Show that $\partial\Gamma/\partial\xi_i = h_i$.

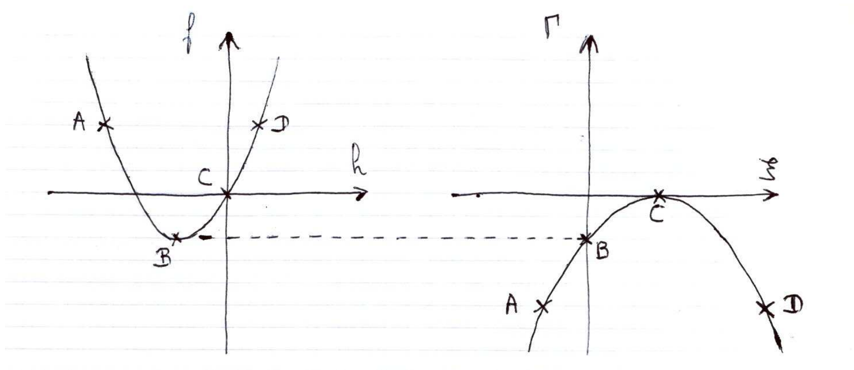
Answer: $d\Gamma = -dW + h_i d\xi_i + \xi_i dh_i = h_i d\xi_i$.

5.4 Let $\Gamma_{ij} = \frac{\partial^2 \Gamma}{\partial \xi_i \partial \xi_j}$ evaluated at $\boldsymbol{\xi} = \langle \boldsymbol{x} \rangle$. Prove that $G = \Gamma^{-1}$.

Answer: We start from $\frac{\partial \Gamma}{\partial \xi_i} = h_i$ and we differentiate a second time wrt ξ_j: $\frac{\partial^2 \Gamma}{\partial \xi_j \partial \xi_i} = \frac{\partial h_i}{\partial \xi_j}$. But given that $\frac{\partial h_i}{\partial \xi_j} G_{jk} = \frac{\partial h_i}{\partial \xi_j} \frac{\partial \xi_j}{\partial h_k} = \delta_{ik}$, we have found that indeed ΓG is the identity matrix.

Physical meaning of $\Gamma(\boldsymbol{\xi})$: In much the same way as W is the proper thermodynamic potential at fixed $\boldsymbol{h}$, we can see Γ as the thermodynamic potential in the conjugate ensemble in which one would be working at fixed average $\langle \boldsymbol{x} \rangle$. In a more standard language, in the canonical ensemble $F(V) = -k_{\mathrm{B}} T \ln Z(V)$ is the free energy at fixed volume and the pressure is $P = -\frac{\partial F}{\partial V}$, but working in the isobaric ensemble leads to the free enthalpy $G(P) = F + PV$ being the natural potential, which verifies $\langle V \rangle = \frac{\partial G}{\partial P}$. In the magnetic language, these results apply as well (fixed magnetic field versus fixed magnetization).

Remember that there exist a number of variants for defining the Legendre transform, with different conventions. A common choice, starting from a function $f(h)$ is to define $\Gamma = f(h) - hf'(h)$, understood as a function of "the slope" $\xi = f'(h)$. It is then important that f be convex, so that h can be expressed univocally as a function of ξ. A similar convexity requirement should hold in the vectorial case, as treated above (where Γ is the Legendre transform of $-W$).
In the mathematical literature, Legendre transformation is defined seemingly differently, through $\Gamma(\xi) = \min_h [f(h) - h\,\xi]$, for a convex-up function $f(h)$. For a given ξ, the minimum is reached for $f'(h) = \xi$ and this definition coincides with the "physicist" one, with the bonus of a compact notation. One also finds the definition $\Gamma(\xi) = \max_h [h\,\xi - f(h)]$, which changes a few signs, but makes sure that the transform is convex-up itself, and can be itself Legendre transformed one more time to yield back the original $f(h)$.
Geometrical interpretation: $\Gamma = f(h) - hf'(h)$ is nothing but the y-intercept of the tangent to the graph of f at abscissa h. This quantity Γ, expressed as a function of the slope $f'(h) = \xi$, can then be sketched graphically as in the picture below (it is useful to train oneself to be able to perform graphically the transformation). The Legendre transform is an important tool in thermodynamics, statistical physics and analytical mechanics.
Further reading : *Making Sense of the Legendre Transform* by Zia *et al.*, `https://arxiv.org/abs/0806.1147`.



