Statistical mechanics and stochastic processes

Master de Physique fondamentale et appliquée

Spécialité : Noyaux, particules, astrophysique, cosmologie

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Résumé

Ce cours présente une introduction aux applications de la mécanique statistique à la théorie de champs, la physique des particules et la cosmologie. Chaque Section est focalisée sur un sujet.

- Dans la première partie nous revisons les fondements de la mécanique statistique d'équilibre et nous discutons l'inéquivalence d'ensembles (microcanonique, canonique et macrocanonique) dans le problème du gaz autogravitant.
- Dans la deuxième partie nous étudions les transitions de phase et leurs réalisations en théorie de champs.
- La troisième partie est dédiée à l'étude statistiques de la distribution de masse (structures) en astrophysique.
- Dans la quatrième partie nous introduisons les processus stochastiques et nous décrivons brièvement la méthode Monte Carlo, utilisée dans l'étude numérique des théories de jauge sur réseau, ainsi que la quantification stochatique basée sur la dynamique de Langevin.
- Finalement, nous analysons la dynamique des transitions de phase du deuxième ordre et les processus de croissance des structures, un problème d'intérêt en cosmologie.

Les notes du cours seront disponibles, en formats postscript et pdf, dans la page web du Master ainsi que dans www.lpthe.jussieu.fr/~leticia/enseignement.html/

Le cours

Calendrier des cours

12 Octobre 9 :00 – 12 :00
20 Octobre 9 :00 – 12 :00
27 October 9 :00 – 12 :00
3 Novembre 9 :00 – 12 :00
10 Novembre 9 :00 – 12 :00
17 Novembre 9 :00 – 12 :00
1 Décembre 9 :00 – 12 :00

Exercises

À la fin des premiers quatre cours je rendrai une fiche d'exercises à résoudre à la maison et à rendre à la prochaine séance. Ces exercises feront partie de la note finale du cours (voir en bas de page).

Lecture d'un article scientifique

Pendant le cours les étudiants doivent lire et comprendre un article scientifique sur le sujet de leur choix. Ils doivent préparer un rapport écrit sur ce sujet selon les consignes données en bas. Ce rapport fera aussi partie de la note finale du cours (voir en bas de page). Ce travail pourra être fait en binôme ; dans ce cas le rapport à rendre sera un seul.

Examen

Il n'y aura pas d'examen final traditionnel.

Remise des rapports

Le 15 Décembre dernier délai.
Fichier pdf à envoyer par email à l'adresse
leticia@lpthe.jussieu.fr
préparé selon les sonsignes décrites en bas.

Note finale

60% TDs ; 40% Rapport.

Notes du cours

Ces notes couvrent un nombre de sujets qui seront presentés en cours ainsi que quelques approfondissement que nous n'aurons pas le temps de discuter en détails. Pour les distinguer on a marqué en rouge les titres des parties traitées en cours.

Table des matières

1 Basic notions

1.1 Background

Equilibrium Statistical Mechanics is a very well-established branch of theoretical physics. Together with Quantum Mechanics, they form the basis of Modern Physics.

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.

<table>
<tr><td></td><td colspan="2">Micro</td><td>Macro</td></tr>
<tr><td>dist (ℓ)</td><td>Solid
10^{-10}m</td><td>Gas
10^{-8}m</td><td>10^{-3}m</td></tr>
<tr><td># part (N)</td><td colspan="2">1</td><td>Solid
$\left(\frac{10^{-3}}{10^{-10}}\right)^{d=3} = 10^{21}$
Gas
$\left(\frac{10^{-3}}{10^{-8}}\right)^{d=3} = 10^{15}$</td></tr>
<tr><td>energy (E)</td><td colspan="2">$1\,eV$</td><td>$1J \approx 6\,10^{18} eV$</td></tr>
<tr><td>time (t)</td><td>Solid
$\hbar/1eV \approx 6\ 10^{-14}\,s$</td><td>Gas
$10^{-9}\,s$</td><td>$1\,s$</td></tr>
</table>

TAB. 1 – Typical length, energy and time scales in the microscopic 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.

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 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* 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.

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 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 is 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 : that of the *equilibration* of the macroscopic system. Some very interesting systems do not match this hypothesis. Still, one would like to use Probabilistic arguments to characterize their macroscopic behavior. This is possible in a number of cases and we shall discuss some of them. Indeed, deriving a theoretical framework to describe the behavior of *macroscopic systems out of equilibrium* is one the present major challenges in theoretical physics.

1.2 This course

In this set of lectures we shall discuss some problems in *equilibrium* and *dynamic* statistical mechanics that either are not fully understood or receive the attention of researchers at present due to their application to problems of interest in physics and other areas of science. We shall play special attention here to applications in particle physics and cosmology.

The plan of the set of lectures is the following :

In the first Section we recall some aspects of Probability Theory and Statistical Mechanics. Basic features of the foundations of Statistical Mechanics are recalled next together with the theory of ensembles (microcanonical, canonical and macrocanonical). As an interesting application, we discuss the *self-gravitating gas*, that is to say, a set of N classical particles confined in a volume V and interacting through Newton's law. Important differences in the thermodynamic behaviour of this system when treated in different ensembles are due to the long-range character of the forces. We discuss these features here.

In Sect. 2 we describe the theory of phase transitions : first we explain the mean-field approach, and then we introduce fluctuations and show how the importance of these led to the development of the renormalization group. We also introduce the standard models of magnetic systems (Ising, xy and Heisenberg), and we discuss their symmetry properties. We explain coarse-graining techniques and how these lead to field theories with different symmetry properties. We pay special attention to the discussion of *field theories at finite temperature* and how phase transitions occur in this context.

In Sect. 3 we use statistical methods to characterize mass distributions and, in particular, *astrophysical structures*.

In the last two Sections we introduce *time* into the discussion. First, in Sect. 4 we define stochastic processes, the Langevin and Fokker-Planck formalisms and we briefly discuss the dynamics of macroscopic systems close to thermal equilibrium. We explain here *Montecarlo techniques* used for instance in the lattice gauge theory for QCD and the method of *stochastic quantization*.

In Sect. 5 we treat the dynamics of phase transitions, discussing separately the case of first and second order ones. We explain how this process has important implications in cosmology with the problem of determining the number of *topological defects* left after going through a phase transition.

It is clear that the correct explanation of all these problems and analytical methods would require many more teaching hours than the ones we have. We shall only give here the main ingredients of each of these subjects and provide the interested students with references to deepen their knowledge.

1.3 Elements in statistical mechanics

Let us here recall some important features of Statistical Mechanics [3, 4, 5, 6, 7].

The state of a classical system with $i = 1, \ldots, N$ particles moving in d-dimensional *real space* is fully characterized 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 $a = 1, \ldots, d$ 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.* $\vec{Y} = (\vec{Q}, \vec{P}) = (q_1^1, q_1^2, q_1^3, q_2^1, q_2^2, q_2^3, \ldots, q_N^1, q_N^2, q_N^3, p_1^1, p_1^2, p_1^3, p_2^1, p_2^2, p_2^3, \ldots, p_N^1, p_N^2, p_N^3)$ in $d = 3$.

The Hamiltonian of the system, H, is a function of the particles' position and momenta. 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. Energy, E, 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 – uncertainty in the initial conditions, deterministic chaos, *etc.* A probabilistic element enters into play. What one really does is estimate the *probability* that the representative point of the system is 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.

Note that if initially one knows the state of the system with great precision, the initial ρ will be concentrated in some region of phase space. At later times, ρ can still be localized – perhaps in a different region of phase – or it can spread. This depends on the system and the dynamics (Newton-Hamilton or else).

We now need to find an equation for the evolution of the probability density ρ knowing the evolution of the phase space coordinates $(\vec{Q},\vec{P})$. ρ can vary in time due to two mechanisms : an explicit time variation, and the time variation of the coordinates and momenta as the representative point wanders in phase space :

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + \frac{\partial\rho}{\partial q_i^a}\dot{q}_i^a + \frac{\partial\rho}{\partial p_i^a}\dot{p}_i^a \ , \tag{1.1}$$

with $\dot{q}_i^a = dq_i^a/dt$ and $\dot{p}_i^a = dp_i^a/dt$, the summation convention over repeated indices (i labels particles and a labels coordinates), and $\rho(\vec{Q},\vec{P},0)$ known.

Probability behaves like an incompressible fluid in phase space and one can then use knowledge of fluid mechanics to analyze the equation above. The partial derivative is taken at fixed $(\vec{Q},\vec{P})$: it represents the time-variation of ρ as the fluid passes by the chosen point in phase space. The total derivative instead is the time-variation as we follow the displacement of a 'piece' of fluid in phase space.

Liouville's theorem states that the ensemble of systems (as represented by a point in phase space) in the vicinity of a given system remains constant in time :

$$\frac{d\rho}{dt} = 0 \ . \tag{1.2}$$

A detailed description of Liouville's theorem is given in [8]. We shall not repeat it here but taken for granted.

In statistical equilibrium one expects the systems to reach stationarity and then the explicit time-variation to vanish

$$\frac{\partial\rho}{\partial t} = 0 \ . \tag{1.3}$$

In this case, the distribution ρ is constant on the phase trajectories. One may wonder whether this solution is reached from generic initial conditions.

Liouville's equation (1.2) is invariant under time-reversal, $t \to -t$ and $\vec{p} \to -\vec{p}$. Indeed, the existence of a conserved current implies, via *Noether's theorem*, the existence of a symmetry. The symmetry is invariance under time translations, and the generator of the symmetry (or Noether charge) is the Hamiltonian.

The time-reversal symmetry implies that, for generic initial conditions the solutions to Liouville's equation oscillate in time and do not approach a single asymptotic stationary solution that could be identified with equilibrium ($\partial_t \rho = 0$). The problem of how to obtain irreversible decay from Liouville's equation is a fundamental one in Statistical Mechanics. We shall come back to this problem in Sect. 2.10.5. 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 looks for solutions that *are stationary* without worrying about how the ensemble reaches them. This can be restated as the following hypothesis :

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

Setting now $\partial_t \rho = 0$ one realizes that the remaining equation admits, as a solution, any function of the energy. The characteristics of the ensemble are then determined by the chosen function $\rho(E)$.

1.4 The ergodic hypothesis

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

$$\overline{A} \equiv \lim_{\tau \to \infty} \frac{1}{2\tau} \int_{-\tau}^{\tau} dt \; A(\vec{Q}(t), \vec{P}(t)) \; . \tag{1.4}$$

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,

$$\langle \, A \, \rangle = c \int \prod_{i=1}^{N} \prod_{a=1}^{d} dq_i^a dp_i^a \; \rho(\vec{Q}, \vec{P}) A(\vec{Q}, \vec{P}) \; , \tag{1.5}$$

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 (1.8) :

$$\langle \, A \, \rangle = c \int \prod_{i=1}^{N} \prod_{a=1}^{d} dq_i^a dp_i^a \; \delta(H(\vec{Q}, \vec{P}) - E) A(\vec{Q}, \vec{P}) \; , \tag{1.6}$$

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

$$\langle \, A \, \rangle = Z^{-1} \int \prod_{i=1}^{N} \prod_{a=1}^{d} dq_i^a dp_i^a \; e^{-\beta H(\vec{Q}, \vec{P})} A(\vec{Q}, \vec{P}) \; . \tag{1.7}$$

Z is the partition function $Z = \int \prod_{i=1}^{N} \prod_{a=1}^{d} dq_i^a dp_i^a \; e^{-\beta H(\vec{Q},\vec{P})}$.

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.

The *ergodic hypothesis* states that time and ensemble averages, (1.4) and (1.5) coincide in equilibrium for all reasonable observables. 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 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 is slow one can hope to derive an extension of equilibrium statistical mechanics concepts to describe their behavior.

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

1.4.1 The microcanonical ensemble

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

– In the same 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 :

$$\rho(\vec{Q},\vec{P}) \;=\; \begin{cases} \rho_0 & \text{if } H(\vec{Q},\vec{P}) \in (E, E+dE) \;, \\ 0 & \text{otherwise} \;, \end{cases} \tag{1.8}$$

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 eq. (1.2).

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

$$\begin{aligned} \langle A \rangle &= \int \prod_{i=1}^{N}\prod_{a=1}^{d} dq_i^a dp_i^a \; \rho(\vec{Q},\vec{P}) A(\vec{Q},\vec{P}) \\ &= \left(\frac{1}{N!g(E)}\right) \int \prod_{i=1}^{N}\prod_{a=1}^{d} dq_i^a dp_i^a \; \delta[E - H(\vec{Q},\vec{P})]\, A(\vec{Q},\vec{P}) \; . \end{aligned} \tag{1.9}$$

The normalization constant $c = \int \prod_{i=1}^{N}\prod_{a=1}^{d} dq_i^a dp_i^a \;\; \delta[E - H(\vec{Q},\vec{P})] = N!g(E)$ is the volume of phase space occupied by the constant energy surface itself. The quantity $g(E)$ is called the *density of states* :

$$g(E) \equiv \frac{1}{N!} \int \prod_{i=1}^{N}\prod_{a=1}^{d} \delta[E - H(\vec{Q},\vec{P})] \; . \tag{1.10}$$

The *microcanonical entropy* is

$$S(E) \equiv k_B \ln g(E) \; . \tag{1.11}$$

Maximization of entropy is thus equivalent to the maximization of the phase volume available to the system.

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.

