Advanced Statistical Physics:
1. Introduction

Leticia F. Cugliandolo
`leticia@lpthe.jussieu.fr`
Sorbonne Université
Laboratoire de Physique Théorique et Hautes Energies
Institut Universitaire de France

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1 Introduction

This is an Advanced Course in Statistical Physics. Good knowledge of the mathematical methods recalled in the Mathematical Support made available during the summer, and standard Thermodynamics and Statistical Physics concepts are assumed.

The Lectures and Exercise Sessions will cover classical and quantum Statistical Physics problems. We will spend some time discussing methods for the study of Phase Transitions and emerging collective phenomena. As we cover the material of the Course we will also mention and present problems on which research is currently carried out by many groups Worldwide.

This first Section (to be covered in one Lecture, TD1 & part of TD2) deals with some aspects of Statistical Physics which are often overlooked in standard Courses: the meaning of the ergodic hypothesis, the (in)equivalence between statistical ensembles, the convenient identification of system and environment, and the "conservation" of the canonical ensemble under "reduction".

1.1 Basic notions

This Subsection defines the class of systems that will be studied in this Course by recalling some basic notions of Statistical Physics. It also puts my Lectures in the context of other Courses of the Master.

1.1.1 Background

Classical Equilibrium Statistical Mechanics is a very well-established branch of theoretical physics. Together with *Quantum Mechanics*, they form the basis of *Modern Physics*. It is based on *Probability Theory and Mathematical Statistics* on the one hand and Hamiltonian Mechanics on the other. Its scope is very wide since it is, in principle, applicable to all states of matter. A nice introduction to the historical development of this theory can be found in the classical book by Pathria [1].

The goal of equilibrium statistical mechanics is to derive the *thermodynamic functions of state* of a *macroscopic* system from the *microscopic laws* that determine the behaviour of its constituents. In particular, it explains the origin of thermodynamic – and intuitive – concepts like pressure, temperature, heat, *etc.*

In Table 1 we recall the typical length, time and energy scales appearing in the microscopic (say, atomistic) and macroscopic World.

A reference number is the number of Avogadro, $N_A = 6.02\ 10^{23}$; it counts the number of atoms in a mol, *i.e.* 12gr of ^{12}C, and it yields the order of magnitude of the number of molecules at a macroscopic level. The ionization energy of the Hydrogen atom is 13.6 eV and sets the microscopic energy scale in Table 1.

	Micro		Macro	
	Solid	Gas	Solid	Gas
dist (ℓ)	10^{-10}m	10^{-8}m	10^{-3}m	
# part (N)	1		$\left(\frac{10^{-3}}{10^{-10}}\right)^{d=3} = 10^{21}$	$\left(\frac{10^{-3}}{10^{-8}}\right)^{d=3} = 10^{15}$
energy (E)	$1\,eV$		$1J \approx 6\,10^{18}eV$	
time (t)	$\hbar/1eV \approx 6\ 10^{-14}\ s$	$10^{-9}\ s$	$1\ s$	

Table 1: Typical length, energy and time scales in the microscopic and macroscopic World.

It is clear from the figures in Table 1 that, from a practical point of view, it would be impossible to solve the equations of motion for each one of the $N \approx N_A$ particles – we keep here the discussion *classical*, including quantum mechanical effects would not change the main conclusions to be drawn henceforth – and derive from their solution the macroscopic behaviour of the system. Moreover, the deterministic equations of motion may present a very high sensitivity to the choice of the initial conditions – *deterministic chaos* – and thus the precise prediction of the evolution of the ensemble of microscopic constituents becomes unfeasible even from a more fundamental point of view.

The passage from the microscopic to the macroscopic is then done with the help of *Statistical Methods*, *Probability Theory* [2] and, in particular, the *Law of Large Numbers*. It assumes – and it has been very well confirmed – that there are no big changes in the fundamental *Laws of Nature* when going through all these orders of magnitude. However, a number of new and interesting phenomena arise due to the unexpected *collective behaviour* of these many degrees of freedom. For example, *phase transitions* when varying an external parameter occur; these are not due to a change in the form of the microscopic interactions but, rather, to the locking of the full system in special configurations.

In the theoretical derivation of phase transitions the necessity to take the infinite size limit clearly appears; this is called the *thermodynamic limit* and corresponds to taking the number of degrees of freedom, say N, to infinity and the volume, say V, also to infinity, while keeping the ratio between the two finite, N/V finite. In this limit, *extensive* quantities scale with N or V while *intensive* ones remain finite.

The main features of statistical mechanics are quite independent of the mechanics that describes the motion of the individual agents (classical or quantum mechanics, relativistic or not). Its foundations do need though different reasonings in different cases. For the sake of concreteness, in the first part of this set of lectures we shall focus on *classical non-relativistic systems*.

In Table I we mentioned energy scales and length scales typical of atomic physics. Particle physics involves even shorter length scales and higher energy scales. Particle physics, and to a certain extent also condensed matter systems, are studied using *field* *theories*. While standard textbooks in Statistical Mechanics do not use a field theoretical formulation, it is indeed pretty straightforward to apply Statistical Mechanics notions to field theories – a theory with 'infinite' degrees of freedom, one for each space-point.

Equilibrium statistical mechanics also makes another very important assumption that we shall explain in more detail below. Namely, that of the equilibration of the macroscopic system. Some very interesting systems do not match this hypothesis. This can arise for several reasons: (i) The *time scales* over which they evolve are too short to reach equilibrium. (ii) The microscopic dynamics are *non conservative*. (iii) There are as many integrals of motion as degrees of freedom in *integrable* systems. Still, one would like to use Probabilistic arguments to characterise the behaviour of macroscopic out of equilibrium systems as well. This is possible in a number of cases although we will not discuss them in these Lectures. Indeed, deriving a theoretical framework to describe the behaviour of *macroscopic systems out of equilibrium* is one the present major challenges in theoretical physics.

Analytic solutions of macroscopic systems (be them in equilibrium or not) are limited to rather simple cases (typically in very low dimension or in the mean-field limit. *Numerical methods*, viz. computer simulations, are very useful to treat such systems.

1.1.2 Elements in statistical mechanics

Let us recall here some important features of Statistical Mechanics [3, 4, 5, 6, 7, 8]. A short account of classical mechanics is given in [9] with special emphasis on the integrability properties. A specially careful discussion of the passage from classical mechanics to statistical physics is given in [10, 11].

The state of a classical system with $i = 1, \dots, N$ particles moving in d-dimensional *real space* is fully characterised by a point in the $2dN$ dimensional *phase space* Γ. The coordinates of phase space are the real space coordinates of the particles, q_i^a, where i is the particle label and $a = 1, \dots, d$ is the label of the real space coordinates, and the particles' momenta, p_i^a. It is convenient to represent a point in phase space with a $2dN$-dimensional vector, *e.g.* $\vec{Y} = (\vec{Q}, \vec{P}) = (q_1^1, q_1^2, q_1^3, q_2^1, q_2^2, q_2^3, \dots, q_N^1, q_N^2, q_N^3, p_1^1, p_1^2, p_1^3, p_2^1, p_2^2, p_2^3, \dots, p_N^1, p_N^2, p_N^3)$ in $d = 3$. This problem has dN *degrees of freedom* and the phase space has *dimension* $2dN$.

The *Hamiltonian* of the system, H, is a function of the particles' position and momenta (we restrict the discussion to Hamiltonian systems). It can be explicitly time-dependent but we shall not consider these cases here. The particles' time evolution, $(\vec{Q}, \vec{P})(t)$, starting from a given initial condition, $(\vec{Q}, \vec{P})(t = 0)$, is determined by Hamilton's equation of motion that are equivalent to *Newton dynamics*. As time passes the representative point in phase space, $(\vec{Q}, \vec{P})(t)$, traces a (one dimensional) path in Γ, the *phase-space trajectory*. Through each point in phase space there passes one and only one trajectory. Any function of the $(\vec{Q}, \vec{P})(t)$ is called a *phase function*. The most important one is the Hamiltonian itself, that determines the evolution of the system *via* the equations of motion. The *energy*, E, or the value the Hamiltonian takes on any point of the trajectory, is conserved if the Hamiltonian does not depend on time explicitly and thus all points in any trajectory lie on a constant energy surface, $H(\vec{Q},\vec{P}) = E$.