6 Functional derivatives

Let $q(t)$ be a function of t and let $S[q]$ be a functional of q. The functional derivative of S wrt $q(t_0)$ is defined as follows. Let $q_{\varepsilon,t_0}(t) = q(t) + \varepsilon \delta(t - t_0)$, then $\frac{\delta S}{\delta q(t_0)} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon}(S[q_{\varepsilon,t_0}] - S[q])$. Another way to put it is 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

$$\delta S = \int \frac{\delta S}{\delta q(t')} \; \delta q(t') \; dt', \tag{3}$$

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

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

Answer: $\delta(t_1 - t_2)$, as obtained from the two definitions.

6.2 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.

Answer: We apply the definition and start from $S[q_{\varepsilon,t_0}] = \int dt L(q_{\varepsilon,t_0}, \dot{q}_{\varepsilon,t_0})$ which we expand to first order in ε: $S[q_{\varepsilon,t_0}] = S[q] + \varepsilon \int dt \left[\delta(t-t_0)\frac{\partial L}{\partial q} + \dot{\delta}(t-t_0)\frac{\partial L}{\partial \dot{q}}\right]$. After an integration by parts and after using the $\delta(t-t_0)$ distribution, we thus arrive at $S[q_{\varepsilon,t_0}] - S[q] = \varepsilon\left[\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\right]$, which is the desired result.

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

Answer: After defining $\phi_{\varepsilon,\boldsymbol{x}_0}(\boldsymbol{x}) = \phi(\boldsymbol{x}) + \varepsilon\delta^{(d)}(\boldsymbol{x} - \boldsymbol{x}_0)$ we repeat the procedure sketched in the previous section and arrive at the Euler-Lagrange equations for the field ϕ (with $t \to \boldsymbol{x}$, $q \to \phi$ and $\frac{d}{dt} \to \boldsymbol{\nabla}\cdot$.

6.4 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 $\frac{\delta^2 S}{\delta\phi(x_2)\delta\phi(x_1)}$.

Answer: $\frac{\delta S}{\delta\phi(x_1)} = -\frac{d^2\phi}{dx^2}(x_1) + r\phi(x_1)$ and thus $\frac{\delta^2 S}{\delta\phi(x_2)\delta\phi(x_1)} = \delta(x_1 - x_2)\left[-\frac{d^2}{dx_1^2} + r\right]$. Note that for any distribution T, $\nabla^2 T = T\,\nabla^2$.

Remember the connection between functional derivatives and Euler-Lagrange equations. Besides, our first order expansion Eq. (3) 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.

7 Pauli matrices *(Soft Matter track can skip)*

Let $\sigma^{1,2,3}$ be the Pauli matrices $\sigma^1 = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$, $\sigma^2 = \begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}$, $\sigma^3 = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$, and σ^0 be the 2-by-2 identity.

