Licence 3 et Magistère de physique

Statistical physics

Exercices

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Contents

Some useful formulae

Euler's Gamma function

$$\boxed{\Gamma(z) \stackrel{\text{def}}{=} \int_0^\infty \mathrm{d}t\, t^{z-1}\, \mathrm{e}^{-t} \qquad \text{for } \operatorname{Re} z > 0} \tag{1}$$

Note that integrals of the form $\int_0^\infty \mathrm{d}x\, x^a\, \mathrm{e}^{-Cx^b}$ may be simply related to the Gamma function.

Functional relation :

$$\boxed{\Gamma(z+1) = z\,\Gamma(z)} \tag{2}$$

This allows to perform an analytic continuation in order to extend the definition of the Gamma fucntion to the other half of the complex plane, $\operatorname{Re} z \leqslant 0$.

Particular values $\boxed{\Gamma(1) = 1 \;\&\; \Gamma(1/2) = \sqrt{\pi}}$, hence, by recurrence,

$$\Gamma(n+1) = n! \tag{3}$$

$$\Gamma(n+\frac{1}{2}) = \frac{\sqrt{\pi}}{2^n}\,(2n-1)!! \tag{4}$$

where $(2n-1)!! \stackrel{\text{def}}{=} 1\times 3\times 5\times\cdots\times(2n-1) = \frac{(2n)!}{(2n)!!}$ and $(2n)!! \stackrel{\text{def}}{=} 2\times 4\times\cdots\times(2n) = 2^n n!$.

Gaussian integrals

An integral related to $\Gamma(1/2)$,

$$\boxed{\int_{\mathbb{R}} \mathrm{d}x\, \mathrm{e}^{-\frac{1}{2}ax^2} = \sqrt{\frac{2\pi}{a}}} \tag{5}$$

An integral related to $\Gamma(3/2)$,

$$\int_{\mathbb{R}} \mathrm{d}x\, x^2\, \mathrm{e}^{-\frac{1}{2}ax^2} = \frac{1}{a}\sqrt{\frac{2\pi}{a}} \tag{6}$$

More generally

$$\int_{\mathbb{R}^+} \mathrm{d}x\, x^n\, \mathrm{e}^{-\frac{1}{2}ax^2} = \frac{1}{2}\left(\frac{2}{a}\right)^{\frac{n+1}{2}}\,\Gamma\left(\frac{n+1}{2}\right) \tag{7}$$

Fourier transform of the Gaussian

$$\int_{\mathbb{R}} \mathrm{d}x\, \mathrm{e}^{-\frac{1}{2}ax^2+\mathrm{i}kx} = \sqrt{\frac{2\pi}{a}}\,\mathrm{e}^{-\frac{1}{2a}k^2} \tag{8}$$

Euler's Beta function

$$B(\mu,\nu) = \int_0^1 \mathrm{d}t\, t^{\mu-1}(1-t)^{\nu-1} = 2\int_0^{\pi/2} \mathrm{d}\theta\, \sin^{2\mu-1}\theta\, \cos^{2\nu-1}\theta = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu+\nu)} \tag{9}$$

Stirling's formula

$$\Gamma(z+1) \simeq \sqrt{2\pi z}\, z^z\, \mathrm{e}^{-z} \qquad \text{i.e} \qquad \boxed{\ln\Gamma(z+1) = z\ln z - z + \frac{1}{2}\ln(2\pi z) + \mathcal{O}(1/z)} \tag{10}$$

which will be used frequently to express $\ln(n!) \simeq n\ln n - n$ or $\frac{\mathrm{d}}{\mathrm{d}n}\ln(n!) \simeq \ln n$.

Binomial formula

$$(p+q)^N = \sum_{n=0}^{N} C_N^n \, p^n \, q^{N-n} \qquad \text{where } C_N^n \stackrel{\text{def}}{=} \frac{N!}{n!(N-n)!} \tag{11}$$

Other useful integrals

$$\int_0^\infty \mathrm{d}x \frac{x^{\alpha-1}}{\mathrm{e}^x - 1} = \Gamma(\alpha)\,\zeta(\alpha) \qquad \text{where } \zeta(\alpha) = \sum_{n=1}^{\infty} n^{-\alpha} \tag{12}$$

is the Euler Zeta function. We give $\zeta(2) = \frac{\pi^2}{6}$, $\zeta(3) \simeq 1.202$, $\zeta(4) = \frac{\pi^4}{90}$, etc.