But, can one really describe the evolution of such a system? In practice, one cannot determine the position and momenta of all particles in a macroscopic system with $N \gg 1$ with great precision – due to uncertainty in the initial conditions, deterministic chaos, *etc.* A probabilistic element enters into play. What one really does is to estimate the probability that the representative point of the system lies in a given region of Γ at time t given that it started in some other region of Γ at the initial time. Thus, one introduces a *time-dependent probability density* $\rho(\vec{Q},\vec{P};t)$ such that $\rho(\vec{Q},\vec{P};t)d\Gamma$ is the probability that the representative point is in a region of volume $d\Gamma$ around the point $(\vec{Q},\vec{P})$ at time t knowing the probability density of the initial condition, $\rho(\vec{Q},\vec{P};t=0)$. Conditions on ρ to make it a probability density, $\rho(\vec{Q},\vec{P};t) \geq 0$ for all $(\vec{Q},\vec{P})$ and t, and $\int_\Gamma d\Gamma\, \rho(\vec{Q},\vec{P};t) = 1$ at all times, need to be satisfied.

Note that if initially one knows the state of the system with great precision, the initial ρ will be concentrated in some tiny region of phase space. At later times, ρ can still be *localised* – perhaps in a different region of phase – or it may *spread*. This depends on the system and the dynamics. If the dynamics is of Newton-Hamilton type, the phase space volume can change form but not volume, while if the dynamics are dissipative or if energy is injected in some way, the scape phase region occupied by the system can also change volume.

For Hamiltonian systems, for which $\vec{Q},\vec{P}$ follow Hamilton's equations, the evolution of the probability density ρ is given by Liouville's equation. A detailed description of some of its properties can be found in [10, 12].

In statistical equilibrium one expects the systems to reach stationarity. The problem of how to obtain irreversible decay from Liouville's equation is a fundamental one in Statistical Mechanics. We shall not deepen this discussion here; let us just mention that the main attempt to understand the origin of irreversibility is in terms of flows in phase space, and this approach is called *ergodic theory*, as founded by Boltzmann by the end of the XIXth century [5].

In the absence of a good way to determine the evolution of ρ and its approach to a stationary state, one simply makes the following hypothesis:

As $t \to \infty$ one expects that the statistical properties of the system be independent of time and $\rho(\vec{Q},\vec{P};t) \to \rho(\vec{Q},\vec{P})$.

Moreover, one assumes that ρ is a function of the coordinate and momenta only *via* the Hamiltonian H.

$$\boxed{\rho(H(\vec{Q},\vec{P}))}$$

The characteristics of the ensemble are then determined by the chosen function $\rho(H)$.

1.1.3 The ergodic hypothesis & Gibbs ensembles

Finally, let us discuss Boltzmann's and Gibb's interpretation of averages and the *ergodic hypothesis*. Boltzmann interpreted macroscopic observations as time averages of the form[1]

$$\overline{A} \equiv \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau dt \; A(\vec{Q}(t), \vec{P}(t)) \tag{1.1}$$

(focusing on observables A that are not explicitly time dependent). The fact that this limit exists is the content of a Theorem in Classical Mechanics initially proven by Birkhoff and later by Kolmogorov [10]. Note that in classical mechanics the choice of the initial time is irrelevant.

With the introduction of the *concept of ensembles* Gibbs gave a different interpretation (and an actual way of computing) macroscopic observations. For Gibbs, these averages are statistical ones over all elements of the statistical ensemble,[2]

$$\langle \, A \, \rangle = \int d\vec{Q} d\vec{P} \; \rho(H(\vec{Q}, \vec{P})) A(\vec{Q}, \vec{P}) \; , \tag{1.2}$$

with ρ the measure.

In the microcanonical ensemble this is an average over micro-states on the constant energy surface taken with the microcanonical distribution (1.6):

$$\langle \, A \, \rangle = \rho_0 \int d\vec{Q} d\vec{P} \; \delta(H(\vec{Q}, \vec{P}) - E) A(\vec{Q}, \vec{P}) \; , \tag{1.3}$$

and the normalization constant $\rho_0^{-1} = \int d\vec{Q} d\vec{P} \, \delta(H(\vec{Q}, \vec{P}) - E)$. In the canonical ensemble the average is computed with the Gibbs-Boltzmann weight:

$$\langle \, A \, \rangle = Z^{-1} \int d\vec{Q} d\vec{P} \; e^{-\beta H(\vec{Q}, \vec{P})} A(\vec{Q}, \vec{P}) \; . \tag{1.4}$$

Z is the partition function $Z = \int d\vec{Q} d\vec{P} \; e^{-\beta H(\vec{Q}, \vec{P})}$.

The *(weak) ergodic hypothesis* states that under the dynamic evolution the representative point in phase space of a classical system governed by Newton laws can get as close as desired to any point on the constant energy surface.

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[1] In practice, in an experiment or numerical simulation initiated at time $t = 0$, averages are computed over a symmetric time interval around a measuring time t, in the form $\overline{A} \equiv \lim_{t_0 \ll \tau \leq t} \frac{1}{2\tau} \int_{t-\tau}^{t+\tau} dt' \; A(\vec{Q}(t'), \vec{P}(t'))$ with the lower bound in the limit representing a microscopic time-scale. The result should be independent of the measuring time t, that is why we did not write it in the expression of the main text.

[2] Here and in the following we assume that ρ is normalized. See also footnote 3 below.

The *ergodic hypothesis* states that time and ensemble averages, (1.1) and (1.2), coincide in equilibrium for *all reasonable observables*:

$$\overline{A} = \langle A \rangle \; . \tag{1.5}$$

This hypothesis cannot be proven in general but it has been verified in a large number of cases. In general, the great success of Statistical Mechanics in predicting quantitative results has given enough evidence to accept this hypothesis.

An important activity in modern Statistical Mechanics is devoted to the study of macroscopic (non-integrable) systems that *do not satisfy the ergodic hypothesis*. A well-understood case is the one of phase transitions and we shall discuss it in the next section. Other cases are related to the breakdown of equilibration. This can occur either because they are externally driven or because they start from an initial condition that is far from equilibrium and their interactions are such that they do not manage to equilibrate. One may wonder whether certain concepts of thermodynamics and equilibrium statistical mechanics can still be applied to the latter problems. At least for cases in which the macroscopic dynamics are slow one can hope to derive an extension of equilibrium statistical mechanics concepts to describe their behaviour.

Finally, let us remark that it is usually much easier to work in the canonical ensemble both experimentally and analytically. Thus, in most of our future applications we will assume that the system is in contact with a heat reservoir with which it can exchange energy and that keeps temperature fixed.

1.2 The statistical (Gibbs) ensembles

In this Subsection we discuss some aspects of the standard Statistical Physics approach to equilibrium systems that are often overlooked in the elementary courses on Statistical Mechanics. They concern the differences encountered in the description of systems with short and long range interactions, as we define below.

Gibbs introduced the notion of statistical ensembles and, usually, equivalence between the thermodynamic descriptions derived from all of them is assumed (in the thermodynamic limit). We discuss here cases in which there can be *inequivalence of ensembles* even when the number of degrees of freedom diverges [13, 14, 15].

To start with, we recall the three ensembles used. These are:

- The microcanonical ensemble describes a completely isolated system at a given energy E.
- The canonical ensemble describes a system that can exchange energy with a large thermal reservoir characterised by its temperature T.

- The grand canonical ensemble describes a system that can exchange energy and particles with a reservoir withs temperature T and chemical potential μ.

As preliminary knowledge, let us define a *microstate* as a precise microscopic state (for example, a given $(\vec{Q}, \vec{P})$). A *macrostate* is defined in terms of a small set of macroscopic or coarse-grained variables and it refers to the (large) set of microstates that yield the same value of the macroscopic variables (for example, all the configurations that share the same kinetic and potential energy values in a system of interacting particles).

1.2.1 The microcanonical ensemble

In the *microcanonical ensemble* one makes the following hypothesis:

In the long-time limit the system does not prefer any special region on the constant energy surface in Γ – there is *a priori* no reason why some region in Γ should be more probable than others! – and thus $\rho(\vec{Q}, \vec{P})$ is expected to be a constant on the energy surface and zero elsewhere:

$$\rho(\vec{Q}, \vec{P}) = \begin{cases} \rho_0 & \text{if } H(\vec{Q}, \vec{P}) \in (E, E + dE) \, , \\ 0 & \text{otherwise} \, , \end{cases} \tag{1.6}$$

The constant ρ_0 is the inverse of the volume of the constant energy surface ensuring normalisation of ρ. This is indeed the simplest stationary solution to the Liouville equation.

These hypotheses can be valid only if the *long-time dynamics is reasonably independent of the initial conditions*.