1.4.2 The canonical ensemble – 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.

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 characterize the statistical properties of the small 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* 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 its volume, $E_1 \propto V_1$ 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 *additivity property*,

$$E = E_1 + E_2 \ , \tag{1.12}$$

for any two subsystems 1 and 2 of a macroscopic system. One defines systems with *short* range interactions as those for which the additivity property applies and systems with *long* range interactions as those for which this property fails.

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

$$\begin{aligned} P(E_1)dE_1 &\propto \int dE_2 g(E_1, E_2)\delta(E - E_1 - E_2)dE_1 \\ &= \int dE_2 g_1(E_1)g_2(E_2)\delta(E - E_1 - E_2)dE_1 \\ &= g_1(E_1)g_2(E - E_1)dE_1 \\ &= g_1(E_1)e^{k_B^{-1}S_2(E-E_1)}dE_1 \\ &\simeq g_1(E_1)e^{k_B^{-1}S_2(E)+k_B^{-1}\partial_E S_2(E)(-E_1)}dE_1 \\ &\propto g(E_1)e^{-\beta E_1}dE_1 \ , \end{aligned} \tag{1.13}$$

and, after fixing the normalization :

$$P(E_1) = Z^{-1}(\beta)\ g(E_1)e^{-\beta E_1} \ , \qquad \text{with} \qquad Z(\beta) = \int dE_1\ g(E_1)e^{-\beta E_1} \ . \tag{1.14}$$

Let us recap the assumptions made : (i) independence, $g(E_1, E_2) = g(E_1)g(E_2)$, (ii) energy additivity $E_2 = E - E_1$, (iii) small system 1 ($E_1 \ll E$), (iv) constant inverse 'temperature' $k_B\beta \equiv \partial_E S(E)$. 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 is not even defined !

Example : the power-law potential

In the field of particle systems with two-body interactions falling-off with distance as a power law

$$V(r) \sim r^{-\alpha} \tag{1.15}$$

one finds that the interactions are
- long-ranged if $\alpha < d$,
- short-ranged 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 and density ρ. The total energy, e, felt by the particle is

$$e = -\int_V d^d x \, \frac{\rho}{r^\alpha} = -\Omega_d \int_\epsilon^R dr \, \frac{r^{d-1}\rho}{r^\alpha} = -\frac{\Omega_d \, \rho}{d-\alpha}\left[R^{d-\alpha} - \epsilon^{d-\alpha}\right] , \tag{1.16}$$

where we adopted the potential $V(r) = r^{-\alpha}$ for all r. Ω_d is the angular volume, $\Omega_d = 2\pi$ in $d = 2$, $\Omega_d = 4\pi$ in $d = 3$, etc. One finds that for $\alpha > d$ the contribution from the surface ($r = R$) is negligible while for $\alpha < d$ it diverges ! In the latter case surface effects cannot be neglected and the energy is not additive.

Another way to express the same wierd fact is that the total energy on a volume $V \propto R^d$, that is to say $E = Ve$, is super-linear on the volume :

$$E \simeq V R^{d-\alpha} \simeq R^{2d-\alpha} = R^{d(2-\alpha/d)} = V^{1+1-\alpha/d} \tag{1.17}$$

for $1 - \alpha/d > 0$.

This definition implies then that the **gravitational interaction**, $V_G(r) = -Gm^2 r^{-1}$ is long-ranged in three spatial dimensions while the Van der Waals interaction, $V_{VW}(r) \propto r^{-6}$, is short-ranged. The long-ranged interactions are sometimes called *non-integrable* in the literature. **Plasma physics** also provides examples of non-additive systems through an effective description.

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 statistical physics of **self-gravitating systems** falls into this class of *bizarre* problems and there is much current research [9, 10, 11] to try to elucidate their properties. We shall discuss some of the many interesting features of this system.

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.

1.4.3 Negative specific heat and phase transitions

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

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

where $S(E) \equiv k_B \ln g(E)$ is the entropy defined from the density of states $g(E)$, see eq. (1.11).

The Taylor expansion of $\ln P(E)$ around $E = U$ yields

$$\ln P(E) \sim -\beta[U - TS(U)] + \frac{1}{2} \left. \frac{\partial^2 \ln P(E)}{\partial E^2} \right|_{E=U} (E-U)^2 + \dots \tag{1.19}$$

$$\sim -\beta[U - TS(U)] - \frac{1}{2}\beta^2 \frac{1}{C_V^{can}} (E-U)^2 + \dots \tag{1.20}$$

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

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

to replace the coefficient of the quadratic term after defining the canonical specific heat :

$$C_V^{can} \equiv -\beta^2 \frac{\partial U(\beta)}{\partial \beta} \, . \tag{1.22}$$

$P(E)$ is a Gaussian centered at U (thus $U = \langle E \rangle$) with dispersion $\sigma = \beta^{-1} C_V^{can\,1/2}$. In a macroscopic system with N particles and *short-range interactions* one expects $E \propto N$ and $C_V^{can} \propto N$ in which case the ratio between dispersion and typical energy, or relative fluctuation, vanishes as $\sigma/E \propto N^{-1/2}$. 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). One thus proves the equivalence between the microcanonical and canonical results.

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 region of parameters 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

$$C_V^{micro} \equiv -\beta^2 \frac{\partial E(\beta)}{\partial \beta} \tag{1.23}$$

[one inverts $\beta(E) = k_B^{-1} \partial_E S(E)$ to write $E(\beta)$] and this quantity is not positive definite. Instead, in the canonical ensemble the constant volume specific heat

$$\begin{aligned} C_V^{can} &= -\beta^2 \frac{\partial U(\beta)}{\partial \beta} = -\beta^2 \frac{\partial \langle E \rangle(\beta)}{\partial \beta} = \beta^2 \frac{\partial \ln Z(\beta)}{\partial \beta} \\ &= \beta^2 \left(\langle E^2 \rangle - \langle E \rangle^2 \right) = \beta^2 \langle (E - \langle E \rangle)^2 \rangle \end{aligned} \tag{1.24}$$

is positive definite. 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 parameters. It turns out that when $C_V^{micro} < 0$ the system undergoes a phase transition in the canonical ensemble (see Sect. 2).

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 :

$$H(\mathbf{P}, \mathbf{Q}, \mathbf{p}, \mathbf{r}) = \frac{P^2}{2M} + \frac{p^2}{2\mu} - \frac{Gm^2}{r} \tag{1.25}$$

where $\mathbf{P}$ and $\mathbf{Q}$ are the momentum and coordinate of the center of mass and $\mathbf{p}$ and $\mathbf{q}$ 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. 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 [9]. 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 heat capacity is positive. As one lowers the energy the effects of gravity begin to be felt. For $E_1 < E < E_2$ the box or the short-distance cut-off do not 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 specific heat. The microcanonical specific heat is shown in Fig. 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 analyze 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. The canonical result is also shown in Fig. 1. 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 (the theory of phase transitions will be discussed in detail in Sect.) 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

$$H = \frac{p^2}{2m} + \sum_{i=1}^{N} \frac{1}{2mr^2} \left(p_{\theta_i}^2 + \frac{p_{\phi_i}^2}{\sin^2 \theta_i} \right) - \frac{Gm^2}{2r} \tag{1.26}$$

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 regularize the $r \to 0$ behaviour of the total interaction potential.
It turns out that an interesting thermodynamic limit of the three ensembles (microcanonical, canonical and macrocanonical) is achieved in the very dilute limit [10, 11]

$$\eta \equiv \frac{Gm^2 N}{V^{1/3} T} \qquad \text{finite} . \tag{1.27}$$

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.

1.4.4 The macrocanonical ensemble

Finally in the macrocanonical ensemble one characterizes 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 $T^{-1} \equiv \frac{\partial S}{\partial E}|_E$. 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.

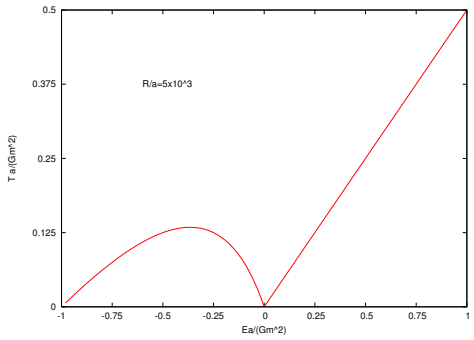

FIG. 1 – The temperature against the energy for the two-body problem with gravitational interaction with cut-off a in a box of size R. The microcanonical curve is non-monotonic with a negative specific heat in the region $E \sim [-0.4, 0]$. The canonical curve is monotonic and almost flat – as in a smoothened phase transition – in the region in which $C_V^{micro} < 0$.

2 Phase transitions

Take a piece of material in contact with an external reservoir. The material will be characterized by certain observables, energy, magnetization, *etc.*. To characterize macroscopic systems it is convenient to consider densities of energy, magnetization, *etc*, by diving the macroscopic value by the number of particles (or the volume) of the system. The external environment will be characterized by some parameters, like the temperature, magnetic field, pressure, *etc.* In principle, one is able to tune the latter and the former will be a function of them.

Sharp changes in the behavior of macroscopic systems at critical points (lines) in parameter space have been observed experimentally. These correspond to phase transitions, a non-trivial collective phenomenon appearing in the thermodynamic limit. In this Section we shall review the main features of, and analytic approaches used to study, phase transitions.

We shall first use the language of magnetic systems, using the Ising model and its variants as the working model. We shall then introduce field theories and briefly discuss phase transitions in this context.

2.1 Standard models

2.1.1 Magnetic systems : the Ising model

Let us analyze, once again, a magnetic system. The Hamiltonian describing all microscopic details is a rather complicated one, depending on the electrons magnetic moments

giving rise the macroscopic magnetization of the sample but also on the vibrations of the atomic crystal, the presence of structural defects, *etc.* If we call α a *microstate*, its probability is $P_\alpha = e^{-\beta H_\alpha}/Z$ with Z the partition function, $Z = \sum_\alpha e^{-\beta H_\alpha}$. It is, however, impossible and not necessarily interesting to keep all details and work with all possible physical phenomena simultaneously. Imagine that we are only interested on the magnetic properties, characterized by the electronic magnetic moments.

The Ising model is a mathematical representation of a magnetic system. It describes magnetic moments as classical *spins*, s_i, taking values ± 1, lying on the vertices of a cubic lattice in d dimensional space, and interacting via nearest-neighbor couplings, $J > 0$. The energy is then

$$H = -\frac{J}{2} \sum_{\langle ij \rangle} s_i s_j - \sum_i h_i s_i \tag{2.1}$$

where h_i is a local external magnetic field. Most typically one works with a uniform field, $h_i = h$ for all sites. The justification for working with an Ising variable taking only two values is that in many magnetic systems the magnetic moment is forced to point along an 'easy axis' selected by crystalline fields.

There are two external parameters in H, the coupling strength J and the external field h. $J > 0$ favors the alignement of the spin in the same direction (ferromagnetism) while $J < 0$ favors the anti-alignement of the spins (antiferromagnetism). The magnetic field tends to align the spins in its direction.

The Ising model is specially attractive for a number of reasons :
(i) It is probably the simplest example of modeling to which a student is confronted.
(ii) It can be solved in some cases : $d = 1$, $d = 2$, $d \to \infty$. The solutions have been the source of new and powerful techniques later applied to a variety of different problems in physics and interdisciplinary fields.
(iii) It has not been solved analytically in the most natural case, $d = 3$!
(iv) It has a phase transition, an interesting collective phenomenon, separating two phases that are well-understood and behave, at least qualitatively, as real magnets with a paramagnetic and a ferromagnetic phase.
(v) There is an upper, d_u, and lower, d_l, critical dimension. Above d_u mean-field theory correctly describes the critical phenomenon. At and below d_l there is no finite T phase transition. Below d_u mean-field theory fails.
(vi) One can see at work generic tools to describe the critical phenomenon like *scaling.* and the *renormalization group.*
(vii) Generalizations in which the interactions and/or the fields are random variables taken from a probability distribution are typical examples of problems with *quenched disorder.*
(viii) Generalizations in which spins are not just Ising variables but vectors with n components with a local constraint on their modulus are also interesting. Their energy is

$$E = -\frac{J}{2} \sum_{\langle ij \rangle} \vec{s}_i \vec{s}_j - \sum_i \vec{h}_i \vec{s}_i \tag{2.2}$$

with $n = 1$ (Ising), $n = 2$ (XY), $n = 3$ (Heisenberg), ... , $n \to \infty$ ($O(n)$) as particular cases. The *local constraint* on the length of the spin is

$$s_i^2 \equiv \sum_{a=1}^{n} (s_i^a)^2 = n \ . \tag{2.3}$$

Note that each component is now a continuous variable bounded in a finite interval, $-\sqrt{n} \leq s_i^a \leq \sqrt{n}$, that actually diverges in the $n \to \infty$ limit. When $n \to \infty$ it is sometimes necessary to redefine the coupling constants including factors of n that yield a sensible $n \to \infty$ limit of thermodynamic quantities.
(ix) One can add a dynamic rule to update the spins and we are confronted to the new World of stochastic processes (Sect. 2.10.5).
(x) Domain growth in these systems is the simplest example of coarsening (Sect. 5).
(xi) Last but not least, it has been a paradigmatic model extended to describe many problems going beyond physics like neural networks, social ensembles, *etc.*

The spins lie on a d dimensional lattice that can have different geometries. For instance, a cubic lattice is such that each vertex has *coordination number*, or number of neighbours, $z = 2d$. Triangular, honeycomb, *etc.* lattices are also familiar.