Finally, we give

$$\int_0^\infty \mathrm{d}x \frac{x^4}{\mathrm{sh}^2\, x} = \frac{\pi^4}{30} \tag{13}$$

(related to the previous integral for $\alpha = 4$).

TD 1 : Random walks and central limit theorem

1.1 Binomial distribution and central limit theorem

We consider the motion of a walker moving along an axis : each time increment, he makes a step to the right with probability $p \in [0,1]$, or to the left with probability $q = 1-p$ (cf. Fig. 1). All steps are equal. We assume each step **independent** from the previous one.

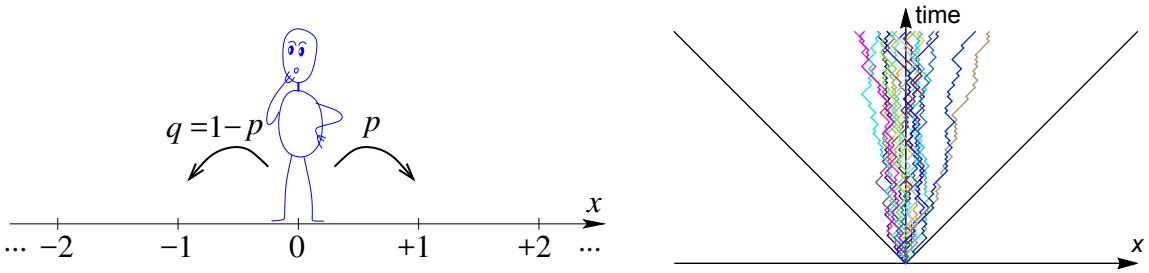

Figure 1: *Walker on a lattice. Right :* 20 *trajectories of* 100 *steps each have been simulated.*

A. Binomial distribution.

1/ Distribution.– After M steps, what is the probability, denoted $\Pi_M(n)$, that the walker has made n steps to the right ? Check the normalisation.

2/ The moments.– Express the kth moment, i.e. $\langle n^k \rangle$, as a sum (careful : n is related to the random variable, while M is a parameter of the problem). Can you calculate this sum ?

3/ Determination of the moments from the generating function.– We introduce an auxiliary function, denoted the "*generating* function",

$$G_M(s) \stackrel{\text{def}}{=} \langle s^n \rangle \,, \tag{14}$$

function of the variable s (which can be complex).

a) Assuming known the function $G_M(s)$, how can you deduce the moments ?

b) For the binomial distribution $\Pi_M(n)$ determined above, calculate explicitly $G_M(s)$; deduce $\langle n \rangle$ and $\langle n^2 \rangle$ and then the variance $\mathrm{Var}(n) \stackrel{\text{def}}{=} \langle n^2 \rangle - \langle n \rangle^2$. Compare the fluctuations and the mean.

c) Optional : we introduce another definition of the generating function : $W_M(\beta) \stackrel{\text{def}}{=} \ln G_M(\mathrm{e}^{-\beta})$, where β is called the "*conjugated variable* " (of the random variable). Check that its $\beta \to 0$ expansion reads $W_M(\beta) = -\beta \langle n \rangle + (\beta^2/2)\,\mathrm{Var}(n) + \cdots$ (thus, given $W_M(\beta)$, one obtains the variance more straightforwardly). Justify this expansion in the general case by comparing the definitions of $G_M(s)$ and $W_M(\beta)$.

4/ Limit $M \to \infty$.– In this question, we analyse directly the distribution in the limit $M \to \infty$. Using the Stirling formula, expand $\ln \Pi_M(n)$ around its maximum at $n = n_*$. Justify that $\Pi_M(n)$ is approximatively Gaussian in the limit $M \to \infty$ (give a condition on p). Plot *neatly* the distribution.

B. Random walker.– We come back to the study of the random walker, with position x. Length of each step is a.

1/ Express x as a function of the number n of steps to the right. Deduce the two first moments of x (use the results of **A**).

2/ Drift.– A time τ elapses between two steps. Express the speed (drift)

$$V \stackrel{\text{def}}{=} \lim_{t\to\infty} \frac{\langle x\rangle_t}{t} \tag{15}$$

as a function of a, τ and the probability p ; $\langle x\rangle_t$ is the mean at time $t = M\tau$.