Even though it is very difficult to show, the solution proposed above is very smooth as a function of $(\vec{Q}, \vec{P})$ and it is then the best candidate to describe the *equilibrium* state – understood as the one that corresponds to the intuitive knowledge of equilibrium in thermodynamics.

This description corresponds to the *microcanonical ensemble* of statistical mechanics, valid for closed systems with fixed energy E and volume V. Each configuration on the constant energy surface is called a *microstate*. In the microcanonical ensemble all *microstates* are equivalent. We can think about all these microstates as being (many) independent *copies* of the original system. This is Gibbs' point of view: he introduced the notion of *ensemble* as the collection of mental copies of a system in identical macroscopic conditions.

The average of any phase space function $A(\vec{Q},\vec{P})$ can now be computed as

$$\begin{aligned}\langle\, A \,\rangle &= \int d\vec{Q}d\vec{P}\; \rho(\vec{Q},\vec{P})A(\vec{Q},\vec{P}) \\ &= \frac{1}{g(E)}\int d\vec{Q}d\vec{P}\; \delta[E-H(\vec{Q},\vec{P})]\, A(\vec{Q},\vec{P})\ . \end{aligned} \tag{1.7}$$

The normalisation constant $\int d\vec{Q}d\vec{P}\; \delta[E-H(\vec{Q},\vec{P})] = g(E) = \rho_0^{-1}$ is the volume of phase space occupied by the constant energy surface itself. The quantity $g(E)$ is called the *density of states*:[3]

$$g(E) \equiv \int d\vec{Q}d\vec{P}\; \delta[E-H(\vec{Q},\vec{P})]\ . \tag{1.8}$$

The *microcanonical entropy* is

$$S(E) \equiv k_B \ln g(E)\ . \tag{1.9}$$

The maximisation of the entropy is thus equivalent to the maximisation of the phase space volume available to the system.[4]

In the microcanonical ensemble the temperature is defined as

$$\frac{1}{T(E)} = \frac{\partial S(E)}{\partial E}\ . \tag{1.10}$$

A positive temperature needs, therefore, that $S(E)$ be an increasing function of E. (See footnote 4 and Ref. [16] for a recent discussion of temperature definitions in different ensembles.)

Note that the nature of the interactions between the constituents has not been mentioned in this discussion. There is no reason to believe that the microcanonical description would fail for some type of interaction as the gravitational one, a case that we shall discuss in detail below.

1.2.2 Extensivity and additivity: short and long range interactions

Once the microcanonical ensemble has been established one usually goes further and derives what is called the canonical ensemble describing the statistical properties of a system that can exchange energy with its surrounding. When trying to derive the canonical

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[3] In order to make the notation concise we ignore here the well-known issues concerning the normalisation of $g(E)$ that ensure that (1) the argument of the ln is dimensionless (also related to the uncertainty principle in quantum mechanics that constraints the number of distinguishable states) and (2) the symmetrisation of the state with respect to exchanges of identical particles.

[4] See [16] for a comparison between the implications of this definition of the entropy, called the "surface" or Boltzmann one in this paper, and the "volume" or Gibbs one in which all energy levels until the selected E one are considered. In most natural systems in large dimensions (large number of particles) the two can be expected to yield equivalent results; however, in some do not and while (1.9) could yield negative microcanonic temperatures, the volume definition does not. Other differences are found in finite size systems.

description from the microcanonical one, the distinction between systems with short and long interactions becomes important. We discuss here two properties that allow one to differentiate these two classes.

First of all, we have to determine how do the constituents of the system interact, that is to say, which are the forces acting between them. We consider systems where the interaction potential is given by the sum, over pairs of the elementary constituents, of a *two-body translationally invariant potential*.

A system of N particles confined inside a volume V is said to be *extensive* if, when the number of particles and the volume are scaled by λ, the internal energy $E(\lambda N, \lambda V)$ of the system scales as $\lambda E(N, V)$.

It is easy to see that systems with short-range forces are extensive[5].

Let us consider a macroscopic system with volume V and divide it in two pieces with volumes V_1 and V_2, with $V = V_1 + V_2$. The aim is to characterise the statistical properties of one subsystem (say 1) taking into account the effect of its interaction with the rest of the macroscopic system (subsystem 2). It is clear that the energy of the subsystems is not fixed since these are not closed: they interact with each other. The total energy, E, is then the sum of the energies of the two sub-ensembles plus the interaction energy between the two pieces, $E = E_1 + E_2 + E_I$.

If the interactions between the constituents of the system are *short-ranged*, in the sense that the interaction energy is proportional to the surface between the two pieces, $E_I \propto S$, while the energy of each subsystem will be extensive and proportional to their volumes, $E_1 \propto V_1$ and $E_2 \propto V_2$. Thus, for a macroscopic system, E_I is negligible with respect to $E_1 + E_2$.

If, instead, the interactions between the constituents are sufficiently *long-ranged* the separation into volume and surface contributions to the total energy does not apply any longer. This remark allows one to define the following property.

The *additivity property*, states that

$$E = E_1 + E_2 \, , \tag{1.11}$$

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[5] If the interaction potential is short-range, each particle will interact only with the particles which are within the range γ of the interaction potential. Suppose that a system is homogeneous, the number of particles within the distance γ of a given particle will then be proportional to $N\gamma^d/V$ and the internal energy must have the form of $E(N,V) = Nf(N/V)$, where $f(x)$ is a function that depends on the microscopic interactions between the particles. Actually, it is not necessary for the interaction potential to be bounded by γ; algebraically decaying potentials will lead to extensive thermodynamics as long as they decay sufficiently rapidly, i.e. if $\alpha > d$.

for any two subsystems 1 and 2 of a macroscopic system. An alternative definition of systems with *short range interactions* applies to those for which the additivity property holds, and systems with *long range interactions* as those for which this property fails.

The long-ranged interactions are sometimes called *non-integrable* in the literature.

In some cases, the energy of a system with long-range interactions can be rendered extensive (instead of super-extensive) by properly scaling the interaction parameters with the number of degrees of freedom. We next investigate some examples.

Examples

One such example is the case of an *Ising spin model with fully-connected ferromagnetic interactions* (the Curie-Weiss model): $H = -J/2 \sum_{i\neq j} s_i s_j$ with $s_i = \pm 1$ and $J > 0$. The sum runs over *all pairs* of spins in the ensemble with the constraint $i \neq j$. The factor $1/2$ ensures that each pair of spins contributes only once to the sum. Clearly, the ferromagnetic configurations have a super extensive energy, since $H(s_i = 1) = -J/2\ N(N-1) \to -J/2\ N^2$ for $N \gg 1$. This problem can be corrected by scaling $J \mapsto J/N$, in which case $H(s_i = 1) = -J/2\,(N-1)$ and energy extensivity is restored. However, the energy remains non-additive since all spins still interact with all other ones in the sample and there is no notion of interface between two subsystems. Indeed, let us explore the additivity property of the energy for the perfectly magnetised state. The total energy is $E = -J(N-1)$. If we now divide the system in two subsystems with $N/2$ spins each the total energy of each subsystem is $E_1 = -J(N/2-1)/4$ and $E_2 = -J(N/2-1)/4$ and one notices that $E \neq E_1 + E_2$. More precisely, $E_I \equiv E - (E_1 + E_2) = -JN/4$, still a macroscopic quantity. One has

$$E \sim E_1 \sim E_I \sim -JN \tag{1.12}$$

all these energies are of the order of the number of spins in the sample. (In contrast, in the usual Ising model defined on a d dimensional lattice with nearest-neighbour interactions the additivity properties holds.)