In the rest of this set of Lectures we shall discuss the physics of this model and we shall study its statics and dynamics with a number of analytic techniques.

2.1.2 Symmetries

Continuous

In the absence of an applied magnetic field the Hamiltonian (2.2) remains invariant under the simultaneous rotation of all spins :

$$\begin{aligned} H[\vec{s}'] &= -\frac{J}{2} \sum_{\langle ij \rangle} \vec{s}_i' \vec{s}_j' = -\frac{J}{2} \sum_{\langle ij \rangle} R^{ab} s_i^b R^{ac} s_j^c \\ &= -\frac{J}{2} \sum_{\langle ij \rangle} R^{tba} R^{ac} s_i^b s_j^c = -\frac{J}{2} \sum_{\langle ij \rangle} s_i^b s_j^b \end{aligned} \tag{2.4}$$

since R is an orthogonal transformation, such that $R^t R = I$. This symmetry is explicitly broken by the external field.
Discrete

The Ising model with no applied field is invariant under $s_i \to -s_i$, a discrete symmetry.

2.1.3 Field theories

A field theory for the magnetic problem can be rather simply derived by coarse-graining the spins over a coarse-graining length ℓ. This simply amounts to computing the averaged

spin on a box of linear size ℓ. In the limit $\ell \gg a$ where a is the lattice spacing many spins contribute to the sum. For instance, an Ising bimodal variable is thus transformed into a continuous real variable taking values in $[-1, 1]$. Studying the problem at long distances with respect to ℓ (or else taking a continuum spatial limit) the problem transforms into a *field theory*. This is the route followed by Landau that we shall discuss later.

Field theories are the natural tool to describe particle physics and cosmology. Indeed, the **Big Bang** leaves a radiation-dominated universe at very high temperature close to the Planck scale. As the initial fireball expands, temperature falls precipitating a sequence of phase transitions. The exact number and nature of these transitions is not known. It is often considered that they are at the origin of the structures (galaxies, clusters, *etc.*) seen in the universe at present, the original seeds being due to density fluctuations left behind after the phase transition. We shall come back to this problem in Sects. 2.10.5 and 4.3.3.

The similarity between the treatment of condensed matter problems and high energy physics becomes apparent once both are expressed in terms of field theories. It is however often simpler to understand important concepts like spontaneous symmetry breaking in the language of statistical mechanics problems.

2.2 Discussion

Let us discuss some important concepts, order parameters, pinning fields, broken ergodicity and broken symmetry, with the help of a concrete example, the Ising model (2.1). The discussion is however much more general and introduces the concepts mentioned above.

2.2.1 Order parameters

An order parameter is generically defined as a quantity – the average of an observable – that vanishes in one phase and is different from zero in another one (or other ones). One must notice though that the order parameter is not unique (any power of an order parameter is itself an order parameter) and that there can exist transition without an order parameter as the Kosterlitz-Thouless one in the $2d$ xy model. In the rest of this course we focus on problem that do have an order parameter defined as the thermal average of some observable.

2.2.2 Thermodynamic limit

The abrupt change in the order parameter at a particular value of the external parameters (T, h) is associated to the divergence of some derivative of the free-energy with respect to one of these parameters. The partition function is a sum of positive terms. In a system with a finite number of degrees of freedom (as, for instance, in an Ising spin model where the sum has 2^N terms with N the number of spins) such a sum is an analytic function of the parameters. Thus, no derivative can diverge. One can then have a phase transition only in the *thermodynamic limit* in which the number of degrees of freedom

diverges.

2.2.3 Pinning field

In the absence of a magnetic field for pair interactions the energy is an even function of the spins, $E(\vec{s}) = E(-\vec{s})$ and, consequently, the equilibrium magnetization density computed as an average over *all* spin configurations with their canonical weight, $e^{-\beta H}$, vanishes at all temperatures.

At high temperatures, $m = 0$ characterizes completely the equilibrium properties of the system since there is a unique paramagnetic state with vanishing magnetization density. At low temperatures instead if we perform an experiment we *do observe* a net magnetization density. In practice, what happens is that when the experimenter takes the system through the transition one cannot avoid the application of tiny external fields – the experimental set-up, the Earth... – and there is always a small *pinning field* that actually selects one of the two possible equilibrium states, with positive of negative magnetization density, allowed by symmetry. In the course of time, the experimentalist should see the full magnetization density reverse, however, this is not see in practice since astronomical time-scales would be needed. We shall see this phenomenon at work when solving mean-field models exactly below.

2.2.4 Broken ergodicity

Introducing dynamics into the problem [1], ergodicity breaking can be stated as the fact that the temporal average over a long (but finite) time window is different from the statical one, with the sum running over all configurations with their associated Gibbs-Boltzmann weight :

$$\overline{A} \neq \langle A \rangle \, . \tag{2.5}$$

In practice the temporal average is done in a long but finite interval $\tau < \infty$. During this time, the system is positively or negatively magnetized depending on whether it is in "one or the other degenerate equilibrium states". Thus, the temporal average of the orientation of the spins, for instance, yields a non-vanishing result $\overline{A} = m \neq 0$. If, instead, one computes the statistical average summing over *all* configurations of the spins, the result is zero, as one can see using just symmetry arguments. The reason for the discrepancy is that with the time average we are actually summing over half of the available configurations of the system. If time τ is not as large as a function of N, the trajectory does not have enough time to visit all configurations in phase space. One can reconcile the two results by, in the statistical average, summing only over the configurations with positive (or negative) magnetization density. We shall see this at work in a concrete calculation below.

2.2.5 Spontaneous broken symmetry

[1] Note that Ising model does not have a natural dynamics associated to it. We shall see in Section 2.10.5 how a dynamic rule is attributed to the evolution of the spins.

In the absence of an external field the Hamiltonian is symmetric with respect to the simultaneous reversal of all spins, $s_i \to -s_i$ for all i. The phase transition corresponds to a *spontaneous symmetry breaking* between the states of positive and negative magnetization. One can determine the one that is chosen when going through T_c either by applying a small *pinning field* that is taken to zero only after the thermodynamic limit, or by imposing adequate boundary conditions like, for instance, all spins pointing up on the borders of the sample. Once a system sets into one of the equilibrium states this is completely stable in the $N \to \infty$ limit. The mathematical statement of spontaneous symmetry breaking is then

$$\lim_{h\to 0^+} \langle\, s_i \,\rangle = - \lim_{h\to 0^-} \langle\, s_i \,\rangle \neq 0 \,. \tag{2.6}$$

Ergodicity breaking necessarily accompanies spontaneous symmetry breaking but the reverse is not true ; an example is provided by systems with quenched disorder that we shall not discuss in these Lectures notes (see, *e.g.* [16]) Indeed, spontaneous symmetry breaking generates disjoint ergodic regions in phase space, related by the broken symmetry, but one cannot prove that these are the only ergodic components in total generality. Mean-field spin-glass models provide a counterexample of this implication.

2.3 Energy *vs* entropy

Let us first use a thermodynamic argument to describe the high and low temperature phases of a magnetic system.

The free energy of a system is given by $F = U - TS$ where U is the internal energy, $U = \langle H \rangle$, and S is the entropy. Here and in the following we measure temperature in units of k_B and then set $k_B = 1$. The equilibrium state may depend on temperature and it is such that it minimizes its free-energy F. A competition between the energetic contribution and the entropic one may then lead to a change in phase at a definite temperature, *i.e.* a different group of microconfigurations, constituting a state, with different macroscopic properties dominate the thermodynamics at one side and another of the transition.

At zero temperature the free-energy is identical to the internal energy U. In a system with ferromagnetic couplings between magnetic moments, the magnetic interaction is such that the energy is minimized when neighboring moments are parallel. Thus the preferred configuration is such that all moments are parallel and the system is fully ordered.

Switching on temperature thermal agitation provokes the reorientation of the moments and, consequently, misalignments. Let us then investigate the opposite, infinite temperature case, in which the entropic term dominates and the chosen configurations are such that entropy is maximized. This is achieved by the magnetic moments pointing in random independent directions. For example, for a model with N Ising spins, the entropy at infinite temperature is $S \sim N \ln 2$.

Decreasing temperature disorder becomes less favorable. The existence or not of a finite temperature phase transitions depends on whether long-range order, as the one observed in the low-temperature phase, can remain stable with respect to fluctuations, or

the reversal of some moments, induced by temperature. Up to this point, the discussion has been general and independent of the dimension d.

The competition argument made more precise allows one to conclude that there is no finite temperature phase transition in $d = 1$ while it suggests there is one in $d > 1$. Take a one dimensional ferromagnetic Ising model with closed boundary conditions (the case of open boundary conditions can be treated in a similar way), $H = -J \sum_{i=1}^{N} s_i s_{i+1}$, $s_{N+1} = s_1$. At zero temperature it is ordered and its internal energy is just

$$U_o = -JN \tag{2.7}$$

with N the number of links and spins. Since there are two degenerate ordered configurations the entropy is

$$S_o = \ln 2 \tag{2.8}$$

The internal energy is extensive while the entropy is just a finite number. At temperature T the free-energy of the completely ordered state is then

$$F_o = U_o - TS_o = -JN - T \ln 2 \, . \tag{2.9}$$

Adding a *domain* of the opposite order in the system, *i.e.* reversing n spins, two bonds are unsatisfied and the internal energy becomes

$$U_2 = -J(N-2) + 2J = -J(N-4) \, , \tag{2.10}$$

for all n. Since one can place the misaligned spins anywhere in the lattice, there are N equivalent configurations with this internal energy. The entropy of this state is then

$$S_2 = \ln(2N) \, . \tag{2.11}$$

The factor of 2 inside the logarithm arises due to the fact that we consider a reversed domain in each one of the two ordered states. At temperature T the free-energy of a state with one reversed spin and two *domain walls* is

$$F_2 = U_2 - TS_2 = -J(N-4) - T \ln(2N) \, . \tag{2.12}$$

The variation in free-energy between the ordered state and the one with one domain is

$$\Delta F = F_2 - F_o = 4J - T \ln N \, . \tag{2.13}$$

Thus, even if the internal energy increases due to the presence of the domain wall, the increase in entropy is such that the free-energy of the state with a droplet in it is much more favorable at any finite temperature T. We conclude that spin flips are favorable and order is destroyed at any finite temperature. The ferromagnetic Ising chain does not have a finite temperature phase transition.

A similar argument in $d > 1$ suggests that one can have, as indeed happens, a finite temperature transition in these cases (see, *e.g.* [16]).

2.4 Droplets and domain-wall stiffness

It is clear the structure of *droplets*, meaning patches in which the spins point in the direction of the opposite state, plays an important role in the thermodynamic behaviour of systems undergoing a phase transition. At criticality one observes ordered domains of the two equilibrium states at all length scales – with *fractal* properties. Right above T_c finite patches of the system are indeed ordered but these do not include a finite fraction of the spins in the sample and the magnetization density vanishes. However, these patches are enough to generate non-trivial thermodynamic properties very close to T_c and the richness of the critical phenomena. M. Fisher and others developed a droplet phenomenological theory for critical phenomena in clean systems. Later D. S. Fisher and D. Huse extended these arguments to describe the effects of quenched disorder in spin-glasses and other random systems ; this is the so-called *droplet model*.

Let us study the stability properties of an equilibrium phase under an applied external field that tends to destabilize it. In the ferromagnetic case the free-energy density cost of a spherical droplet of radius R of the equilibrium phase parallel to the applied field embedded in the dominant one (see Fig. 2-left) is

$$f(R) = 2\Omega_d R^d h m_{eq} + \Omega_{d-1} R^{d-1} \sigma_0 \tag{2.14}$$

where σ_0 is the inter-facial free-energy density and Ω_d is the volume of a d-dimensional unit sphere. We assume here that the droplet has a regular surface and volume such that they are proportional to R^{d-1} and R^d, respectively. If the magnetic field is negative, $h < 0$, the excess free-energy reaches a maximum

$$f_c = \Omega_d \sigma_0^d \left(\frac{d-1}{2|h| m_{eq}} \right)^{d-1} \tag{2.15}$$

at the critical radius

$$R_c = \frac{(d-1)\sigma_0}{2|h| m_{eq}} \, , \tag{2.16}$$

see Fig. 2. This means that as long as the critical size is not reached the droplet is not favorable and the system remains positively magnetized.

The study of droplet fluctuations is useful to establish whether an ordered phase can exist at low (but finite) temperatures. One then studies the free-energy cost for creating large droplets with thermal fluctuations that may destabilize the ordered phase, in the way we have done with the simple Ising chain. Indeed, a fundamental difference between an ordered and a disordered phase is their stiffness (or rigidity). In an ordered phase the free-energy cost for changing one part of the system with respect to the other part far away is of the order $k_B T$ and usually diverges as a power law of the system size. In a disordered phase the information about the reversed part propagates only a finite distance (of the order of the correlation length, see below) and the stiffness vanishes.