3/ Diffusion constant.– In order to characterize the spreading of the walker's distribution, we introduce the diffusion constant

$$D \stackrel{\text{def}}{=} \lim_{t\to\infty} \frac{\langle x^2\rangle_t - \langle x\rangle_t^2}{2t} \tag{16}$$

Express D as a function of the microscopic parameters.

4/ Give the probability density $P_t(x)$ of the walker's position at time t. Check the normalisation (when $p = 1/2$, one can try to relate directly $\Pi_M(n)$ and $P_t(x)$).

C. Continuous distribution for the jumps – Universality.– We study another model of random walker, where its position is not restricted to a lattice but can vary continuously. At each time interval, the walker makes a jump h distributed with the law $p(h)$.

1/ Justify that the distribution at time t obeys the recurrence

$$P_{t+\tau}(x) = \int \mathrm{d}h\, p(h)\, P_t(x-h)\,. \tag{17}$$

Choose one of the two methods exposed below in order to solve this equation.

2/ Method 1 : symmetric Gaussian walk.– we consider the case where the jump distribution is Gaussian $p(h) = (\sqrt{2\pi}\,\sigma)^{-1} \exp\left\{-h^2/(2\sigma^2)\right\}$. Using known results on the convolution of Gaussians, deduce $P_{M\tau}(x)$. Express the diffusion constant as a function of τ and σ.

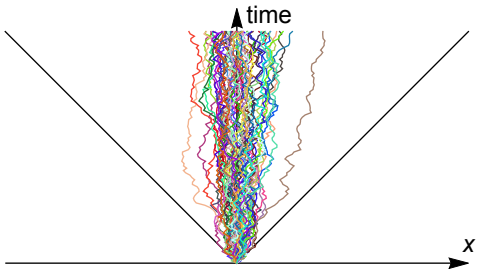

Figure 2: 50 *random walks of* 100 *steps distributed by a Gaussian law.*

3/ Method 2 : general case.– we don't assume any specific form for the law $p(h)$, which only decays sufficiently fast in order to ensure $\langle h\rangle < \infty$ and $\langle h^2\rangle < \infty$. We consider "small" time interval, $\tau \to 0$, and "small" jumps (i.e. the width of $p(h)$ is "small").

a) In the integral equation (17), expand the left hand side at first order, $P_{t+\tau}(x) \simeq P_t(x) + \tau\,\partial_t P_t(x)$, and the distribution in the integral at second order, $P_t(x-h) \simeq P_t(x) - h\,\partial_x P_t(x) + h^2\,\partial_x^2 P_t(x)$.

b) We assume that the three parameters $\tau \propto \epsilon$, $\langle h\rangle \propto \epsilon$ and $\langle h^2\rangle \propto \epsilon$ goes simultaneously to zero, all proportionally to the parameter $\epsilon \to 0^+$. Deduce a partial differential equation for $P_t(x)$, written in terms of V and D.

c) Give the solution of this partial differential equation (the most efficient method to solve the equation is to go to Fourierize in space, but keep the time variable).

4/ Universality.– Justify why the different models for the random walkers all lead to the same universal law $P_t(x)$, in the limit of a large number of steps.

D. d-dimensionnal case and application.

1/ We now consider a walker in $\mathbb{R}^d$. At each time step, he makes a jump $\vec{\delta x} = h_1\,\vec{e}_1 + \cdots + h_d\,\vec{e}_d$, where the variables h_i are d *independent* random variables, obeying the same symmetric law $p(h)$. Deduce the distribution of the walker's position in $\mathbb{R}^d$ (use the result of **C** for $d = 1$).

2/ Express $\langle \vec{x}^{\,2} \rangle$ as a function of the diffusion constant defined above in the one-dimensional case (one will thus have to consider $\langle x_i x_j \rangle$ for $i = j$ and $i \neq j$).

3/ Optional : **Joint law *versus* marginal law.**– $\vec{x} \in \mathbb{R}^2$ is distributed by the Gaussian law obtained for the walker after a large number of steps. How one can relate the joint distribution $P_t(x, y)$ to the *marginal law* $Q_t(r)$ for $r = \sqrt{x^2 + y^2}$? Compare the determinantion of $\langle \vec{x}^{\,2} \rangle$ from $P_t(x, y)$ and $Q_t(r)$. Compute the mean $\langle r \rangle$ and the typical value r_{typ} (the value for which $Q_t(r)$ is maximum). Plot neatly $Q_t(r)$.