The *the power-law potential* is another relevant case in which particle systems have non-additive potentials in sufficiently low dimensions. In the field of particle systems with two-body interactions falling-off with distance as a power law

$$V(r) \sim r^{-\alpha} \tag{1.13}$$

one finds that the interactions are

- long-ranged (non-additive) if $\alpha < d$,
- quasi long-ranged (marginal) if $\alpha = d$,
- short-ranged (additive) if $\alpha > d$,

with d the dimension of space. A simple way of showing this general result is the following. Take a point particle with unit mass and place it at the origin of coordinates. Consider its interaction with a homogeneous massive spherical shell with internal radius ϵ and external radius R. The energy, e, felt by the central particle is

$$e = -\int_V d^d x \, \frac{J\rho}{r^\alpha} = -\Omega_d \, J\rho \int_\epsilon^R dr \, \frac{r^{d-1}}{r^\alpha} = -\frac{\Omega_d \, J\rho}{d-\alpha} \left[R^{d-\alpha} - \epsilon^{d-\alpha} \right] \ , \tag{1.14}$$

where we adopted the potential $V(r) = Jr^{-\alpha}$ for all r, and the particle density is ρ. Ω_d is the angular volume, $\Omega_d = 2\pi$ in $d = 2$, $\Omega_d = 4\pi$ in $d = 3$, etc. For $\alpha > d$ the contribution from the external surface ($r = R$) is negligible while for $\alpha \leq d$ it grows with the volume $V \propto R^d$ as $V^{1-\alpha/d}$. In the latter case surface effects cannot be neglected and the total energy $E = Ve$, is super-linear with the volume:

$$E \simeq JVR^{d-\alpha} \simeq JR^{2d-\alpha} = JR^{d(2-\alpha/d)} = JV^{1+1-\alpha/d} \tag{1.15}$$

for $1 - \alpha/d > 0$, or is *super extensive*. This problem can be solved by scaling the interactions analogously to what was done in the fully-connected spin model (defined on the complete graph), *i.e.* one can redefine the coupling constant $J \mapsto J \ V^{\alpha/d-1}$ and get an extensive system, $E \propto V$. However, the lack of additivity will not be resolved if $\alpha < d$, as there is no clear distinction between *bulk* and *surface* in models with long-range interactions.

Another example is the *self-gravitating gas in a low dimensional space*. As the interaction, $V_G(r) = -Gm^2 r^{-1}$, is attractive, one and two dimensional gravitational systems are self-confining. One can then safely take the infinite volume limit $V \to \infty$ and focus on the scaling of the energy with the number of particles. In order to avoid the non-extensivity of the energy, the gravitational constant can be rescaled by a factor $1/N$, the so-called *Kac prescription*. However, the energy remains non-additive after this rescaling, in particular, in three spatial dimensions. The statistical physics of self-gravitating systems falls into this class of *bizarre* problems and there is much current research [17, 18, 19] to try to elucidate their properties.

The *Van der Waals interaction*, $V_{VW}(r) \propto r^{-6}$, is instead short-ranged in $d = 3$. *Plasma physics* provides another exampl of non-additive systems through an effective description.

Note that that non-additivity also occurs in systems with short-range interactions in which surface and bulk energies are comparable; this is realised in *finite size* problems, of special importance nowadays in the context of biological or quantum mesoscopic systems, for example.

1.2.3 The canonical ensemble

Let us review the derivation of the canonical distribution. Consider a system with volume V, divide it in two pieces with volumes V_1 and V_2, with $V = V_1 + V_2$, and energies

E_1 and E_2. If we assume that the two systems are *independent* with the constraint that $E_1 + E_2 = E$, *i.e.* the *additivity property*, the probability of subsystem 1 to get an energy E_1 is

$$
\begin{aligned}
P(E_1)\, dE_1 &\propto \int dE_2\; g(E_1, E_2)\; \delta(E - E_1 - E_2)\; dE_1 \\
&= \int dE_2\; g_1(E_1) g_2(E_2)\; \delta(E - E_1 - E_2)\; dE_1 \\
&= g_1(E_1) g_2(E - E_1)\; dE_1 \\
&= g_1(E_1) e^{k_B^{-1} S_2(E-E_1)}\; dE_1 \\
&\simeq g_1(E_1)\; e^{k_B^{-1} S_2(E) + k_B^{-1} \partial_E S_2(E)(-E_1)}\; dE_1 \\
&\propto g(E_1) e^{-\beta_2(E) E_1}\; dE_1
\end{aligned}
\qquad (1.16)
$$

where we used the definition of the microcanonic inverse temperature of the second component, $\beta_2(E) = 1/(k_B T_2(E))$. Note that in the next to last passage we dropped all higher order terms in the Taylor expansion assuming that $E_1 \ll E$. After fixing the normalisation, re-expanding $\beta_2(E) \simeq \beta_2(\langle E \rangle)$ and dropping the energy fluctuations of the bath with respect to its average or expectation value $\langle E \rangle$, we can call $\beta_2(E) \simeq \beta_2(\langle E \rangle) \to \beta$, and

$$
\boxed{P(E_1) = Z^{-1}(\beta)\; g(E_1) e^{-\beta E_1} \qquad \text{with} \qquad Z(\beta) = \int dE_1\; g(E_1) e^{-\beta E_1}\;. \qquad (1.17)}
$$

Let us recap the assumptions made: (i) energy additivity $E_2 = E - E_1$, (ii) independence, $g(E_1, E_2) = g(E_1) g(E_2)$, (iii) small system 1 ($E_1 \ll E$), (iv) constant inverse 'temperature' $k_B \beta \equiv \partial_E S_2(E)$. Note that assumptions (i) and (ii) fail in systems with long-range interactions. In these cases the microcanonical ensemble is well-defined though difficult to use, and the canonical one is not even defined!

The failure of energy additivity is at the origin of the unusual equilibrium and dynamic behaviour of systems with long-range interactions. Surprisingly enough, one finds that many usual thermodynamic results are modified with, for example, systems having negative microcanonical specific heat; moreover, the statistical ensembles (microcanonic, canonic and macrocanonic) are no longer equivalent, as we saw above with the failure of the derivation of the canonical ensemble from the microcanonical.

The canonical ensemble does not describe the fluctuations of a small subsystem of a system with constituents interacting via long-range interactions. One can, however, argue that it will describe the fluctuations of a system with long-range internal interactions connected, *via* short-range interactions, with another larger systems that acts as a heat-bath and, itself, with only internal short-range interactions. This claim leads us to the issue of the *reduction* of a larger system into a smaller one by integrating away a large part of the combined ensemble, a problem that we will discuss in Sec. 1.3.1.

1.2.4 Gaussian energy fluctuations in the canonical ensemble

The probability distribution $P(E)$ in the canonical ensemble, $P(E) = g(E)e^{-\beta E}/Z$, has an extremum at $E = U(\beta)$, with $U(\beta)$ given by[6]

$$\partial_E S(E)|_{E=U(\beta)} = k_B\beta = T^{-1} , \tag{1.18}$$

where $S(E) \equiv k_B \ln g(E)$ is the (microcanonic) entropy defined from the density of states $g(E)$, see eq. (1.9). The stability of this extremum depends on the sign of $\partial_E^2 S(E)|_{E=U(\beta)}$ and we examine it below.

The Taylor expansion of $\ln[ZP(E)]$ around $E = U$ (not writing the β dependence of U to lighten the notation) yields

$$\begin{aligned} \ln[ZP(E)] &\sim -\beta[U - TS(U)] + \frac{1}{2k_B} \left.\frac{\partial^2 S(E)}{\partial E^2}\right|_{E=U} (E-U)^2 + \dots \\ &\sim -\beta[U - TS(U)] - \frac{k_B}{2}\beta^2 \frac{1}{\overline{C}_V^{can}} (E-U)^2 + \dots \end{aligned} \tag{1.19}$$

where we took the derivative of (1.18) with respect to β

$$k_B = \left.\frac{\partial^2 S(E)}{\partial E^2}\right|_{E=U(\beta)} \frac{\partial U(\beta)}{\partial \beta} \tag{1.20}$$

to replace the coefficient of the quadratic term as a function of the *canonical specific heat*[7]

$$\overline{C}_V^{can}(\beta) \equiv \frac{\partial U(T)}{\partial T} = -k_B\beta^2 \frac{\partial U(\beta)}{\partial \beta} = -k_B^2\beta^2 \frac{1}{\left.\frac{\partial^2 S(E)}{\partial E^2}\right|_{E=U(\beta)}} . \tag{1.21}$$

Within the quadratic approximation of eq. (1.19) that neglects all higher order terms, and the supposition $\overline{C}_V^{can}(\beta) > 0$, the energy probability density $P(E)$ is a Gaussian centred at U (thus $U = \langle E \rangle \equiv U(\beta)$) with variance $\sigma^2 = \overline{C}_V^{can}/(k_B\beta^2)$ (thus $\langle (E - U)^2 \rangle = \overline{C}_V^{can}/(k_B\beta^2)$).

---

[6] One proves it by taking the ln (a monotonic function of its argument), replacing $g(E)$ by its relation to $S(E)$, and taking the derivative.

[7] In order to check the presence of the k_B factors one can do a dimensional analysis and see that $[C_V^{can}] = [k_B]$.