The calculation of the stiffness is usually done as follows. Anti-parallel configurations (or more generally the two ground states) are imposed at the opposite boundaries of the

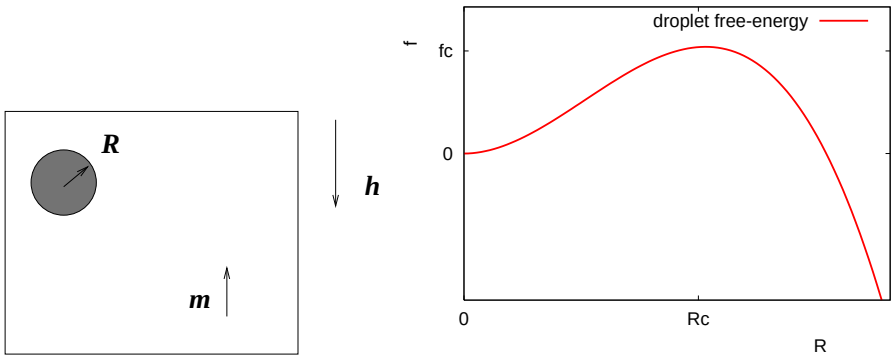

FIG. 2 – Left : the droplet. Right : the free-energy density $f(R)$ of a spherical droplet with radio-us R.

sample. A domain wall is then generated somewhere in the bulk. Its free-energy cost, *i.e.* the difference between the free-energies of the modified configuration and the equilibrium one, is then measured and one tests when creating a wall is favorable.

Note that these arguments are easy to implement when one knows the equilibrium states.

2.5 Classification

Phase transitions are commonly classified by their *order*. In Ehrenfest's classification a phase transition is of nth order if $\partial^n F/\partial y^n$ is the lowest discontinuous derivative where y is any argument of f. The more common transitions are those of first and second order.

In first order phase transition the order parameter jumps at the critical point from a vanishing value in the disordered side to a finite value right on the ordered side of the critical point. This is accompanied by discontinuities in various thermodynamic quantities and it is related to the fact that a first derivative of the free-energy density diverges. In such a transition the high and low temperature phases coexist at the critical point. Well-known examples are the melting of three dimensional solids and the condensation of a gas into a liquid. These transitions often exhibit hysteresis or memory effects since the system can remain in the metastable phase when the external parameters go beyond the critical point.

In second order phase transition the order parameter is continuous at the transition, *i.e.* it smoothly departs from zero at the critical point, but its variation with respect to the conjugate field in the zero field limit, or linear susceptibility, diverges. This is a second derivative of the free-energy density. At the critical point there is no phase coexistence, the system is in one critical state ; the two phases on either side of the transition become identical at the critical point.

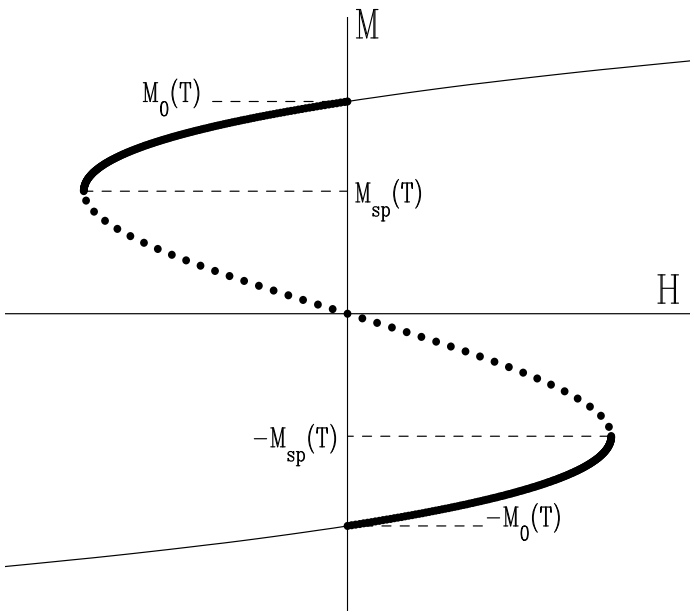

FIG. 3 – The magnetization against the applied field in a ferromagnet.

In disordered systems (problems with the interactions, J_{ij}'s, or other parameters taken from a probability distribution) a mixed case occurs in which the order parameter is discontinuous at the transition but all first derivatives of the free-energy density are finite. This is called a *random first order* transition and it provides a scenario for the glassy arrest [40].

2.6 Mean-field theory (Ising class)

In spite of their apparent simplicity, the statics of ferromagnetic Ising models has been solved analytically only in one and two dimensions. The mean-field approximation allows one to solve the Ising model in *any* spatial dimensionality. Even if the qualitative results obtained are correct, the quantitative comparison to experimental and numerical data shows that the approximation fails below an *upper critical dimension* d_u. It is however very instructive to see the mean-field approximation at work.

2.6.1 The naive mean-field approximation

The naive mean-field approximation consists in assuming that the probability density of the system's spin configuration is factorizable in independent factors

$$P(\{s_i\}) = \prod_{i=1}^{N} P_i(s_i) \qquad \text{with} \qquad P_i(s_i) = \frac{1+m_i}{2}\delta_{s_i,1} + \frac{1-m_i}{2}\delta_{s_i,-1} \tag{2.17}$$

and $m_i = \langle\, s_i \,\rangle$, where the thermal average has to be interpreted in the restricted sense

described in the previous sections, *i.e.* taken over one ergodic component, in a way that $m_i \neq 0$. Note that one introduces an order-parameter dependence in the probabilities. Using this assumption one can compute the total free-energy

$$F = U - TS \tag{2.18}$$

where the average is taken with the factorized probability distribution (2.17) and the entropy S is given by

$$S = -\sum_{\{s_i\}} P(\{s_i\}) \ln P(\{s_i\}) \; . \tag{2.19}$$

One can use this approximation to treat finite dimensional models [2] Applied to the d-dimensional pure ferromagnetic Ising model with nearest-neighbor interactions on a cubic lattice $J_{ij} = J/2$ for nearest-neighbors and zero otherwise. One finds the internal energy

$$U = -\frac{J}{2}\sum_{\langle ij\rangle}\langle s_i s_j\rangle - h\sum_i \langle s_i\rangle = -\frac{J}{2}\sum_{\langle ij\rangle} m_i m_j - h\sum_i m_i \; , \tag{2.20}$$

and the entropy

$$\begin{aligned} S &= -\sum_{s_i=\pm 1}\prod_{k=1}^{N} P_k(s_k) \ln \prod_{l=1}^{N} P_l(s_l) = -\sum_{l=1}^{N}\sum_{s_l=\pm 1} P_l(s_l)\ln P_l(s_l) \\ &= -\sum_i \frac{1+m_i}{2}\ln\frac{1+m_i}{2} + \frac{1-m_i}{2}\ln\frac{1-m_i}{2} \; . \end{aligned} \tag{2.21}$$

For a uniformly applied magnetic field, all local magnetization equal the total density one, $m_i = m$, and one has the 'order-parameter dependent' free-energy density :

$$f(m) = -dJm^2 - hm + T\left[\frac{1+m}{2}\ln\frac{1+m}{2} + \frac{1-m}{2}\ln\frac{1-m}{2}\right] \; . \tag{2.22}$$

The extrema, $df(m)/dm = 0$, are given by

$$m = \tanh\left(\beta 2dJm + \beta h\right) \; , \tag{2.23}$$

with the factor $2d$ coming from the connectivity of the cubic lattice. The stable states are those that also satisfy $d^2 f/dm^2 > 0$. This *equation of state* predicts a second order phase transition at $T_c = 2dJ$ when $h = 0$. This result is qualitatively correct in the sense that T_c increases with increasing d but the actual value is incorrect in all finite dimensions. In particular, this treatment predicts a finite T_c in $d = 1$ which is clearly wrong. The critical behavior is also incorrect in all finite d, with exponents (see Sect. 2.6.3) that do not depend on dimensionality and take the mean-field values. Still, the nature of the *qualitative* paramagnetic-ferromagnetic transition in $d > 1$ is correctly captured. We

[2] Note that this approximation amounts to replace the exact equation $m_i = \langle \tanh\beta(h + \sum_j J_{ij}s_j)\rangle$ by $m_i = \tanh\beta(h + \sum_j J_{ij}m_j)$.

postpone the study of the solutions to eq. (2.23) to the next Subsection where we shall treat a similar, and in some respects, more general case. Having an expression for the free-energy density as a function of the order parameter, that is determined by eq. (2.23), one can compute all observables and, in particular, their critical behavior. We shall discuss it below.

The Taylor expansion of the free-energy in power of m, close to the critical point where $m \sim 0$, yields the familiar cross over from a function with a single minima at m to the double well form :

$$-\beta F(m) \sim \frac{1}{2}(T - 2dJ)m^2 + \frac{T}{12}m^4 - hm \; . \tag{2.24}$$

Indeed, below $T = 2dJ = T_c$ the sign of the quadratic term becomes negative and the function develops two minima away from $m = 0$.

Taking the derivative of m with respect to h and the limit $h \to 0^{\pm}$ one easily finds that χ diverges as $|T - T_c|$.

Another way of deriving the mean-field approximation is to write

$$s_i = m + \delta s_i \tag{2.25}$$

in one factor in the quadratic term in the energy, where m is the global magnetization density and expanding the Hamiltonian in powers of δs_i keeping only first order terms. This leads to a model with N non-interacting Ising spins coupled to a field that depends on m, $H(m) = -\sum_i s_i(Jzm + h)$, where h is a uniform external field, that one has to determine self-consistently. This way of presenting the approximation makes the "mean field" character of it more transparent.

One can see that the more spins interact with the chosen one the closer the spin sees an average field, *i.e.* the mean-field. The number of interacting spins increases with the range of interaction and the dimension in a problem with nearest neighbour interactions on a lattice.

2.6.2 The fully-connected Ising ferromagnet

Let us now solve exactly the fully-connected Ising ferromagnet with interactions between all p uplets of spins in an external field :

$$H = -\sum_{i_1 \neq \ldots \neq i_p} J_{i_1 \ldots i_p} s_{i_1} \ldots s_{i_p} - \sum_i h_i s_i \; , \tag{2.26}$$

$s_i = \pm 1$, $i = 1, \ldots, N$. For the sake of generality we use a generic interaction strength $J_{i_1 \ldots i_p}$. The ferromagnetic model corresponds to

$$J_{i_1 \ldots i_p} = \frac{J}{p! N^{p-1}} \tag{2.27}$$

with $0 < J = O(1)$, *i.e.* finite, and p is a fixed integer parameter, $p = 2$ or $p = 3$ or ..., that defines the model. The normalization with N^{p-1} of the first term ensures an extensive

energy in the ferromagnetic state at low temperatures, and thus a sensible thermodynamic limit. The factor $p!$ is chosen for later convenience. This model is a source of inspiration for more elaborate ones with dilution and/or disorder Using the factorization of the joint probability density that defines the mean-field approximation, one finds

$$\begin{aligned} F(\{m_i\}) &= -\sum_{i_1\neq\ldots\neq i_p} J_{i_1\ldots i_p} m_{i_1}\ldots m_{i_p} - \sum_i h_i m_i \\ &\quad + T\sum_{i=1}^{N}\left[\frac{1+m_i}{2}\ln\frac{1+m_i}{2} + \frac{1-m_i}{2}\ln\frac{1-m_i}{2}\right] . \end{aligned} \tag{2.28}$$

Note that a Taylor expansion of the entropic contribution around $m_i = 0$ leads to a polynomial expression that is the starting point in the Landau theory of phase transitions (see Sect. 2.6.3).

The local magnetizations, m_i, are then determined by requiring that they minimize the free-energy density, $\partial f(\{m_j\})/\partial m_i = 0$ and a positive definite Hessian, $\partial^2 f(\{m_j\})/\partial m_i \partial m_j$ (*i.e.* with all eigenvalues being positive at the extremal value). This yields

$$m_i = \tanh\left(p\beta \sum_{i_2\neq\ldots\neq i_p} J_{ii_2\ldots i_p} m_{i_2}\ldots m_{i_p} + \beta h_i\right) \tag{2.29}$$

If $J_{i_1\ldots i_p} = J/(p!N^{p-1})$ for all p uplets and the applied field is uniform, $h_i = h$, one can take $m_i = m$ for all i and these expressions become (2.31) and (2.34) below, respectively. The mean-field approximation is exact for the fully-connected pure Ising ferromagnet, as we shall show below. [Note that the fully-connected limit of the model with pair interactions ($p = 2$) is correctly attained by taking $J \to J/N$ and $2d \to N$ in (2.23) leading to $T_c = J$.]