Remember that the Pauli matrices satisfy the algebra $\sigma^\ell\sigma^n = \delta_{\ell n}\,\sigma^0 + i\sum_{j=1}^3 \epsilon_{\ell n j}\sigma^j$ ($\ell, n \in \{1,2,3\}$) and the commutation relations $[\sigma^\ell, \sigma^n] = 2i\sum_{j=1}^3 \epsilon_{\ell n j}\sigma^j$, where $\delta_{\ell n}$ is the Kronecker delta ($\delta_{\ell n}$ is nonzero only if $\ell = n$, in which case it is equal to 1) and $\epsilon_{\ell n j}$ is the (antisymmetric) Levi-Civita symbol ($\epsilon_{\ell n j}$ is nonzero only if the three indices are different; in that case, it is equal to $(-1)^p$, where p is the number of transpositions that bring $\{\ell, n, j\}$ into $\{1,2,3\}$). In short, $[\sigma^1, \sigma^2] = 2i\sigma^3$ (plus permutations, as for angular momentun operators, which they almost are). Besides, $(\sigma^1)^2 = (\sigma^2)^2 = (\sigma^3)^2 = \sigma^0 = I$ and the matrices anticommute $\sigma^1\sigma^2 + \sigma^2\sigma^1 = 0$, etc. Thus, $\sigma^1\sigma^2 = i\,\sigma^3$, $\sigma^2\sigma^3 = i\,\sigma^1$ etc.

7.1 Show that, for any real number λ and vector $\vec{v}$ with real components, the eigenvalues $\mu_\pm$ of $M_{\lambda,\vec{v}} = \lambda\sigma^0 + \vec{v}\cdot\vec{\sigma} \overset{def}{=} \lambda\sigma^0 + \sum_{j=1}^3 v_j\sigma^j$ are $\mu_\pm = \lambda \pm |\vec{v}|$, where $|\vec{v}| = \sqrt{v_1^2 + v_2^2 + v_3^2}$.

Answer: The eigenvalues can be determined by computing the trace of $M_{\lambda,\vec{v}}$ and of $M_{\lambda,\vec{v}}^2$. The result is readily obtained using that the Pauli matrices are traceless: $\mathrm{tr}[M_{\lambda,\vec{v}}] = \mu_+ + \mu_- = 2\lambda$ and $\mathrm{tr}[M_{\lambda,\vec{v}}^2] = \mu_+^2 + \mu_-^2 = \mathrm{tr}[(\lambda^2 + |\vec{v}|^2)\sigma^0 + 2\lambda\vec{v}\cdot\vec{\sigma}] = 2(\lambda^2 + |\vec{v}|^2)$.

7.2 Show that $\Pi_\pm = \left(\sigma^0 \pm \frac{\vec{v}\cdot\vec{\sigma}}{|\vec{v}|}\right)/2$ are the projectors on the eigenvectors of $M_{\lambda,\vec{v}}$ ($\Pi_\pm^2 = \Pi_\pm$ and $M_{\lambda,\vec{v}}\Pi_\pm = (\lambda \pm |\vec{v}|)\Pi_\pm$; consequently, one has the spectral decomposition

$$M_{\lambda,\vec{v}} = (\lambda + |\vec{v}|)\Pi_+ + (\lambda - |\vec{v}|)\Pi_-.$$

Answer: $\Pi_\pm^2 = \Pi_\pm$ because the eigenvalues of $\frac{\sigma^0 \pm \frac{\vec{v}\cdot\vec{\sigma}}{|\vec{v}|}}{2}$ are $\{0, 1\}$. They project on the eigenvectors of $M_{\lambda,\vec{v}}$, indeed

$$M_{\lambda,\vec{v}}\Pi_{\pm} \;=\; (\lambda\sigma^0 + \vec{v}\cdot\vec{\sigma})\,\frac{\sigma^0 \pm \frac{\vec{v}\cdot\vec{\sigma}}{|\vec{v}|}}{2} \;=\; \lambda\frac{\sigma^0 \pm \frac{\vec{v}\cdot\vec{\sigma}}{|\vec{v}|}}{2} + \frac{\vec{v}\cdot\vec{\sigma} \pm \frac{(\vec{v}\cdot\vec{\sigma})^2}{|\vec{v}|}}{2} \;=\; (\lambda \pm |\vec{v}|)\Pi_{\pm}\,.$$

7.3 A function $f(M)$ of a diagonalizable matrix M is the matrix with the same eigenvectors of M and with eigenvalues $f(m_i)$, where m_i are the eigenvalues of M. Calculate $\mathrm{Tr}[(\tanh(\sin(\vec{v}\cdot\vec{\sigma}))^7]$.