Is the assumption $\overline{C}_V^{can} > 0$ true? Indeed, it should be. In the canonical ensemble the constant volume specific heat (note that it is defined through $U(\beta) = \langle E \rangle$ an entity that is canonical by construction)

$$\begin{aligned} C_V^{can}(\beta) &= -k_B\beta^2 \frac{\partial U(\beta)}{\partial \beta} = -k_B\beta^2 \frac{\partial \langle E \rangle(\beta)}{\partial \beta} = k_B\beta^2 \frac{\partial^2 \ln Z(\beta)}{\partial \beta^2} \\ &= k_B\beta^2 \left[-\frac{1}{Z^2(\beta)} \left(\frac{\partial Z(\beta)}{\partial \beta} \right)^2 + \frac{1}{Z(\beta)} \frac{\partial^2 Z(\beta)}{\partial \beta^2} \right] = k_B\beta^2 \, \left[\langle E^2 \rangle(\beta) - \langle E \rangle^2(\beta) \right] \\ &= k_B\beta^2 \, \langle (E - \langle E \rangle)^2 \rangle(\beta) > 0 \end{aligned} \tag{1.22}$$

is positive definite. All averages in these expressions have to be computed with the full canonical pdf (no Gaussian approximation used).

In this process we have proven a form of *fluctuation-dissipation* theorem or, in other words, a relation between a *susceptibility* (to changes in temperature) and *connected fluctuations* (of the energy):

$$-\frac{\partial \langle E \rangle}{\partial \beta} = \langle (E - \langle E \rangle)^2 \rangle \qquad \Rightarrow \qquad \frac{\partial \langle E \rangle}{\partial T} = k_B\beta^2 \, \langle (E - \langle E \rangle)^2 \rangle \, . \tag{1.23}$$

In an extensive macroscopic system with N particles, $\langle E \rangle = U \propto N$ and $C_V^{can} \propto N$ in which case the ratio between dispersion and typical energy, or relative fluctuation, vanishes as $\sigma/U \propto N^{-1/2}$, and the Gaussian approximation is fully satisfied. In the large N limit, fluctuations are ‘killed’, the energy in the canonical ensemble does not fluctuate, it is locked to the value U, and it is related to the temperature through (1.18).

In the thermodynamic limit $N \to \infty$ the relative fluctuations $\sigma/U \propto N^{-1/2} \to 0$ and $E \to U(\beta)$. This implies that the microcanonical and canonical descriptions should coincide as, in practice, in the canonical formalism the energy of a macroscopic system is concentrated on a single value U determined by the temperature $T = 1/(k_B\beta)$.

One thus proves the equivalence between the microcanonical and canonical results.

1.2.5 Negative specific heat and convex entropy function in the microcanonic ensemble

What happens when the equivalence fails? What kind of peculiar effect can one expect to find? One of the simplest mismatches found is the possibility of having negative specific heat in some range of energies in the microcanonical description of systems with long-range interactions. This is impossible in a canonical formalism. Indeed, the *microcanonical constant volume specific heat* is defined as

$$C_V^{micro} \equiv -k_B \beta^2 \, \frac{\partial E(\beta)}{\partial \beta} = \frac{\partial E(T)}{\partial T} \tag{1.24}$$

[one inverts $\beta(E) = k_B^{-1} \partial_E S(E)$ to write $E(\beta)$ or $1/T(E) = \partial_E S(E)$ to write $E(T)$] and this quantity is not positive definite if the *entropy is not concave*. Indeed, after the simple manipulation,

$$\frac{\partial^2 S}{\partial E^2} = \frac{\partial}{\partial E}\left(\frac{\partial S}{\partial E}\right) = \frac{\partial}{\partial E}\left(\frac{1}{T}\right) = -\frac{1}{T^2}\frac{\partial T}{\partial E} = -\frac{1}{C_V^{micro}}\frac{1}{T^2} \tag{1.25}$$

and

> the *convexity of the entropy*, $\partial^2 S/\partial E^2 > 0$ for some values of the energy implies that $C_V^{micro} < 0$ for those same values.

When the two ensembles are equivalent the micronanonical C_V^{micro} should be identical to the canonical one, C_V^{can}, and thus positive. However, it is possible to construct models, for instance those with long-range interactions, such that C_V^{micro} is negative in some range of energies (these are usually related to first order phase transitions in the canonical ensemble).

It turns out that when $C_V^{micro} < 0$ the system undergoes a first-order phase transition in the canonical ensemble.

> In a nutshell, the energy interval in which there is a convex entropy in the microcanonical setting, corresponds to a single value of the temperature in the canonical ensemble at which the system undergoes a *first order phase transition*.

We will revisit this problem in the Chapter in which we will review phase transitions.

1.2.6 The macrocanonical ensemble

Finally in the macrocanonical ensemble one characterises the macroscopic state with the volume V, the temperature T, and the chemical potential μ.

Summarizing, in the microcanonical ensemble the system is isolated and temperature is defined as $T^{-1} \equiv \partial S/\partial E|_E$. In the canonical ensemble the system is in contact with a reservoir – considered to be a much larger system – with which it can exchange energy to keep temperature fixed to be the one of the external environment. In the macrocanonical ensemble the system is in contact with a reservoir with which it can exchange energy *and* particles. The equivalence between them is ensured only for systems with short-range interactions.

1.2.7 Equivalence of ensembles

The practical consequence of ensemble equivalence is that one has the freedom to choose the ensemble in which calculations are easier. In spite of its fundamental importance in the construction of statistical mechanics, the microcanonical ensemble is practically never used to perform analytical calculations, since calculations are much harder in its setting than in the canonical one. The microcanonical ensemble is, however, commonly used in numerical simulations, since it is at the basis of molecular dynamic simulations.

Paraphrasing H. Touchette [20], the questions as to whether there is equivalence of ensembles can be posed in different ways:

- *Thermodynamic equivalence.* Are the microcanonical thermodynamic properties of a system determined from the entropy as a function of energy the same as the canonical thermodynamic properties determined from the free energy as a function of temperature? Are energy and temperature always one-to-one related?
- *Macrostate equivalence.* Is the set of equilibrium values of macrostates (e.g., magnetization, energy, velocity distribution, etc.) determined in the microcanonical ensemble the same as the set of equilibrium values determined in the canonical ensemble? What is the general relationship between these two sets?
- *Measure equivalence.* Does the Gibbs distribution defining the canonical ensemble at the microstate level converge (in some sense to be made precise) to the microcanonical distribution defined by Boltzmann's equiprobability postulate?

Equivalence of ensembles holds at the thermodynamic level whenever the entropy is concave, that is to say, $\partial^2 S(E)/\partial E^2 < 0$.

(see the proof below). This also implies, under additional conditions, the equivalence of the microcanonical and canonical ensembles at the macrostate level. Less is known about the measure equivalence. A survey of recent research on this field can be found in [20]. Systems with short-range interactions have concave entropies and for them equivalence of ensembles is ensured. Systems with long-range interactions can have non-concave[8] entropies and, therefore, inequivalence of ensembles can apply to them [13, 14, 15].

The proof goes as follows. The partition function Z and the free-energy density f are linked by

$$Z(\beta, V, N) = e^{-\beta N f(\beta, v)} \tag{1.26}$$

---

[8] A concave entropy density, $\lim_{N\to\infty} S(E,V,N)/N$, function satisfies $s(ce_1+(1-c)e_2,v) \geq cs(e_1,v)+(1-c)s(e_2,v)$ for any choice of $e_1 = E_1/V$, $e_2 = E_2/V$, $v = N/V$ and $0 \leq c \leq 1$.

with $v = V/N$ and the large N limit assumed. For a system of N identical particles, the partition function can be expressed as

$$\begin{aligned} Z(\beta, V, N) &= \frac{1}{N!}\int dE \int d\vec{Q}d\vec{P}\;\delta(E - H(\vec{Q},\vec{P}))\,e^{-\beta E} \\ &= \int dE\; g(E,V,N)\,e^{-\beta E} \\ &= \int dE\; e^{-N[\beta\varepsilon - k_B^{-1}s(\varepsilon,v)]} \end{aligned} \tag{1.27}$$

where, for large N, we replaced $S(E,V,N) = Ns(\varepsilon,v)$ with $\varepsilon = E/N$ and $v = V/N$. In the large N limit we can evaluate the last integral by saddle-point *iff* the entropy is concave, $\partial^2 S(E)/\partial E^2 < 0$, otherwise the Gaussian corrections would make the remaining integral explode. Assuming concavity,

$$\beta f(\beta, v) = \inf_{\varepsilon}\,[\beta\varepsilon - k_B^{-1}s(\varepsilon,v)] \tag{1.28}$$

obtaining that $\beta f(\beta,v)$ is the Legendre transform of $s(\varepsilon,v)$. One can proceed backwards and derive that s is the Legendre transform of βf

$$k_B^{-1}s(\varepsilon,v) = \inf_{\beta}\,[\beta\varepsilon - \beta f(\beta,v)]\;. \tag{1.29}$$

For each value of β there is a value of ε that satisfies (1.28) and viceversa for (1.29).