Let us solve the ferromagnetic model exactly. The sum over spin configurations in the partition function can be traded for a sum over the variable, $x = N^{-1}\sum_{i=1}^{N} s_i$, that takes values $x = -1, -1+2/N, -1+4/N, \ldots, 1-4/N, 1-2/N, 1$. Neglecting sub-dominant terms in N, one then writes

$$Z = \sum_x e^{-N\beta f(x)} \tag{2.30}$$

with the x-parameter dependent 'free-energy density'

$$f(x) = -\frac{J}{p!}x^p - hx + T\left[\frac{1+x}{2}\ln\frac{1+x}{2} + \frac{1-x}{2}\ln\frac{1-x}{2}\right] . \tag{2.31}$$

The first two terms are the energetic contribution while the third one is of entropic origin since $N!/(N(1+x)/2)!(N(1-x)/2)!$ spin configurations have the same magnetization density. The average of the parameter x is simply the averaged magnetization :

$$\langle\, x\,\rangle = \frac{1}{N}\sum_{i=1}^{N}\langle\, s_i\,\rangle = m \tag{2.32}$$

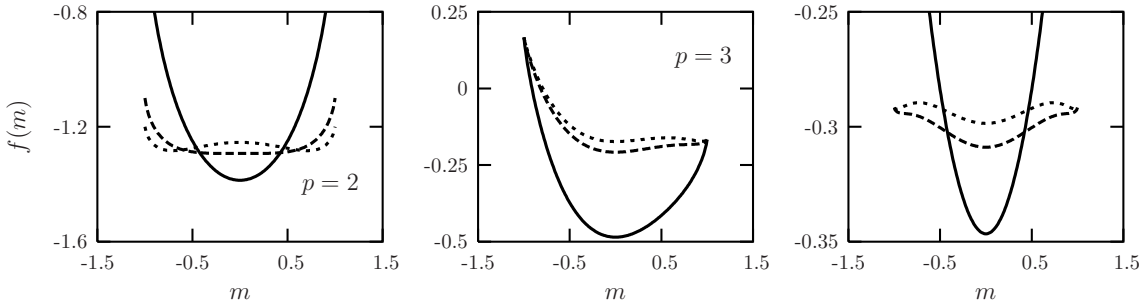

FIG. 4 – The free-energy density $f(m)$ of the $p = 2$ (left), $p = 3$ (center) and $p = 4$ (right) models at three values of the temperature $T < T_c$ (light dashed line), $T = T_c$ (dark dashed line) and $T > T_c$ (solid line) and with no applied field. (The curves have been translated vertically.)

In the large N limit, the partition function – and all averages of x – can be evaluated using the saddle-point method (see Appendix C)

$$Z \approx \sum_{\alpha} e^{-N\beta f(x_{sp}^{\alpha})} \quad , \tag{2.33}$$

where x_{sp}^{α} are the absolute minima of $f(x)$ given by the solutions to $\partial f(x)/\partial x|_{x_{sp}} = 0$,

$$x_{sp} = \tanh\left(\frac{\beta J}{(p-1)!}\, x_{sp}^{p-1} + \beta h\right) \ , \tag{2.34}$$

together with the conditions $d^2 f(x)/dx^2|_{x_{sp}^{\alpha}} > 0$. Note that the contributing saddle-points should be degenerate, *i.e.* have the same $f(x_{sp}^{\alpha})$ for all α. The sum over α then just provides a numerical factor of two in the present case ($h = 0$). Now, since

$$x_{sp} = -\partial f(x)/\partial h|_{x_{sp}} = \langle\, x \,\rangle = m \ , \tag{2.35}$$

as we shall show below, the solutions to these equations determine the order parameter.

High temperature

In a finite magnetic field, eq. (2.34) has a unique positive – negative – solution for positive – negative – h at all temperatures. The model is ferromagnetic at all temperatures and there is no phase transition in this parameter.

2nd order transition for $p = 2$

In the absence of a magnetic field this model has a paramagnetic-ferromagnetic phase transition at a finite T_c. The order of the phase transition depends on the value of p. This

can be seen from the temperature dependence of the free-energy density (2.31). Figure 4 displays $f(x)$ in the absence of a magnetic field at three values of T for the $p = 2$ (left), $p = 3$ (center) and $p = 4$ (right) models (we call the independent variable m since the stationary points of $f(x)$ are located at the magnetization density of the equilibrium and metastable states, as we shall show below). At high temperature the unique minimum is $m = 0$ in all cases. For $p = 2$, when one reaches T_c, the $m = 0$ minimum splits in two that slowly separate and move towards higher values of $|m|$ when T decreases until reaching $|m| = 1$ at $T = 0$ (see Fig. 4-left). The transition occurs at $T_c = J$ as can be easily seen from a graphical solution to eq. (2.34), see Fig. 5-left. Close but below T_c, the magnetization increases as $m \sim (T_c - T)^{\frac{1}{2}}$. The linear magnetic susceptibility has the usual Curie behavior at very high temperature, $\chi \approx \beta$, and it diverges as $\chi \sim |T - T_c|^{-1}$ on both sides of the critical point. The order parameter is continuous at T_c and the transition is of second-order thermodynamically.

1st order transition for $p > 2$

For $p > 2$ the situation changes. For even values of p, at T^* two minima (and two maxima) at $|m| \neq 0$ appear. These coexist as metastable states with the stable minimum at $m = 0$ until a temperature T_c at which the three free-energy densities coincide, see Fig. 4-right. Below T_c the $m = 0$ minimum continues to exist but the $|m| \neq 0$ ones are favored since they have a lower free-energy density. For odd values of p the free-energy density is not symmetric with respect to $m = 0$. A single minimum at $m^* > 0$ appears at T^* and at T_c it reaches the free-energy density of the paramagnetic one, $f(m^*) = f(0)$, see Fig. 4-center. Below T_c the equilibrium state is the ferromagnetic minimum. For all $p > 2$ the order parameter is discontinuous at T_c, it jumps from zero at T_c^+ to a finite value at T_c^-. The linear magnetic susceptibility also jumps at T_c. While it equals β on the paramagnetic side, it takes a finite value given by eqn. (2.37) evaluated at m^* on the ferromagnetic one. In consequence, the transition is of first-order.

Pinning field, broken ergodicity and spontaneous broken symmetry

The saddle-point equation (2.34) for $p = 2$ [or the mean-field equation (2.23)] admits two equivalent solutions in no field. What do they correspond to ? They are the magnetization density of the equilibrium ferromagnetic states with positive and negative value. At $T < T_c$ if one computes $m = N^{-1} \sum_{i=1}^{N} \langle s_i \rangle = \sum_x e^{-\beta N f(x)} x$ summing over the two minima of the free-energy density one finds $m = 0$ as expected by symmetry. Instead, if one computes the averaged magnetization density with the partition sum restricted to the configurations with positive (or negative) x one finds $m = |m_{sp}|$ (or $m = -|m_{sp}|$).

In practice, the restricted sum is performed by applying a small magnetic field, computing the statistical properties in the $N \to \infty$ limit, and then setting the field to zero. In other words,

$$m_\pm \equiv \frac{1}{N} \sum_{i=1}^{N} \langle s_i \rangle_\pm = \left(\frac{1}{\beta N} \frac{\partial \ln Z}{\partial h} \right) \Big|_{h \to 0^\pm} = - \frac{\partial f(m_{sp})}{\partial h} \Big|_{h \to 0^\pm} = \pm |m_{sp}| \, . \qquad (2.36)$$

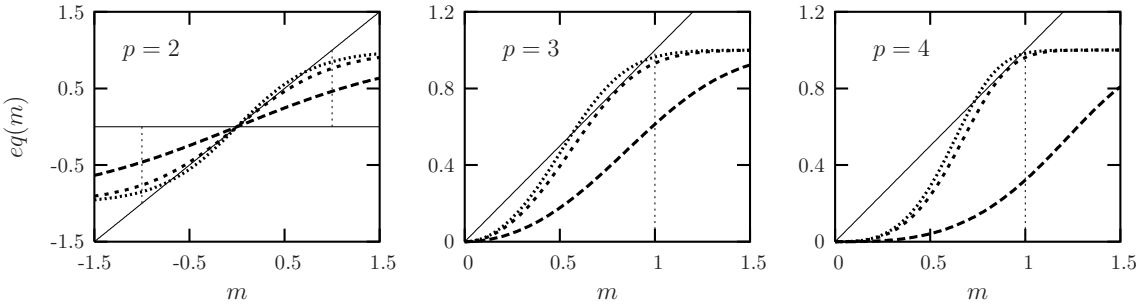

FIG. 5 – Graphical solution to the equation fixing the order parameter x for $p = 2$ (left), $p = 3$ (center) and $p = 4$ (right) ferromagnetic models at three values of the temperature $T < T^*$, $T = T^*$ and $T > T^*$ and with no applied field. Note that the rhs of this equation is antisymmetric with respect to $m \to -m$ for odd values of p while it is symmetric under the same transformation for even values of p. We show the positive quadrant only to enlarge the figure. T^* is the temperature at which a second minimum appears in the cases $p = 3$ and $p = 4$.

The limit $N \to \infty$ taken in a field selects the positive (or negatively) magnetized states.

For odd values of p there is only one non-degerate minimum of the free-energy density at low temperatures and the application of a pinning field is then superfluous.

The existence of two degenerate minima of the free-energy density, that correspond to the two equilibrium ferromagnetic states at low temperatures, implies that ergodicity is broken in these models. In pure static terms this means that one can separate the sum over all spin configurations into independent sums over different sectors of phase space that correspond to each equilibrium state. In dynamic terms it means that temporal and statistical averages (taken over all configurations) do not coincide.

For any even value of p and at all temperatures the free-energy density in the absence of the field is symmetric with respect to $m \to -m$, see the left and right panels in Fig. 4. The phase transition corresponds to a *spontaneous symmetry breaking* between the states of positive and negative magnetization. One can determine the one that is chosen when going through T_c either by applying a small *pinning field* that is taken to zero only after the thermodynamic limit, or by imposing adequate boundary conditions. Once a system sets into one of the equilibrium states this is completely stable in the $N \to \infty$ limit.

For all odd values of p the phase transition is not associated to symmetry breaking, since there is only one non-degenerate minimum of the free-energy density that corresponds to the equilibrium state at low temperature.

The magnetic linear susceptibility is given by

$$\chi \equiv \left.\frac{\partial m}{\partial h}\right|_{h\to 0^{\pm}} = \left.\frac{\partial x_{sp}}{\partial h}\right|_{h\to 0^{\pm}} = \frac{\beta}{\cosh^2(\frac{\beta J}{(p-1)!}\, x_{sp}^{p-1}) - \frac{\beta J}{(p-2)!} x_{sp}^{p-2}} \,. \tag{2.37}$$

For $p = 2$ the two magnetized states have the same divergent susceptibility, $\chi \sim (k_B T - J)^{-1}$, at T_c. For $p > 2$ the magnetization takes the Curie form $\chi = \beta$ in the full high-T phase and it jumps to a different value at the transition.

2.6.3 The Bethe lattice

Another way of achieving a model for which mean-field theory is exact is to use a Cayley tree or a lattice with a tree-like structure (and no loops). A slightly different case is the one of the Bethe lattice defined as a random graph with N nodes and $M = 2zN$ edges. On average, each node has z neighbours. In the $N \to \infty$ limit the distribution of the number of neighbours of a given node is a Poisson distribution. These lattices are locally tree-like and loops have length $\sim \ln N$ or longer. The name is based on the fact that the Bethe approximation is exact for models defined on these lattices. In the pure case the interactions are normalized in such a way that $J_{ij} \sim z^{-1}$ and when $z \to \infty$ one recovers the fully-connected ferromagnetic model. These models are now recieving renewed attention since many combinatorial optimizations problems can be written as disordered spin models on such lattices. We shall not develop this line here.

2.6.4 Landau theory : a field theory

The exercise in the last subsection is a fully solvable model for which mean-field theory is exact. Now, can one attack more generic phase transitions in a similar manner ? Can one also get an idea of the limit of validity of mean-field theory and when it is expected to fail ?

Landau proposed an extension of Weiss mean-field theory for ferromagnets (Sect. 2.4) that has a much wider range of application, includes space and allows to predict when it applies and when it fails. In a few words, in Landau theory one first identifies the order parameter for the phase transition, that is to say, a quantity with zero average in the disordered phase and non-zero average on the ordered side. Next, one proposes a field theory for a coarse-grained field that represents the averaged relevant variable – giving rise to the order parameter – over a *mesoscopic scale* ℓ that is, by definition, much larger than the interatomic distance a. In the case of an Ising spin system, the field in each coarse-graining volume $v = \ell^d$ within the sample is defined as :

$$\phi(\vec{x}) \equiv \frac{1}{\ell^d} \sum_{j \in v_{\vec{x}}} s_j \ , \tag{2.38}$$

see Fig. 6. The *field* ϕ is a continuous variable taking real values. One can construct a field ϕ that takes a different value per lattice site (using overlapping coarse-graining volumes) in which case the coordinates of the space variable $\vec{x}$ vary by steps of a, the lattice spacing. Instead, one can use non-overlapping coarse-graining volumes in which

case the coordinates of the space variable $\vec{x}$ vary by steps of ℓ, the coarse-graining linear size.

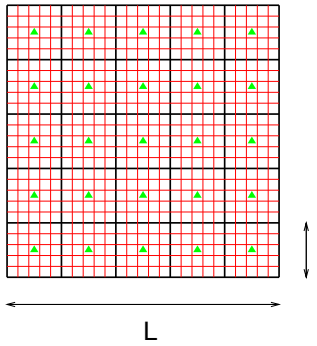

FIG. 6 – Coarse-graning

The next step consists in constructing (or proposing) an effective free-energy of the interacting system. One can procede as for the fully-connected Ising model, where we transformed the sum over the N spin variables into a sum over possible values of the averaged magnetization taking into account the associated degeneracy (entropy). In this vein

$$Z = \sum_{\{conf\}} e^{-\beta H_{conf}} = \int \mathcal{D}\phi \sum_{\{conf/\phi\}} e^{-\beta H_{conf}} \tag{2.39}$$

where the constrained sum runs over all microstates $conf$ that are compatible with a field value ϕ and the integral is a functional integral over all possible spatial realizations of the field : $\mathcal{D}\phi = \prod_{\vec{x}} d\phi(\vec{x})$. The factor $\sum_{\{conf/\phi\}} e^{-\beta H_{conf}}$ is a positive definite function of ϕ. We can then define a *free-energy at fixed field*, $F(\phi)$, using

$$e^{-\beta F(\phi)} \equiv \sum_{\{conf/\phi\}} e^{-\beta H_{conf}} \tag{2.40}$$

where

$$F(\phi) = -k_B T \ln \sum_{\{conf/\phi\}} e^{-\beta H_{conf}} \tag{2.41}$$

The partition function (2.39) became

$$Z = \int \mathcal{D}\phi \, e^{-\beta F(\phi)} \tag{2.42}$$

and we now have a *statistical field theory* that is described by a functional $F(\phi)$ that plays the rôle of a generalized Hamiltonian.

