The purpose of this set of problems[1] 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 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 $\widetilde{f}_q = \sum_{n=1}^{N} e^{iqna} f_n$.

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

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.

1.2 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?

1.3 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 $A = 1$).

1.4 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.

1.5 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.

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 $\widetilde{M}(q)\widetilde{M^{-1}}(q) = 1$, assuming M is invertible. 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 $m(x)$. We note in passing that circulant matrices (of the same size) are diagonal in the same basis, and thus any two such matrices do commute.

[1] prepared with F. van Wijland and M. Lenz

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

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

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 $f(x)$ is periodic of period L, then $q = 2\pi n/L$, where $n \in \mathbb{Z}$. The Fourier transform becomes a Fourier series. Let us check this with the traditional choice $A = 1$. We start from

  $$f(x) = \int_{\mathbb{R}} \widetilde{f}(q)\, e^{-iqx}\, \frac{dq}{2\pi} \quad \text{with the added constraint} \quad \sum_{n\in\mathbb{Z}} \delta\left(n - \frac{qL}{2\pi}\right).$$

  We obtain

  $$f(x) = \frac{1}{L}\sum_{n\in\mathbb{Z}} \widetilde{f}(2\pi n/L)\, e^{-i2\pi n x/L} \quad \text{with} \quad \widetilde{f}(q) = \int_0^L f(x)e^{iqx}\, dx.$$

- If f is defined on an N-site lattice with constant a, then $q = 2\pi n/(Na)$, where $n = 0, 1, \ldots N-1$ (or, if N is even, $n = -N/2+1, \ldots, N/2-1, N/2$. 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 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.

2 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.

2.1 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.

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

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

We finish with two more examples that connect with other areas of physics. First, $\Gamma(x,t;x',t') = \delta(t-t')\delta(x-x')\left[\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right]$, with $D>0$. 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).

3 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 $W(\boldsymbol{h}) = \ln Z(\boldsymbol{h})$.

3.1 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 $\langle x_i\rangle = \left.\dfrac{\partial W}{\partial h_i}\right|$.

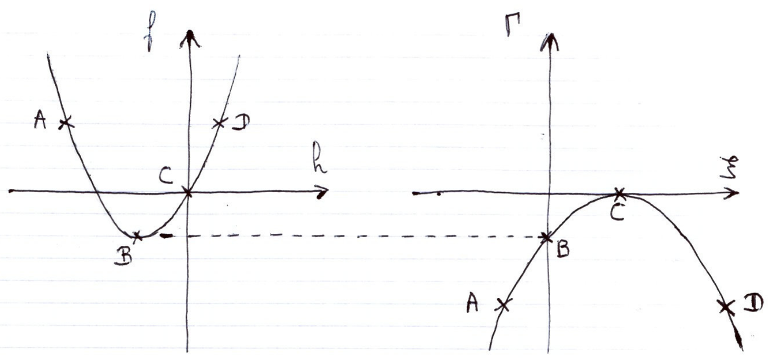
3.2 Show that $G_{ij} = \langle x_i x_j\rangle - \langle x_i\rangle\langle x_j\rangle = \left.\dfrac{\partial^2 W}{\partial h_i \partial h_j}\right|$.

3.3 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 $\partial\Gamma/\partial\xi_i = h_i$.

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

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 $F(V) = -k_{\text{B}}T\ln Z(V)$ 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, the transformation is defined seemingly differently, through $\Gamma(\xi) = \min_h[f(h) - h\,\xi]$, and is known as the Legendre-Fenchel transform. The transformed function need not be differentiable, nor convex. We do not enter in the distinction between Legendre and Legendre-Fenchel; we restrict here to convex and differentiable functions $f(h)$. 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`.



4 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

$$\delta S = \int \frac{\delta S}{\delta q(t')}\ \delta q(t')\ dt', \tag{1}$$

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'.

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

4.2 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.

4.3 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 $\boldsymbol{x}_0$).

4.4 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. (1) 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.

Remember also the "**be wise, discretize**": should you feel at a loss with a functional, the discrete formulation will be more transparent. After having overcome the difficulty (such as computing a derivative), you can go back to the continuum limit and proceed…