In cases in which the entropy has a convex region, the inverse Legendre transform leading from βf to s yields the concave envelope of s (and cannot access its convex piece).

Ensemble inequivalence is not merely a mathematical drawback, but it is the cause of physical properties that can be experimentally verified.

1.2.8 Non-equilibrium steady states

The dynamics of systems with long-range interactions can be extremely slow and the approach to equilibrium can take a very long time, that increases with the number N of elementary constituents. This feature is induced by the long-range nature of the interaction itself and it is not a consequence of the existence of a collective phenomenon. The state of the system during this long transient is quasi-stationary but it is not a thermodynamic metastable state, as it does not lie on local extrema of equilibrium thermodynamic potentials. The nature of quasi-stationary states can depend on the initial condition. In addition, a variety of macroscopic structures can form spontaneously in out-of-equilibrium conditions for isolated systems: a fact that should not be a surprise given that already the equilibrium states of long-range systems are usually inhomogeneous.

1.2.9 Many physical examples

Computing the microcanonical distribution function of macroscopic systems with realistic long-range interactions is usually prohibitly difficult. One then works with *toy models* that are much simpler but capture the essential features of the realistic problems. Some of the toy models that have been studied in detail are

- The *self-gravitating two-body problem*:

$$H(\vec{P},\vec{Q},\vec{p},\vec{r}) = \frac{P^2}{2M} + \frac{p^2}{2\mu} - \frac{Gm^2}{r} \tag{1.30}$$

  where $\vec{P}$ and $\vec{Q}$ are the momentum and coordinate of the center of mass and $\vec{p}$ and $\vec{q}$ are the relative moment and coordinate, $M = 2m$ is the total mass, $\mu = m/2$ is the reduced mass and m is the mass of the individual particles. The distance r is the modulus of the vector $\vec{q}$. One also restricts the range of the r coordinate to the interval (a, R). The short-distance cut-off mimics hard spherical particles of radius $a/2$. In the limits $a \to 0$ and $R \to \infty$ this is the standard Kepler problem.

  The statistical mechanics of this system are described in detail in [17]. The system has two natural energy scales $E_1 = -Gm^2/a$ and $E_2 = -Gm^2/R$ with $E_1 < E_2$. For $E \gg E_2$ gravity is irrelevant, there is a long distance between the particles ($r > R$) and the system behaves like a gas, confined by a container. The microcanonic heat capacity is positive. As one lowers the energy the effects of gravity begin to be felt. For $E_1 < E < E_2$ neither the box nor the short-distance cut-off have an effect and there is a negative specific heat. As $E \sim E_1$ the hard core nature of the particles becomes important and gravity is again resisted, this is the low energy phase with positive microcanonic specific heat. The $T(E)$ dependence (and hence the microcanonical specific heat) is shown in Fig. 1.1. It must be noticed that astrophysical systems are in the intermediate energy scales with negative specific heat; moreover, this range is pretty wide since $E_1 \ll E_2$.

  One can also analyse the canonical partition function – knowing already that it should predict a different behaviour from the above in the region $[E_1, E_2]$. In particular, one can compute the mean energy and its relation with temperature to compare with the microcanonical behaviour. One finds that at very low and very high energies the curves coincides. In the intermediate region the canonical $T(E)$ relation is almost flat and the canonical specific heat takes a very large value, almost a divergent one. This is similar to a phase transition in which the specific heat would diverge. The divergence is smoothened in this case due to the fact that there is a finite number of degrees of freedom in the two body problem.

- The *Lynden-Bell model* is a model of $(2N + 1)$ coordinates evolving through the Hamiltonian

$$H = \frac{p^2}{2m} + \sum_{i=1}^{N} \frac{1}{2mr^2}\left({p_{\theta}}_i^2 + \frac{{p_{\phi}}_i^2}{\sin^2\theta_i}\right) - \frac{Gm^2}{2r} \tag{1.31}$$

with r constrained to take values in (a, R). In this model one can take the large N limit and recover a true phase transition in the canonical formulation.

- The *Thirring model* is one with a set of N particles in a volume V. The particles interact with a constant potential if they come within an interaction volume V_o. In both the Lynden-Bell and Thirring models in the high energy regime the particles occupy space uniformly: it is a homogeneous phase. In the low energy regime instead the particles are close together in a collapsed phase.

- The *self-gravitating gas.* Consider a system of N particles interacting through Newtonian gravitational forces alone. The properties of this system depend on N. If $N = 2$ it is the exactly solvable Kepler problem, for $N = 3 - 50$, say, it cannot be solved exactly but it can be tackled with a computer. For larger N, $N = 10^5 - 10^{11}$, say, one is interested in averaged properties and statistical methods should be used.

  First, one must recall that a short-distance cut-off is necessary to render all phase space integrals convergent. This is justified by arguing that at very short distances not only the gravitational force acts on the particles and other forces regularise the $r \to 0$ behaviour of the total interaction potential.

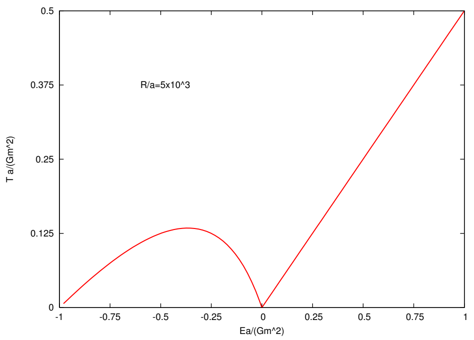

Figure 1.1: The temperature against the energy for the two-body problem with gravitational interaction with cut-off a in a box of size R. The microcanonical curve is non-monotonic with a negative specific heat in the region $E \sim [-0.4, 0]$. The canonical curve is monotonic and almost flat – as in a smoothened phase transition – in the region in which $C_V^{micro} < 0$.

It turns out that an interesting thermodynamic limit of the three ensembles (microcanonical, canonical and macrocanonical) is achieved in the very dilute limit [18, 19]

$$\eta \equiv \frac{Gm^2 N}{V^{1/3} T} \qquad \text{finite} \; . \tag{1.32}$$

In this limit the thermodynamic quantities (free energy, energy, *etc.*) are functions of η and T and scale with N. Instead, the chemical potential and specific heat are just functions of T and η. The system undergoes collapse phase transitions in microcanonical and canonical ensembles though their location is different.

- The fully-connected *Blume-Capel* lattice spin-1 model,

  $$H = \Delta \sum_{i=1}^{N} s_i^2 - \frac{J}{2N} \left(\sum_{i=1}^{N} s_i \right)^2 \;, \tag{1.33}$$

  with s_i taking three values, $s_i = \pm 1, 0$, $J > 0$ the ferromagnetic coupling, $\Delta > 0$ the parameter that controls the energy difference between the ferromagnetic ± 1 states and the paramagnetic $s_i = 0$ state. The normalisation of the interaction term with N ensures that the total energy is extensive, *i.e.* $E = \mathcal{O}(N)$. This model has a phase diagram with two phases, ferromagnetic and paramagnetic, separated by a transition curve that is of second order for small Δ (the Curie-Weiss limit is attained for $\Delta = 0$) and of first order for large Δ. Details on the solution of this mean-field model are found in [13].

- The *Hamiltonian mean-field model* is defined by

  $$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{J}{2N} \sum_{ij} [1 - \cos(\theta_i - \theta_j)] \tag{1.34}$$

  It represents unit mass particles moving on a unit circle with momenta p_i and position represented by an angular variable $\theta_i \in [0, 2\pi)$. The interactions are such that each particle interacts with all other ones in the same attractive ($J > 0$) or repulsive ($J < 0$) way (classical XY rotors).

1.3 Reduced systems

In this section we will consider the reduction operation that consists in integrating away a portion of the system and investigate which are the statistical properties of what remains. We will distinguish the weak and strong coupling between the part retained and the part integrated away. This procedure is great importance when, for example, trying to describe the statistical properties of a small system strongly coupled to an environment.

1.3.1 The reduced partition function in the canonical setting

In the rest of this lecture we always think of the system of interest being coupled to a mega environment with which it can exchange energy. In this section we will consider the operation that consists in integrating away a portion of the system and investigate which are the statistical properties of what remains. We will distinguish the weak and strong coupling between the two parts.