In general, we do not know how to compute $F(\phi)$. Landau's proposal is to expand $F(\phi)$ in powers of ϕ and its gradients $\vec{\nabla}\phi$ and then determine, depending on the problem at hand, which terms vanish and which among the non-vanishing ones are the most relevant. The first question is answered using *symmetry arguments*. Let us illustrate the argument in the magnetic problem modelled by the Ising model.

– The Hamiltonian under no applied field is invariant under simultaneous reversal of all spins $s_i \to -s_i$. The free-energy $F(\phi)$ should then be such that $F(\phi) = F(-\phi)$.
– The expansion is expected to be valid close to T_c where $\langle \phi \rangle \sim 0$ and then $\phi \sim 0$ too (if ℓ is sufficiently large to avoid large local fluctuations). In this case, one keeps only the first terms in the power expansion.
– The terms with high order derivatives, $c'(\nabla^2\phi)^2$, should be negligible with respect to the first one, $c\nabla^2\phi$. Indeed, writing $\phi(\vec{x})$ using a Fourier expansion

$$\phi(\vec{x}) = \sum_{\vec{q}} e^{i\vec{q}\vec{x}}\phi(\vec{q}) \tag{2.43}$$

where the sum runs over wave-vectors that satisfy $q \ll \ell^{-1}$ due to the cut-off introduced by the size of the coarse-graning box (we are here considering non-overlapping boxes, otherwise the condition is $q \ll a^{-1}$. Since $(c'/c)^{1/2}$ is usually of the order of the microscopic interactions, $c'/c \ll \ell^2$, for each q such that $q \ll \ell^{-1}$ one has

$$c'q^4|\phi(\vec{q})|^2 \ll cq^2|\phi(\vec{q})|^2 \; . \tag{2.44}$$

Based on the arguments itemized above, the Landau free-energy reads

$$F(\phi) = \int d^dx \left[\frac{c}{2}(\nabla\phi(\vec{x}))^2 + \frac{\lambda}{4!}\phi^4(\vec{x}) + \frac{T-T_c}{T_c}\phi^2(\vec{x})\right] \; . \tag{2.45}$$

The coefficients are *chosen* in such a way to reproduce a second order phase transition when going through T_c. The first term mimics an elastic energy related to the ferromagnetic interactions. The second term can also be estimated as an expansion, upto fourth order, of the entropic contribution in powers of $T - T_c$ that is expected to be valid only close to T_c. The entropic contribution in the fully connected model with $p = 2$, see eq. (2.31) combined with the energetic term proportional to J (that is equal to T_c for $p = 2$) leads to exactly this expansion. Note that this 'order-parameter dependent' free-energy is not quadratic due to the term ϕ^4. The averages can be computed by introducing an applied field and adding the following term to the free-energy :

$$\int d^dx \; h(\vec{x})\phi(\vec{x}) \tag{2.46}$$

and taking the corresponding functional derivatives (see App. C). The values of the parameters in the expansion of the free-energy are not known in general. They are determined by comparison to experiments or from first-principle approaches.

If one realizes that the free-energy in the exponential is proportional to the volume of the system, the integral over all ϕ configurations in the partition function can be evaluated with a *saddle-point approximation* (expected to be accurate in the limit $V \to \infty$). This evaluation is what is usually called the *Landau approximation* or *mean-field approximation*. Calling ϕ_{sp} the value of the field that renders the exponent minimum, *i.e.* the *state of the system*, one has

$$Z \sim e^{-\beta F(\phi_{sp})} \; . \tag{2.47}$$

Including the fluctuations (see Appendix C) one can see when these ones become too important and render the saddle-point evaluation invalid. This analysis is called the *Ginzburg criterion*, see Sect. 2.6.3.

2.6.5 The correlation length

A very important concept in critical phenomena is that of a *correlation length* usually denoted by ξ.

Discussion

The correlation length is the distance over which the *fluctuations* of the microscopic degrees of freedom are significantly correlated. A simple way to understand its meaning is the following. Take a macroscopic sample and measure some macroscopic observable under some external conditions, *i.e.* temperature T and pressure P. Now, repeat the measurement after cutting the sample in two pieces and keeping the external conditions unchanged. The result for the macroscopic observable is the same. Repeating this procedure, one finds the same result until the system size reaches the correlation length of the material.

When the correlation length is finite, a fluctuation within a region of length ξ has no effect outside of it. There is a separation of length-scales. When describing the system at a short length scale, $a \ll \ell \ll \xi$, the other boxes act as constant parameters with respect to the chosen one. At a longer length scale, $\xi \ll \ell$, the microscopic details enter only through average values like the mean density or the averaged magnetization.

Systems with finite correlation lengths look uniform, that is to say, they are statistically translational invariant over distances $\ell \gg \xi$. The measurement of any observable on different boxes of linear size ℓ is Gaussian distributed about its mean and the variance decreases with ℓ/ξ (due to the central limit theorem). Global measurements do not reflect the microscopic details.

At finite temperature, $T < T_c$, one can have *droplets* of the wrong phase within the correct one, due to thermal agitation. The size of these droplets will be a function of temperature and at a given instant, a snapshot of the system reveals the existence of a number of them with different sizes. One expects though that they have a well-defined average (taken, for instance, over different snapshots taken at different times). This average size can be taken as a qualitative indication of the value of the correlation length (we shall give a more precise definition below).

Systems with diverging correlation length have fluctuations, or droplets, of all sizes. The fact that one finds coherent structures at all lengths at the critical point means that there is no spatial scale left in the problem and then all scales participate in the critical behaviour. These systems are no longer translational invariant over any finite length scale. Instead, they are *scale invariant* under simultaneous rescaling of the quantities of interest and the length, meaning that if one looks at it with different microscopes one essentially

sees the same. Otherwise stated, the structure is self-similar. A localized fluctuation has an effect over the whole system and no subsystem is statistically independent of the others. Still, knowledge of the behaviour at a given scale allows one to derive what happens at all scales through the scaling transformation.

In first order phase transition the correlation length is finite for all values of the parameters. In second order phase transitions, the correlation length is usually very short, of the order of a few lattice spacing, at low temperature. It increases when approaching T_c, it diverges at T_c, and then decreases again in the high temperature phase when getting away from the critical point. See Fig. 7.

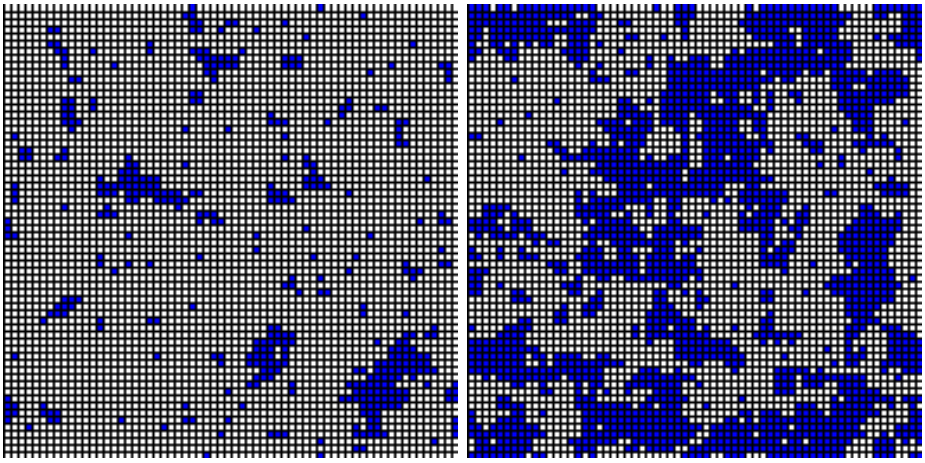

FIG. 7 – Two snapshots of an equilibrium spin configuration in a $2d$ Ising model. Left : below T_c ; right : at T_c.

Definition

The actual definition of the correlation length is based on the use of the *static susceptibility sum rule*.

A simple calculation allows one to show that the linear susceptibility is related to the connected correlation function as

$$\chi \equiv \left.\frac{\partial m_h}{\partial h}\right|_{h=0} = -\left.\frac{\partial^2 f}{\partial h^2}\right|_{h=0} = \frac{\beta}{N}\sum_{ij} G(\vec{r}_i, \vec{r}_j) \tag{2.48}$$

with the spin-spin connected correlation function

$$G(\vec{r}_i, \vec{r}_j) \equiv \langle (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \rangle = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \ . \tag{2.49}$$

Nothing indicates that spatial translational invariance should be violated, thus, the correlation should be a function of the distance between the points $\vec{r}_i$ and $\vec{r}_j$ only :

$$G(\vec{r}_i, \vec{r}_j) = G(\vec{r}_i - \vec{r}_j) \ . \tag{2.50}$$

One then has

$$\chi \equiv \left.\frac{\partial m_h}{\partial h}\right|_{h=0} = \beta \sum_i G(\vec{r}_i) = \frac{\beta}{a^d}\int_V d^d r\; G(\vec{r}) \; . \tag{2.51}$$

This means that the divergence of the susceptibility at the critical point must be accompanied by a special behavior of the correlation function. Indeed, one finds that

$$G(\vec{r}) \sim r^{2-d-\eta} f\left(\frac{r}{\xi}\right) \quad \text{with} \quad \left\{ \begin{array}{l} f(0) = 1 \; , \\ f(x \to \infty) \sim x^\eta e^{-x} \; , \end{array} \right. \tag{2.52}$$

with η another critical exponent that takes a very small value. This expression is integrable over the full volume unless the exponential factor disappears. This is indeed what happens at T_c where the correlation length ξ diverges, again as a power law of the distance to the critical point

$$\xi \sim |T - T_c|^{-\nu} \; . \tag{2.53}$$

Finally, one observes that the correlation function right at the critical point also diverges as a power law :

$$G(\vec{r}) \sim r^{-(d-2+\eta)} \; . \tag{2.54}$$

An example : the Ising chain

Let us discuss the correlation length in a simple solvable case, the Ising model in $d = 1$ with, say, open boundary conditions. In this case, the finite temperature correlation function is

$$G_{kl} \;\; = \;\; \langle s_k s_l \rangle - \langle s_k \rangle \langle s_l \rangle = \langle s_k s_l \rangle \tag{2.55}$$

since $\langle s_k \rangle = 0$ at any $T > 0$. Introducing, for convenience, different coupling constants $K_i = \beta J_i$ on the links, G_{kl} reads

$$G_{kl} = Z^{-1} \sum_{\{s_i = \pm 1\}} e^{\sum_i K_i s_i s_{i+1}} s_k s_l = Z^{-1} \frac{\partial}{\partial K_k} \frac{\partial}{\partial K_{k+1}} \cdots \frac{\partial}{\partial K_{l-1}} Z \; . \tag{2.56}$$

At the end of the calculation one takes $K_i = K = \beta J$ for all i. Thus, at finite temperature the connected correlation between any two spins can be computed as a number of derivatives (depending on the distance between the spins) of the partition function conveniently normalized. Using the change of variables $\eta_i = s_i s_{i+1}$, one finds

$$Z = \sum_{\{\eta_i = 1\}} e^{\sum_i K_i \eta_i} = 2 \prod_{i=1}^{N-1} 2\cosh(K_i) \to 2(2\cosh \beta J)^{N-1} \; . \tag{2.57}$$

Taking the distance between the chosen spins s_k and s_l to be $k - l = r$ the correlation function is then given by

$$G(r) \;\; = \;\; [\tanh(\beta J)]^r = e^{r \ln[\tanh(\beta J)]} = e^{-r/\xi} \tag{2.58}$$

with

$$\xi = \frac{1}{\ln \coth(\beta J)} \sim e^{4J/(T-T_c)} , \qquad T \sim 0 . \tag{2.59}$$

In this one dimensional example we found an essential singularity, an exponential divergence, of the correlation length when approaching $T_c = 0$. In general, in higher d, one has a power law divergence of the form (2.54).

2.6.6 The Ginzburg criterium

The Ginzburg criterium states that the Landau mean-field theory breaks down when

$$\langle\, \delta\phi_{coh}^2 \,\rangle \sim \langle\, \phi \,\rangle^2 \tag{2.60}$$

where

$$\delta\phi_{coh} \equiv V_{coh}^{-1} \int d^d r \, (\phi(\vec{r}) - \langle\, \phi \,\rangle) , \tag{2.61}$$

$V_{coh} = \xi^d$ with ξ the coherence length, to be defined below, and $\langle\, \phi \,\rangle$ the equilibrium order parameter. The left-hand-side in (2.60) is

$$\langle\, \delta\phi_{coh}^2 \,\rangle = V_{coh}^{-1} \int d^d r \, G(\vec{r}) \tag{2.62}$$

where G is the connected correlation function

$$G(\vec{r}, \vec{r}') \equiv \langle (\phi(\vec{r}) - \langle \phi(\vec{r}) \rangle) \, (\phi(\vec{r}') - \langle \phi(\vec{r}') \rangle) \tag{2.63}$$

$G(\vec{r}, \vec{r}') = G(|\vec{r} - \vec{r}'|) = G(r)$ can be computed within the same Landau theory and compared to the right-hand-side. Landau theory, thus, establishes its own limits of validity : it is valid until the fluctuations of the order parameter become of the order of the order parameter itself when both are coarse-grained over a volume determined by the correlation length.