4/ Application : molecule in a gas.– The speed of molecules in a gas at room temperature is typically $v \approx 500$ m/s. Typically, a molecule makes a collision with another molecule every $\tau \approx 2$ ns. Compare the typical distance between two consecutive collisions with the typical distance to the closest molecule in normal conditions ($p = 1$ atm, $T = 300$ K). Compare the diffusive motion of the molecule after one second (number of colllisions, typical distance finally covered) , with the ballistic motion.

TD 3 : Density of states

3.1 Two-level systemS

A single two-level system is characterised by two eigenstates, denoted $|+\rangle$ and $|-\rangle$, with energies $\varepsilon_\pm = \pm\varepsilon_0$ where ε_0 is a microscopic scale. An example is a spin in magnetic field.

We consider N such two-level systems, *identical* and *independent* (for example N spins 1/2 at the nodes of a crystal). We denote $\varepsilon_\sigma^{(i)}$ the energy of subsystem i, with $\sigma = +$ or $-$, and $E = \sum_{i=1}^N \varepsilon_{\sigma_i}^{(i)}$ the total energy.

1/ Energy spectrum : Describe the microstates of the system. Writing $E = M\varepsilon_0$, how does the integer M vary ?

2/ If the energy is fixed, give the number $N_\pm$ of subsystems in state $|\pm\rangle$. Deduce the degeneracy g_M of level $E_M = M\varepsilon_0$. Relate g_M to the density of states $\rho(E_M)$.

3/ We consider the limit $N \gg 1$. Find an approximation for $\ln g_M$ by using the Stirling formula (assuming $N_\pm \gg 1$). Plot $\ln g_M$ as a function of E_M. Show that the density of states is Gaussian for $E \ll N\varepsilon_0$,

$$\rho(E) \simeq \rho(0)\, \mathrm{e}^{-E^2/(2N\varepsilon_0^2)} \,. \tag{18}$$

Compare the width of the function to the width of the full spectrum. What is the total number of states ? Deduce the value of $\rho(0)$.

Optional : Using $\ln N! = N\,\ln N - N + \frac{1}{2}\ln(2\pi N) + \mathcal{O}(N^{-1})$, recover $\rho(0)$ more directly.

3.2 Volume of a hypersphere

A hypersphere of radius R in $\mathbb{R}^d$ is the domain defined by $x_1^2 + x_2^2 + \cdots + x_d^2 \leqslant R^2$. By studying the integral $\int_{\mathbb{R}^d} \mathrm{d}\vec{x}\, \mathrm{e}^{-\vec{x}^{\,2}}$, calculate the surface of the hypersphere $S_d(R)$ and show that the volume is given by

$$V_d(R) = \mathscr{V}_d\, R^d \qquad \text{where} \quad \boxed{\mathscr{V}_d = \frac{\pi^{d/2}}{\Gamma(\frac{d}{2}+1)}} \tag{19}$$

is the volume of the sphere of unit radius (consider the cases $d = 1$, 2, and 3).

Hint: (i) Use separability of integral ; (ii) Use rotational invariance of the function integrated.

3.3 Density of states of free particles

We consider a gas of N free atoms in a cubic box of volume $V = L^3$. The Hamiltonian of the system is

$$H = \sum_{i=1}^N \frac{\vec{p}_i^{\,2}}{2m} \,. \tag{20}$$

1/ Distinguishable atoms.– By (incorrectly) considering the atoms as distinguishable, show that the volume $\Phi_{\text{disc}}(E)$ of phase space occupied by states of energy less than E is

$$\Phi(E) = \frac{1}{\Gamma(\frac{3N}{2}+1)} \left(\frac{E}{\epsilon_0}\right)^{3N/2} \qquad \text{where} \quad \epsilon_0 \stackrel{\text{def}}{=} \frac{2\pi\hbar^2}{mL^2} \tag{21}$$

2/ Inistinguishable atoms.– Identical atoms are indistinguishable. Give $\Phi_{\text{indisc}}(E)$ and simplify the result with the help of the Stirling formula. Find the corresponding density of states.

Numerical example: Calculate ϵ_0 (in J and then in eV) for helium atoms in a box of size $L = 1$ m.

3.4 Density of state of a free relativist particle

1/ Non relativistic case.– Recall the density of states for a non relativistic free particle, $\varepsilon_{\vec{k}} = \hbar^2 \vec{k}^{\,2}/(2m)$ (cf. previous exercice).