We analyze the statistical static properties of a *classical canonical system* in equilibrium at inverse temperature β and itself formed by two sub-parts, one that will be treated as an

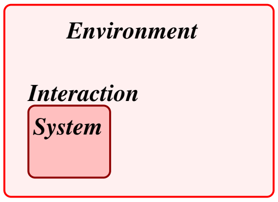

Figure 1.2: Sketch of the system and bath coupling.

environment (not necessarily of infinite size) and another one that will be the (sub-)system of interest. We study the *partition function* or Gibbs functional, $Z_{\rm tot}$:

$$Z_{\rm tot}[\eta] = \sum_{\substack{\text{conf env}\\ \text{conf syst}}} \exp(-\beta H_{\rm tot}) \tag{1.1}$$

where the sum represents an integration over the phase space of the full system, i.e. the system's and the environmental ones. We take

$$H_{\rm tot} = H_{\rm syst} + H_{\rm env} + H_{\rm int} \; . \tag{1.2}$$

For simplicity we use a single particle moving in $d = 1$: $H_{\rm syst}$ is the Hamiltonian of the isolated particle,

$$H_{\rm syst} = \frac{p^2}{2M} + V(x) \; , \tag{1.3}$$

with p and x its momentum and position. $H_{\rm env}$ is the Hamiltonian of a 'thermal bath' that, for simplicity, we take to be an ensemble of N independent harmonic oscillators with masses m_a and frequencies ω_a, $a = 1, \dots, N$

$$H_{\rm env} = \sum_{a=1}^{N} \frac{\pi_a^2}{2m_a} + \frac{m_a\omega_a^2}{2} q_a^2 \tag{1.4}$$

with π_a and q_a their momenta and positions. This is indeed a very usual choice since it may represent phonons. (These oscillators could be the normal modes of a generic Hamiltonian expanded to quadratic order around its absolute minimum, written in terms of other pairs of conjugate variables; the bath could be, for instance, a chain of harmonic oscillators with nearest-neighbor couplings.) $H_{\rm int}$ is the coupling between system and environment. We will restrict the following discussion to a linear interaction in the oscillator coordinates, q_a, and in the particle coordinate,

$$H_{\rm int} = x \sum_{a=1}^{N} c_a q_a \; , \tag{1.5}$$

with c_a the coupling constants.

The generalization to more complex systems and/or to more complicated baths and higher dimensions is straightforward. The calculations can also be easily generalized to an interaction of the oscillator coordinate with a more complicated dependence on the system's coordinate, $\mathcal{V}(x)$, that may be dictated by the symmetries of the system at the expense of modifying the counter-term. Non-linear functions of the oscillator coordinates cannot be used since they render the problem unsolvable analytically (although, of course, they can exist in Nature!).

Having chosen a quadratic bath and a linear coupling, the integration over the oscillators' coordinates and momenta can be easily performed. This yields the *reduced* partition function

$$Z_{\rm red} \propto \sum_{\rm conf\ syst} \exp\left[-\beta\left(H_{\rm syst} - \frac{1}{2}\sum_{a=1}^{N} \frac{c_a^2}{m_a\omega_a^2}\, x^2\right)\right] . \tag{1.6}$$

We notice that a quadratic term in x has been generated by the integration of the q_a variables. The reduced partition function can be written as

$$Z_{\rm red} \propto \sum_{\rm conf\ syst} \exp(-\beta H^*) \qquad \text{with} \qquad H^* = H_{\rm syst} - \frac{1}{2}\sum_{a=1}^{N} \frac{c_a^2}{m_a\omega_a^2}\, x^2 . \tag{1.7}$$

At this level different choices can be made.

- One can argue that the coupling constants are small enough, say $c_a^2 = \mathcal{O}(N^{-2})$, and drop the last term to recover the partition function of the selected system. This is a *weak coupling limit* between the selected system and the rest.
- One can claim that $c_a^2 = \mathcal{O}(N^{-1})$ and keep the modification of the Hamiltonian of the reduced system as a relevant one (and start in this way a *renormalisation* procedure by reproducing these steps many times).
- One can argue that, although the couplings are not small, say $c_a^2 = \mathcal{O}(N^{-1})$, the original Hamiltonian of the coupled system needs to be modified by adding a counter-term in order to recover only the Hamiltonian of the selected system after integrating away the oscillators. We explain this procedure in detail below.

In the last item above we propose to work with

$$H_{\rm tot} = H_{\rm syst} + H_{\rm env} + H_{\rm int} + H_{\rm counter} = H_{\rm syst} + \tilde{H}_{\rm env} \tag{1.8}$$

with

$$H_{\rm counter} = \frac{1}{2}\sum_{a=1}^{N} \frac{c_a^2}{m_a\omega_a^2} x^2 \tag{1.9}$$

so that the combination of the environmental, interaction and *counter-term* Hamiltonians take a rather simple and natural form

$$\tilde{H}_{\text{env}} = H_{\text{env}} + H_{\text{int}} + H_{\text{counter}} = \sum_a \frac{m_a \omega_a^2}{2} \left(q_a + \frac{c_a}{m_a \omega_a^2} x \right)^2 . \tag{1.10}$$

In this way,

$$H^* = H_{\text{syst}} + H_{\text{counter}} - \frac{1}{2} \sum_{a=1}^{N} \frac{c_a^2}{m_a \omega_a^2}\, x^2 = H_{\text{syst}} \tag{1.11}$$

and

$$Z_{\text{red}}[\eta] \propto \sum_{\text{conf syst}} \exp\left[-\beta \left(H_{\text{syst}}\right)\right] = Z_{\text{syst}} . \tag{1.12}$$

The counter-term H_{counter} is chosen to cancel the term generated by the integration over the oscillators and it avoids the renormalization of the coefficient of the quadratic term in the potential that could have even destabilized the potential by taking negative values. For a non-linear coupling $H_{\text{int}} = \sum_{a=1}^{N} c_a q_a \mathcal{V}(x)$ the counter-term is

$$H_{\text{counter}} = \frac{1}{2} \sum_{a=1}^{N} \frac{c_a^2}{m_a \omega_a^2} [\mathcal{V}(x)]^2 . \tag{1.13}$$

The interaction with the reservoir does not modify the statistical properties of the particle since $Z_{\text{red}} \propto Z_{\text{syst}}$, independently of the choices of c_a, m_a, ω_a and N.

If one is interested in the *dynamics* of a coupled problem, the characteristics of the sub-system that will be considered to be the bath have an influence on the reduced dynamic equations found for the system, that are of generic Langevin kind. To take a weak coupling limit $c_a^2 \to 0$ to get rid of the generated force might be problematic since it implies also a very slow relaxation. One usually adds a counter-term in the dynamic formalism to get a good Langevin for the system.

Appendices

1.A Some useful mathematical tools

1.A.1 Stirling

Stirling formula for the factorial of a large number reads:

$$\ln N! \sim N \ln N - \ln N \; , \qquad \text{for} \qquad N \gg 1 \; . \tag{1.A.1}$$

1.A.2 Moments

Introducing a source h that couples linearly to a random variable x one easily computes all moments of its distribution $p(x)$. Indeed,

$$\langle \, x^k \, \rangle = \frac{\partial^k}{\partial h^k} \int dx \; p(x) e^{hx} \bigg|_{h=0} \; . \tag{1.A.2}$$

1.A.3 Gaussian integrals

The Gaussian integral is

$$I_1 \equiv \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \; e^{-\frac{(x-\mu)^2}{2\sigma^2}} = 1 \; . \tag{1.A.3}$$

It is the normalization condition of the Gaussian probability density written in the *normal form*. One has

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \; e^{-\frac{(x-\mu)^2}{2\sigma^2}} \; x &= \mu \; , \\ \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \; e^{-\frac{(x-\mu)^2}{2\sigma^2}} \; x^2 &= \sigma^2 \; . \end{aligned} \tag{1.A.4}$$

From (1.A.3) one has

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \; e^{-\frac{x^2}{2\sigma^2} + \frac{\mu x}{\sigma^2}} = e^{\frac{\sigma^2 \mu^2}{2}} \; . \tag{1.A.5}$$

The generalization to N variables

$$I_N \equiv \int_{-\infty}^{\infty} \prod_{i=1}^{N} dx_i e^{-\frac{1}{2}\vec{x}^t A \vec{x} + \vec{x}^t \vec{\mu}} \tag{1.A.6}$$