For the $l\lambda\phi^4$ problem one finds an upper critical dimension,

$$d_u = 4 \tag{2.64}$$

above which the mean-field description of the ferromagnetic transition is *exact*! Below d_u mean-field theory fails. However, it does not fail everywhere in parameter space. It just fails when very close to the critical point, in a system-dependent *critical region*. The behavior away from the critical region is still well-described by the Landau-Ginzburg phenomenological theory. A signature of the failure of the Landau-Ginzburg theory is that it predicts the mean-field exponents in (2.93) for all d which is clearly incorrect for small d.

Landau (1962) and Ginzburg (2003) got Nobel Prizes in Physics for their work along these lines (Landau on superfluidity, Ginzburg on superconductors and superfluids). The

strategy of Ginzburg and Landau proved to be very useful to describe phase transitions of very different type using, as a starting point, the identification of the order parameter and a proposal for the field theory describing the physical problem one is interested in. It is particularly well-suited for problems with *long-range interactions* such as superconductors and ferroelectrics since in these cases fluctuations are suppressed.

In the Ψ-theory of superconductivity that got Ginzburg the 2003 Nobel Prize a scalar complex field Ψ is the order parameter and it is coupled to a vector electromagnetic field potential $\vec{A}$. A link between Bardeen-Cooper-Shrieffer's microscopic theory of superconductivity and the Landau-Ginzburg phenomenological model can be established.

2.6.7 Euclidean quantum field theories and statistical systems in equilibrium

A very simple analogy can be drawn between quantum field theories defined in Eurclidean space and statistical systems in equilibrium if one uses the path-integral formulation developed by Feynman to describe the former [1]. Let us show this equivalence using the quantum scalar field as an example. The *expectation value* of the n-point correlation function

$$C_n \equiv \langle\, \phi(\vec{r}_1) \,\ldots\, \phi(\vec{r}_n) \,\rangle \tag{2.65}$$

where $\vec{r}_j$, $j = 1, \ldots, n$ are generic points in the $1 + d$ dimensional Euclidean space (with the usual Euclidean metric such that $r^2 = x_0^2 + \ldots + x_d^2$ and x_0 is the Euclidean time) is given by

$$C_n = \frac{\int \mathcal{D}\phi \; e^{-\frac{1}{\hbar} S_E[\phi]} \; \phi(\vec{r}_1) \,\ldots\, \phi(\vec{r}_n)}{\int \mathcal{D}\phi \; e^{-\frac{1}{\hbar} S_E[\phi]}} \; . \tag{2.66}$$

S_E is the Euclidean action, $\hbar$ is Planck's constant, and $\mathcal{D}\phi$ is the measure in the path integral. Note that working in Euclidean space-time there is no i in the exponential. If we simply identify $\hbar = k_B T$ we can also interpret (2.66) as the statistical expectation value of a *classical field theory* in equilibrium with an environment at temperature T. The normalization constant is then the *vacuum-to-vacuum permanence amplitude* or *partition function*

$$Z \equiv \int \mathcal{D}\phi \; e^{-\frac{1}{\hbar} S_E[\phi]} \; . \tag{2.67}$$

In Sects. 4.3.3 and 4.3.3 we shall see how this remark allows one to develop the **Monte-carlo study of lattice field theory** and a quantization method based on a stochastic Langevin dynamics, the so-called **Stochastic quantization** method of Parisi and Wu.

2.7 Continuous broken symmetry and Goldstone modes

The energy of spin models with continuous variables, such as the XY, Heisenberg or generic O(N) models introduced in (2.2) and (2.3) in the absence of an applied field ($\vec{h} = \vec{0}$), is invariant under the simultaneous rotation of all the spin variables by the same angle. This is a *continuous global symmetry* to be confronted to the *discrete global* reversal invariance, $s_i \to s_i$, of the Ising case.

The spontaneous magnetization at low temperatures can point in any of the infinite equivalent directions constrained to satisfy (2.3). This gives rise to an infinite degeneracy of equilibrium states that are translational invariant (in real space). These equilibrium states are controlled by a continuous variable, determining the direction on the N-dimensional hypersphere of radius 1.

2.7.1 The d-dimensional XY model : spin-waves

Let us consider one such equilibrium state and call it $\vec{s}_i^{\,eq}$. It is clear that if one slightly modifies the angle of the $\vec{s}$ vector on neighbouring space points, the energy cost of such a perturbation would vanish in the limit of vanishing angle. More precisely, these configurations are called *spin-waves* and they differ from the equilibrium state by an arbitrarily small amount.

In the particular case of the XY model, the local spin has only two components ($N = 2$) and it can be parametrized as

$$\vec{s}_i = (s_i^1, s_i^2) = |\vec{s}_i|(\cos\phi_i, \sin\phi_i) = (\cos\phi_i, \sin\phi_i) \ , \tag{2.68}$$

where $0 \leq \phi_i \leq 2\pi$ is the angle with respect to the x axis on each d-dimensional lattice site i, and $|\vec{s}_i| = 1$. The energy (2.2) then becomes

$$E = -J \sum_{\langle ij \rangle} \cos\phi_{ij} \tag{2.69}$$

where $\phi_{ij} = \phi_i - \phi_j$ is the angle between the spins at neighbouring sites i and j. It remains invariant under the global change $\phi_i \to \phi_i + \phi_0$. The ground state is the fully aligned state $\phi_i = \phi$ for all i, with ϕ in $[0, 2\pi]$, and ground state energy $E_0 = -JNz/2$ (z is the coordination number of the lattice). If one assumes that at low enough T the angles change smoothly $|\phi_i - \phi_j| \ll 2\pi$ for all nearest-neighbours the cosine in the energy can be approximated at second order and

$$E \ \simeq \ E_0 + \frac{J}{2} \sum_{\langle ij \rangle} (\phi_i - \phi_j)^2 \ = \ E_0 + \frac{J}{4} \sum_{\vec{r},\vec{a}} [\phi(\vec{r} + \vec{a}) - \phi(\vec{r})]^2 \ . \tag{2.70}$$

If $\phi(\vec{r})$ is a slowly varying function of $\vec{r}$ one can approximate the finite difference by a derivative, *e.g.* $\phi(\vec{r} + a\hat{e}_x) - \phi(\vec{r}) \simeq a\partial_x\phi(\vec{r})$ the sum over lattice sites by an integral $\sum_{\vec{r}} \simeq a^{-d} \int d^d r$, and write

$$E \ \simeq \ E_0 + \frac{J}{2a^{d-2}} \int d^d r \ [\vec{\nabla}\phi(\vec{r})]^2 \ . \tag{2.71}$$

We ended up with a quadratic form that, if we relax the constraint $\phi \in [0, 2\pi]$, acts on a field on the real axis, $-\infty < \phi < \infty$.

The interest is in computing the correlation function

$$C(r) \equiv \langle \vec{s}(\vec{r})\vec{s}(\vec{0}) \rangle = \mathrm{Re} \langle e^{i[\phi(\vec{r}) - \phi(\vec{0})]} \rangle = e^{-\frac{1}{2}\langle [\phi(\vec{r}) - \phi(\vec{0})]^2 \rangle} \equiv e^{-\frac{1}{2}g(r)} \ , \tag{2.72}$$

where the second identity holds for Gaussian fields and $C(r)$ plays a similar role to the one in eq. (**??**) although it is not connected (we have not subtracted the average values $\langle \vec{s}(\vec{r}) \rangle$. One should analyze whether at long distances it converges to a finite value (long-range order) or zero (no long-range order). We shall not give the details of this calculation which can be found in many textbooks (and your field-theory lectures, I presume) and just give the results :

$$\frac{Ja^{2-d}}{T}\, g(r) \simeq \begin{cases} \Omega_d/(d-2)\ (\pi/L)^{d-2} & d>2\ , \\ (2\pi)^{-1}\ \ln(r/L) & d=2\ , \\ r/2 & d=1\ , \end{cases}$$

that imply

$$C(r) \simeq \begin{cases} e^{-\text{const }T} & d>2 & \text{long-range order}\ , \\ (r/L)^{-\eta(T)} & d=2 & \text{quasi-long-range order}\ , \\ \exp[-T/(2Ja)\ r] & d=1 & \text{short-range order}\ . \end{cases}$$

The exponent η continuously depends on temperature, $\eta = T/(2\pi J)$. These results imply that the order parameter is non-zero in $d > 2$ but vanishes in $d \leq 2$. Interestingly enough, we find that the $2d$ XY model does not support long-range order but its correlation function decays algebraically at *all* temperatures. This is the kind of decay found *at* a critical point, $G(r) \simeq r^{-d+2-\eta}$, so the system behaves as at criticality at all temperatures. This does not seem feasible physically and, indeed, we shall see that other excitations, not taken into account by the continuous expansion above, are responsible for a phase transition of a different kind. The low-T phase remains well described by the spin-wave approximation but the high-T one is dominated by the proliferation of topological defects.

2.7.2 The $2d$ XY model : Kosterlitz-Thouless transition

The energy (2.70) has a *local discrete symmetry* that is lost in the continuous approximation (2.71) :

$$\phi_i \to \phi_i \pm 2\pi \tag{2.73}$$

and permits the existence of vortices [20]. These are configurations, $\phi(\vec{r})$, in which the angle winds around a topological defect :

$$\oint d\vec{l}\ \vec{\nabla}\phi(\vec{r}) = 2\pi n \qquad\qquad \vec{\nabla}\phi(\vec{r}) = \frac{n}{r}\ \hat{\theta}\ . \tag{2.74}$$

Let us evaluate the energy of a vortex configuration

$$\phi(\vec{r}) = \phi(r,\theta) = n\theta \tag{2.75}$$

where, without loss of generality, we set the origin of coordinates at the center of the vortex, θ is the angle of the position $\vec{r}$ with respect to the x axis, and n is its strength using the expression (2.71). Thus,

$$E_{1\ vortex} = \frac{J}{2}\int d^2r\ [\vec{\nabla}\phi(\vec{r})]^2 = \pi J n^2 \int_a^L dr\ \frac{1}{r} = \pi J n^2 \ln\frac{L}{a} \tag{2.76}$$

with L the linear dimension of the system. The energy of a single vortex diverges in the infinite size limit and one might conclude that these configurations are not favorable. However, as already discussed in the Ising chain (see Sect.), at finite T one needs to estimate the *free-energy* difference between configurations with and without a vortex to conclude about their existance. The entropy of a single vortex is $S = k_B \ln \mathcal{N} = k_B \ln(L/a)^2$ since in a $2d$ lattice the center of the vortex can be located on $(L/a)^2$ different sites. Then

$$\Delta F = F_{1\ vortex} - F = (\pi J n^2 - 2k_B T) \ln(L/a) \ . \tag{2.77}$$

This quantity changes sign at $k_B T = \pi J n^2/2$ therefore *no isolated vortex* occurs below $k_B T_{KT} = \pi J/2$. At higher temperatures, $T > T_{KT}$, isolated vortices proliferate (favored by the entropic contribution), destroy the quasi long-range order and correlations decay exponentially on a length-scale given by the typical spacing between vortices

$$G(r) \simeq e^{-r/\xi(T)} \qquad\qquad \xi(T) \simeq e^{-b|T-T_{KT}|^{-1/2}} \tag{2.78}$$

close to T_{KT}. This very fast decay of the correlation length, loosely $|T - T_{KT}|^{-\nu}$ with $\nu \to \infty$, follows from an RG analysis that we shall not present here.

Below T_{KT} vortices exist only in bound pairs with opposite vorticity (the arrows turning in opposite direction) held together by a logarithmic confining potential

$$E_{pair}(\vec{r}_1, \vec{r}_2) = -2\pi J n_1 n_2 \ln(|\vec{r}_1 - \vec{r}_2|/a) \ . \tag{2.79}$$

This is proven by an electrostatic analogy that we shall not develop further. Note that the energy increases if one tries to unbind – separate – the vortices in the pair. The correlation still decays as a power-law and there is no spontaneous symmetry breaking in this phase since the order parameter vanishes – in agreement with the Mermin-Wagner theorem that we discuss below.

This argument shows that two qualitatively different equilibrium states exist at high and low T but it does not characterize the transition. The order parameter vanishes on both sides of the transition but there is still one, with the correlation decaying exponentially on one side (high T) and as a power law on the other (low T).

2.7.3 O(N) model : Ginzburg-Landau field theory

Let us now focus on the generic $O(N)$ model. Symmetry arguments à la Landau lead to the free-energy

$$F[\vec{\phi}] = \int d^d r \left[[\vec{\nabla}\vec{\phi}(\vec{r})]^2 + \frac{T - T_c}{T_c} \phi^2(\vec{r}) + \frac{\lambda}{4!} \phi^4(\vec{r}) - \vec{h}\vec{\phi}(\vec{r}) \right] \tag{2.80}$$

where $\phi^2 \equiv \sum_{a=1}^{N} \phi_a^2$ is the result of a sum over a N components.