2/ Ultrarelativist case.– Compute the density of states for an ultrarelativist particle, with $\varepsilon_{\vec{k}} = \hbar||\vec{k}||\, c$.

Indication : Use the representation $\rho(\varepsilon) = \sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}})$.

3/ Relativist case.– (Optional) Using the semi-classical rule, compute the density of states for a massive relativist particle, $\varepsilon_{\vec{k}} = \sqrt{(\hbar\vec{k}c)^2 + m^2c^4}$. Recover the two previous limiting behaviours.

3.5 Classical and quantum harmonic oscillators

We consider a system of N independent identical 1D harmonic oscillators.1D, The Hamiltonian of the system is

$$H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 q_i^2 \right) . \tag{22}$$

1/ Semi-classical treatment.– We suppose that the oscillators are classical.

a/ We denote by $\mathcal{V}(E)$ the volume occupied by states of energy $\leqslant E$ in phase space (the dimension of which will be specified). Express $\mathcal{V}(E)$ in terms of the constant $\mathscr{V}_{2N}$, the volume of the hypersphere of unit radius (exercise 3.2).

b/ Using the semi-classical hypothesis that a quantum state occupies a cell of volume h^N in phase space, calculate the number of quantum states of energy less than E (written $\Phi(E)$), and then the density of states $\rho(E)$.

2/ Quantum treatment.– We now suppose that the N oscillators are quantum mechanical. We know that the energy levels of each oscillator are nondegenerate and given by $\varepsilon_n = (n + 1/2)\hbar\omega$ (where n is an integer $\geqslant 0$).

a/ Calculate the number of accessible states of the system when its energy is equal to E.

Indications: We wish to calculate the number of different ways of choosing N nonnegative integers (n_1, n_2, n_3...n_N) such that their sum $\sum_{i=1}^{N} n_i$ equals a given integer M. To do so we use the following method: each choice may be represented by a diagram of n_1 balls, then one bar, then n_2 balls, then one bar, ... The total number of balls is M and the total number of bars is $N - 1$. Permutations of balls and bars each among themselves do not count. Only matter the number of different ways of placing $N - 1$ bars in a linear array of M balls.

c/ Calculate the quantum density of states of the system. Show that, in the limit $E \gg N\hbar\omega$, one recovers the semi-classical result of question (2).

Appendix 2.A: Semi-classical rule for counting states in phase space

When the degrees of freedom can be described in classical terms, the semi-classical rule allows to determine the density of states very efficiently : this is the case for translation degree of freedom of atomes, but not for a spin 1/2 which has no classical equivalent.

For a system with D degrees of freedom the phase space of vectors $(q_1, \cdots, q_D, p_1, \cdots, p_D)$ has dimension $2D$. The correspondence between classical and quantum counting of micro-states is ensured by considering that one *quantum state* occupies a volume h^D in *classical phase space*.

Integrated density of states.– Let $H(\{q_i, p_i\})$ be the Hamiltonian governing the dynamics of a system. We denote by $\Phi(E)$ the number of micro-states of energy less than E. In the semi-classical limit, we have

$$\boxed{\Phi(E) = \frac{1}{h^D} \int_{H(\{q_i,p_i\})\leqslant E} \prod_{i=1}^{D} \mathrm{d}q_i \mathrm{d}p_i \equiv \frac{1}{h^D} \int \prod_{i=1}^{D} \mathrm{d}q_i \mathrm{d}p_i \ \theta_{\mathrm{H}}\left(E - H(\{q_i, p_i\})\right)} \tag{23}$$

where $\theta_{\mathrm{H}}(x)$ is the Heaviside function.

Density of states.– The density of states is given by

$$\rho(E) = \Phi'(E) \tag{24}$$

i.e. $\rho(E)\mathrm{d}E$ represents the number of quantum states of energy in the interval $[E, E + \mathrm{d}E)$.

Indistinguishable particles.– If the system contains N indistinguishable particles (for instance an ideal gas of N particles moving in three-dimensional space, $D = 3N$), we must multiply by an extra factor $1/N!$ to take into account the fact that the particles are indistinguishable (*i.e.* that micro-states differing only by a permutation of particles are equivalent):

$$\Phi_{\mathrm{indist}}(E) = \frac{1}{N!} \Phi_{\mathrm{dist}}(E) \tag{25}$$

Notice, however, that this expression accounts only partially for the symmetrization postulate of quantum mechanics. The full consequences of the latter will be studied in detail in tutorials 8 and 9.