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

$$-\frac{1}{2}\vec{x}^t A\vec{x} + \vec{x}^t\vec{\mu} \tag{1.A.7}$$

is the most generic quadratic form. Note that A plays here the role σ^{-2} in the single variable case. 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 vectors $\vec{x}$ and its transposed. Focusing now on a symmetric matrix, $A^t = A$, that we still call A we can ensure that it is diagonalizable 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 $\vec{x}^t A\vec{x} = (\vec{x}^t A^{1/2})(A^{1/2}\vec{x}) = \vec{y}\vec{y}$, the integral I_N in (1.A.6) becomes

$$I_N = \int_{-\infty}^{\infty} \prod_{i=1}^{N} dy_i J e^{-\frac{1}{2}\vec{y}^t\vec{y}+\vec{y}^t(A^{-1/2}\mu)} \tag{1.A.8}$$

where $J = \det(A^{1/2})^{-1} = (\det A)^{-1/2}$ is the Jacobian of the change of variables. Calling $\vec{\mu}'$ the last factor one has the product of N integrals of the type I_1; thus

$$I_N = (2\pi)^{N/2}(\det A)^{-1/2}e^{\frac{1}{2}\vec{\mu}^t A^{-1}\vec{\mu}} \tag{1.A.9}$$

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

$$\vec{x} \equiv (x_1, \dots, x_N) \to \phi(\vec{x}) \tag{1.A.10}$$

and

$$I = \int \mathcal{D}\phi \; e^{-\frac{1}{2}\int d^dx d^dy \; \phi(\vec{x})A(\vec{x},\vec{y})\phi(\vec{y}) + \int d^dx \; \phi(\vec{x})\mu(\vec{x})} \; . \tag{1.A.11}$$

The sum runs over all functions $\phi(\vec{x})$ with the spatial point $\vec{x}$ living in d dimensions. The first and the second term in the exponential are quadratic and linear in the field, respectively. In analogy with the I_N case the result of the *path integral* is

$$I \propto e^{\frac{1}{2}\int d^dx d^dy \; \mu(\vec{x}) \, A^{-1}(\vec{x},\vec{y}) \, \mu(\vec{y})} \tag{1.A.12}$$

where we ignore the proportionality constant. Indeed, this one depends on the definition of the path-integral measure $\mathcal{D}\phi$. Usually, the actual value of this constant is not important since it does not depend on the relevant parameters of the theory. The inverse A^{-1} is defined by

$$\int d^dy \; A^{-1}(\vec{x},\vec{y})A(\vec{y},\vec{z}) = \delta(\vec{x} - \vec{z}) \; . \tag{1.A.13}$$

1.A.4 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 pdf is

$$p(x) = (2\pi\sigma^2)^{-1/2}\, e^{-(x-\mu)^2/(2\sigma^2)} \; . \qquad (1.A.14)$$

All moments $\langle\, x^k\,\rangle$ can be computed with (1.A.2). One finds

$$\langle\, e^{hx}\,\rangle = e^{\frac{h^2\sigma^2}{2}+h\mu} \qquad (1.A.15)$$

and then

$$\langle\, x^k\,\rangle = \frac{\partial^k}{\partial h^k}\, e^{\frac{h^2\sigma^2}{2}+\mu h}\Big|_{h=0} \qquad (1.A.16)$$

from where

$$\begin{array}{ll} \langle\, x\,\rangle = \mu \; , & \langle\, x^2\,\rangle = \sigma^2 + \mu^2 \; , \\ \langle\, x^3\,\rangle = 3\sigma^2\mu + \mu^3 \; , & \langle\, x^4\,\rangle = 3\sigma^4 + 6\sigma^2\mu^2 + \mu^4 \end{array}$$

etc. One recognizes the structure of Wick's theorem: given k factors x one organises them in pairs leaving the averages μ aside. The simplest way of seeing Wick's theorem in action is by drawing examples.

The generalization to N Gaussian variables is immediate. Equation (1.A.15) becomes

$$\langle\, e^{\vec h\vec x}\,\rangle = e^{\frac{1}{2}\vec h A^{-1}\vec h + \vec h\vec\mu} \qquad (1.A.17)$$

and the generalization of (1.A.16) leads to

$$\langle\, x_i\,\rangle = \mu_i \; , \qquad \langle\, x_i x_j\,\rangle = {A^{-1}}_{ij} + \mu_i\mu_j \; , \qquad (1.A.18)$$

etc. In other words, whereever there is σ^2 in the single variable case we replace it by ${A^{-1}}_{ij}$ with the corresponding indices.

The generalization 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 here

$$\langle\, \phi(\vec x)\,\rangle = \mu(\vec x) \; , \qquad \langle\, \phi(\vec x)\phi(\vec y)\,\rangle = A^{-1}(\vec x,\vec y) + \mu(\vec x)\mu(\vec y) \; , \qquad (1.A.19)$$

etc.

1.A.5 The Hubbard-Stratonovich or Gaussian decoupling

$$e^{bm^2} = \sqrt{\frac{b}{\pi}} \int_{-\infty}^{\infty} dx\; e^{-bx^2+2bmx} \qquad (1.A.20)$$

for all b and m.

1.A.6 Functional analysis

A functional $F[h]$ is a function of a 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 $\delta F \equiv F[h+\delta h] - F[h]$ and one tries to write this as $\delta F = \int d^dx\, \alpha(\vec{x})\delta h(\vec{x}) + \frac{1}{2}\int d^dx d^dy\, \beta(\vec{x},\vec{y})\, \delta h(\vec{x})\delta h(\vec{y}) + \dots$ and one defines the functional derivative of F with respect to h evaluated at the spatial points $\vec{z}$, in the limit $\delta h(\vec{x}) \to 0$ for all $\vec{x}$, as

$$\left.\frac{\delta F}{\delta h(\vec{z})}\right|_{\delta h(\vec{x})\to 0} = \alpha(\vec{z}) \ . \tag{1.A.21}$$

Similarly, for a second order variation evaluated at $\vec{u}$ and $\vec{v}$, for $\delta h(\vec{x}) \to 0$ for all $\vec{x}$,

$$\left.\frac{\delta^2 F}{\delta h(\vec{u})\delta h(\vec{v})}\right|_{\delta h(\vec{x})\to 0} = \beta(\vec{u},\vec{v}) \ . \tag{1.A.22}$$

All usual properties of partial derivatives apply.

1.A.7 Fourier transform

We define the Fourier transform (FT) of a function $f(\vec{x}$ defined in a volume V as

$$\tilde{f}(\vec{k}) = \int_V d^dx\, f(\vec{x})\, e^{-i\vec{k}\vec{x}} \tag{1.A.23}$$

This implies

$$f(\vec{x}) = \frac{1}{V}\sum_{\vec{k}} \tilde{f}(\vec{k})\, e^{i\vec{k}\vec{x}} \tag{1.A.24}$$

where the sum runs over all $\vec{k}$ with components k_i satisfying $k_i = 2m\pi/L$ with m an integer and L the linear size of the volume V.

In the large V limit these equations become

$$\tilde{f}(\vec{k}) \ = \ \int_V d^dx\, f(\vec{x})\, e^{-i\vec{k}\vec{x}} \tag{1.A.25}$$

$$\tilde{f}(\vec{x}) \ = \ \int_V \frac{d^dk}{(2\pi)^d}\, f(\vec{k})\, e^{i\vec{k}\vec{x}} \tag{1.A.26}$$

The Fourier transform of a real function $f(\vec{x})$ satisfies $\tilde{f}^*(\vec{k}) = \tilde{f}(-\vec{k})$.

1.A.8 Volume of a sphere in n dimensions

Take a sphere with radius R in an n dimensional space. The sphere has volume

$$V_n(R) = \pi^{n/2}/\Gamma(n/2+1)\, R^n \; . \tag{1.A.27}$$

1.A.9 The saddle-point method

Imagine one has to compute the following integral

$$I \equiv \int_a^b dx\; e^{-Nf(x)} \; , \tag{1.A.1}$$

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, one then Taylor expands $f(x)$ upto second order

$$f(x) \sim f(x_0) + \frac{1}{2} f''(x_0)(x-x_0)^2 \tag{1.A.2}$$

and obtains

$$I \sim e^{-Nf(x_0)} \int_a^b dx\; e^{-N\frac{1}{2}f''(x_0)(x-x_0)^2} = e^{-Nf(x_0)} [Nf''(x_0)]^{-1/2} \int_{y_a}^{y_b} dy\; e^{-\frac{1}{2}(y-y_0)^2} \; , \tag{1.A.3}$$

with $y_0 \equiv \sqrt{Nf''(x_0)}x_0$ and similarly for y_a and y_b. The Gaussian integral is just an error function that one can find in Tables.

This argument can be extended to multidimensional integrals, cases in which there is no absolute minimum within the integration interval, cases in which the function f is not positive definite, etc.

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