Answer: Every odd function of the Pauli matrices is traceless.

7.4 Show that, if $\vec{v}\cdot\vec{w} = \sum_{j=1}^{3} v_j w_j = 0$, then $e^{\lambda\vec{v}\cdot\vec{\sigma}}\,\vec{w}\cdot\vec{\sigma} \;=\; \vec{w}\cdot\vec{\sigma}\,e^{-\lambda\vec{v}\cdot\vec{\sigma}}$.

Answer: Using the spectral decomposition of $\vec{v}\cdot\vec{\sigma}$, we find $e^{\lambda\vec{v}\cdot\vec{\sigma}} = e^{\lambda|\vec{v}|}\frac{\sigma^0 + \frac{\vec{v}\cdot\vec{\sigma}}{|\vec{v}|}}{2} + e^{-\lambda|\vec{v}|}\frac{\sigma^0 - \frac{\vec{v}\cdot\vec{\sigma}}{|\vec{v}|}}{2}$. Indeed, $\vec{v}\cdot\vec{\sigma} = v\Pi_+ - v\Pi_-$ with $v = |\vec{v}|$, $\Pi_+\Pi_- = 0$, $\exp(\lambda v\Pi_{\pm}) = \sigma^0 + \left(e^{\pm\lambda v} - 1\right)\Pi_{\pm}$ since $\Pi_{\pm}^2 = \Pi_{\pm}$. The final result follows from $\vec{v}\cdot\vec{\sigma}\vec{w}\cdot\vec{\sigma} = -\vec{w}\cdot\vec{\sigma}\vec{v}\cdot\vec{\sigma}$.

7.5 Prove

$$e^{i\frac{\pi}{4}\frac{3\sigma^2+4\sigma^3}{5}}\,\sigma^1\,e^{-i\frac{\pi}{4}\frac{3\sigma^2+4\sigma^3}{5}} \;=\; \frac{3\sigma^3 - 4\sigma^2}{5}$$

(hint: define the vector $\vec{v}$ in such a way that $\vec{v}\cdot\vec{\sigma} = \frac{3\sigma^2+4\sigma^3}{5}$, what is $|\vec{v}|$?).

Answer: The vector $\vec{v}$ has a magnitude of 1 ($|\vec{v}| = 1$), and it is given by $\vec{v} = \begin{bmatrix} 0 \\ \frac{3}{5} \\ \frac{4}{5} \end{bmatrix}$. Thus we have

$$e^{i\frac{\pi}{4}\frac{3\sigma^2+4\sigma^3}{5}}\sigma^1 e^{-i\frac{\pi}{4}\frac{3\sigma^2+4\sigma^3}{5}} \;=\; e^{i\frac{\pi}{4}\vec{v}\cdot\sigma}\sigma^1 e^{-i\frac{\pi}{4}\vec{v}\cdot\sigma} = \sigma^1 e^{-i\frac{\pi}{2}\vec{v}\cdot\sigma}\,,$$

where we applied the identity proved in the previous point. We now use the spectral decomposition of $e^{-i\frac{\pi}{2}\vec{v}\cdot\vec{\sigma}}$

$$\sigma^1 e^{-i\frac{\pi}{2}\vec{v}\cdot\sigma} = \sigma^1\left(e^{-i\frac{\pi}{2}}\Pi_+ + e^{i\frac{\pi}{2}}\Pi_-\right) = \sigma^1\left(-i\Pi_+ + i\Pi_-\right) = -i\sigma^1\vec{v}\cdot\vec{\sigma} = \frac{3\sigma^3 - 4\sigma^2}{5}\,.$$