In the XY case, $N = 2$, but with no constraint on the modulus of the vector field $\vec{\phi}$, it is simple to derive a continuum limit of the lattice model in analogy with the Landau

approach. Coarse-graining the two-component spin to construct a two-component field $\vec{\psi}(\vec{r}) = \ell^{-d} \sum_{i \in V_{\vec{r}}} \vec{s}_i$, proposing a Landau ψ^4 action for the field $\vec{\psi}$, and parametrising the field by its modulus and angle, $\vec{\psi}(\vec{r}) = \phi_0(\vec{r})|(\cos\phi(\vec{r}), \sin\phi(\vec{r}))$, one finds

$$E[\phi_0, \phi] = \int d^d r \left[(\vec{\nabla}\phi_0(\vec{r}))^2 + \frac{T - T_c}{T_c}\phi_0^2(\vec{r}) + \frac{\lambda}{4!}\phi_0^4(\vec{r}) \right] \tag{2.81}$$

$$+ \frac{\phi_0^2}{2} \int d^d r \, [\vec{\nabla}\phi(\vec{r})]^2 \tag{2.82}$$

The first term is just similar to the energy of a scalar field configuration in the Ising model. The second-term quantifies the energy of the spin-wave configurations. The local angle is simply a *massless scalar field* in d dimensional space. Its correlation functions behave as (see the next Section)

$$\langle \, \phi(\vec{r})\phi(\vec{r}') \, \rangle \sim (2-d)^{-1} |\vec{r} - \vec{r}'|^{2-d} \tag{2.83}$$

in the large $|\vec{r} - \vec{r}'|$ limit. The behaviour is logarithmic in $d = 2$ and it is long-ranged in all other dimensions.

In the general N case the correlation functions, $C_{ab} = \langle (\phi_a(\vec{r}) - \langle \phi_a(\vec{r}) \rangle)(\phi_b(\vec{0}) - \langle \phi_b(\vec{0}) \rangle) \rangle$ can be written as

$$C_{ab}(\vec{r}) = \delta_{ab} \left[C_L(r)\delta_{aN} + C_T(r)(1 - \delta_{aN}) \right] \, . \tag{2.84}$$

a and b label the components in the N-dimensional space. C_L is the *longitudinal* correlation (parallel to an infinitesimal applied field that selects the ordering direction) and C_T is the *transverse* (orthogonal to the applied field) one. A simple calculation shows that the longitudinal component behaves just as the correlation in the Ising model. It is a *massive* scalar field. The transverse directions, instead, are massless : there is no restoring force to the tilt of the full system. These components behave just as the angle in the XY model, $C_T(\vec{r}) \sim r^{2-d}$ (the power law decay becomes a logarithm in $d = 2$). These are called *Goldstone modes* (in the field theory literature the name 'Goldstone modes' is sometimes restricted to the massless excitations about a non-zero order parameter, *i.e.* when there is spontaneous symmetry breaking).

2.7.4 The Mermin-Wagner theorem

What happens in $d = 2$ and below ? Indeed, the logarithmic behaviour of the angle correlation function in the XY model or the transverse correlation in the generic $O(N)$ model is a signature of the fact that this is a special dimensionality. The *Mermin-Wagner theorem* states that for any system with short-range interactions there is a *lower critical dimension* below which no spontaneous broken symmetry can exist at finite temperature. In other words, fluctuations are so large that any ordering that breaks a continuous symmetry is destroyed by thermal fluctuations. $d_L = 1$ for discrete symmetries and $d_L = 2$

for continuous symmetries. [3] The absence of long-range order in the $2d$ XY case, for example, is demonstrated by the fact that the finite temperature correlation decays to zero at long distances – albeit as a power law – and thus there is no net magnetization in the system.

The Mermin-Wagner theorem is known as Coleman-Weinberg theorem/result in quantum field theory for particle physics.

2.8 The Higgs mechanism

A particular feature of models with continuous symmetry breaking in gauge theories is that gauge fields acquire a mass through the process of spontaneous symmetry breaking. Take the classical Abelian field theory

$$\mathcal{L}[A_\mu, \phi] = \int d^d r \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + (D_\mu \phi)^* (D^\mu \phi) + V(\phi) \right] \tag{2.85}$$

with $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, $D_\mu = \partial_\mu + ieA_\mu$ and ϕ a complex field that is to say a field with two independent components (ϕ_R, ϕ_I). The potential is

$$V(\phi) = \mu(\phi^*\phi) + \frac{\lambda}{4}(\phi^*\phi)^2 \, . \tag{2.86}$$

$\mathcal{L}$ is invariant under any global rotation of the complex field, $\phi \to e^{i\epsilon}\phi$ with ϵ real (U(1) symmetry) and local gauge transformation

$$\begin{aligned} \phi(\vec{x}) &\to e^{-i\epsilon(\vec{x})}\phi(\vec{x}) \\ \phi^*(\vec{x}) &\to e^{i\epsilon(\vec{x})}\phi^*(\vec{x}) \\ A_\mu(\vec{x}) &\to A_\mu(\vec{x}) + \partial_\mu \epsilon(\vec{x}) \, . \end{aligned} \tag{2.87}$$

Let us forget about the gauge field for a moment and look for static and uniform configurations that render V minimum. If $\mu > 0$ and $\lambda > 0$ the only solution is $\phi_0 = 0$ and it is invariant under the transformation $\phi_0 \to e^{i\epsilon}\phi_0 = 0$. Instead, if $\mu < 0$ and $\lambda > 0$ the ϕ configuration that renders V minimum is such that $\phi_0^*\phi_0 = -2\mu/\lambda$. V has a continuum of minima lying on a circle of radius $\sqrt{-2\mu/\lambda}$. Any such minima is not invariant under global rotation by an angle ϵ. This is called an *spontaneously broken U(1) symmetry*.

Without loss of generality one can choose ϕ_0 to be real through a uniform rotation over all space. It is easy to verify that replacing ϕ by $(\phi_0 + \delta\phi) + i\phi_2$ where ϕ_2 is an

[3] The fact that d_L is smaller for continuous than for discrete symmetries is due to the fact that it is easier to create interfaces in the latter than in the former and hence to destroy the ordered phase. Indeed, in a continuous spin model the cost of an interface is proportional to its surface divided by its thickness (note that spins can smoothly rotate from site to site to create a thick interface). The thickness of the interface depends on the details of the model, temperature, *etc.* This means that interfaces are much easier to create in continuous spin models than in discrete ones.

	Ising $d=1$	Ising $d>1$	XY $d=2$	XY $d>2$
T_c	$=0$	>0	$=T_{KT}>0$	>0
$\langle\vec{\phi}\rangle$ at $T\leq T_c$	1	$\neq 0$	$\vec{0}$	$\neq\vec{0}$
Fluctuations		droplets	Pairs of vortices	Goldstone modes $\perp\langle\vec{\phi}\rangle$

imaginary part (playing the role of the transverse components in the analysis of the $O(N)$ model) one finds that the quadratic Lagrangian does not have a ϕ^2 term (massless field) but instead a quadratic term in A appears. The gauge field acquired a mass (there is also a $A_\mu\partial^\mu\phi_2$ term that can be eliminated with a change of variables).

This phenomenon has been discovered in the study of superconductors, in particular by P. W. Anderson, and later used in the context of particle physics by Brout, Englert and Higgs.

2.9 Comments

Note that all the features we have discussed)phase transitions, spontaneous symmetry breaking, Goldstone modes, HIggs mechanisms, etc.) have been found in classical statistical physics and hence they are not due to quantum mechanics.

2.10 Towards an understanding of critical phenomena

The rest of the discussion will focus on second order phase transitions for which the order parameter smoothly departs from zero when entering the ordered phase.

2.10.1 Critical exponents and universality

When studying the observables close to the critical point one realizes that they depend on the distance from the critical point in the form of power laws

$$X\sim\theta^n \tag{2.88}$$

where X is the observable, θ the distance to criticality and n the exponent. It is clear that this and the other exponents measure the *strength* of the singularity at the critical point in the sense that all derivatives $d^mX/d\theta^m$ with $m>n$ diverge and the smaller n the sooner this happens.

For instance, in zero field the order parameter increases as

$$m\sim(T_c-T)^\beta\ . \tag{2.89}$$

At T_c and as a function of the conjugate field it behaves as

$$m\sim h^{1/\delta}\ . \tag{2.90}$$

The divergence of the linear susceptibility at T_c is characterized by two exponents

$$\chi \sim \begin{cases} (T-T_c)^{-\gamma} & T > T_c \ , \\ (T_c-T)^{-\gamma'} & T < T_c \ . \end{cases} \tag{2.91}$$

The specif heat also diverges at T_c :

$$C_V \sim \begin{cases} (T-T_c)^{-\alpha} & T > T_c \ , \\ (T_c-T)^{-\alpha'} & T < T_c \ . \end{cases} \tag{2.92}$$

While the values of T_c are material dependent, all ferromagnetic transitions of systems in $d = 3$ with an order parameter of the same dimensionality can be described by the same – within error bars – critical exponent ! This feature indicates the existence of *universality classes*, *i.e.* groups of systems for which the details of the microscopic interactions do not matter and whose macroscopic critical behavior is identical.

It is simple to compute the exponents in the naive mean-field approximation for any d or for the fully connected model with $p = 2$. They read

$$\alpha = 0 \ , \qquad \beta = \frac{1}{2} \ , \qquad \gamma = 1 \ , \qquad \delta = 3 \ , \qquad \eta = 0 \ , \qquad \nu = \frac{1}{2} \ , \tag{2.93}$$

and they are independent of d. η and ν are exponents characterizing the correlation function and the correlation length that we define in (2.96) and (2.53). These values are to be confronted to the experimental values. In ferromagnetic phase transitions with Ising symmetry they are

d	β	α	γ	δ	ν	η	
2	1/8	0	7/4	15	1	1/4	exact
3	0.325	0.11	1.24	4.82	0.63	0.032	approx

TAB. 2 – Critical exponents in the Ising universality class.

The fact that very different systems share the same critical properties, the mere existence of universality classes, suggested that it should be possible to describe critical behavior of all these systems with a very general framework. The fact that the mean-field critical exponents were slightly different from the ones observed was not very important as a quantitative disagreement but it was from a fundamental point of view. Something important was going on and needed an explanation.

In the rest of this Subsection we introduce and discuss the concepts that allowed one to acquire a qualitative and quantitative understanding of critical phenomena. The ideas and methods introduced actually go beyond this problem and have been exported to other situations like dynamical processes in and out of equilibrium (see Sects. 2.10.5 and 4.3.3).

2.10.2 Scaling

Scaling concepts are fundamental in describing the behaviour of systems made of a large number of constituents, interacting non-linearly and according to laws that are sometimes poorly understood. The idea is to isolate a few relevant variables that characterize the behaviour at a certain length and time scale and to postulate simple *scaling relations* between them. When there is only one independent variable, the scaling relations take the form of power laws with exponents that are not rational numbers.

Systems that may be microscopically very different but share the same scaling relations belong to the same *universality class*.

Scaling arguments apply to many different physical situations (in and out of equilibrium) and they can be explained using *renormalization* ideas. In most cases, the renormalization approach does not have a formal basis yet. It is in the context of critical phenomena in equilibrium that scaling and renormalization can be derived systematically.

Phenomenological relations

In the discussion of critical phenomena we have defined 6 critical exponents (α for the specific heat, β for the order parameter, γ for the susceptibility, δ for the order parameter at the critical point as a function of the conjugate field, η for the correlation function and ν for the correlation length). But, actually, not all these exponents are independent. It was soon observed that the experimental data pointed to simple relations between the exponents, and one example is the *Rushbrooke scaling law*

$$\alpha + 2\beta + \gamma = 2 \; . \tag{2.94}$$

Let us first take a practical viewpoint and discuss a way to collapse data close to a critical point, a property closely related to scaling. The power law expressions (2.89) and (2.90) suggest *Widom scaling* for the order parameter :

$$m(t,h) \sim |t|^{\beta} \; \Phi_{\pm}\left(\frac{h}{|t|^{\beta\delta}}\right) \qquad t \equiv \frac{|T-T_c|}{T_c} \; , \tag{2.95}$$

with $\Phi_{\pm}(0) = 1$ and $\Phi_{\pm}(x \to \infty) \sim x^{1/\delta}$. With these limits, (2.90) is recovered on the critical isotherm and (2.89) follows at strictly zero field and for $|t| \ll 1$. An example of *data collapse* is given in Fig. 8.

Surprisingly enough, *all* systems undergoing a ferromagnetic transition can be *scaled* in this way using the *same* functions $\Phi_{\pm}$ above and below the critical temperature, respectively ! The way of checking this hypothesis is by plotting $m/|t|^{\beta}$ against $|h|/|t|^{\beta\delta}$ for different systems and looking for *data collapse*. Of course, we do not know the values of the universal exponents β and δ and the material dependent critical temperature T_c *a priori*, so we need to manipulate a bit the data before obtaining collapse. Note that the scaling law (2.95) is independent of the dimension d.

Scaling relations that involve the dimension are called *hyperscaling*. Again, it was phenomenologically observed that the correlation function satisfies

$$G(\vec{r};t,h) = \frac{1}{r^{d-2+\eta}}\, g\left(r|t|^{\nu}, \frac{h}{|t|^{\beta\delta}}\right) . \tag{2.96}$$

It is interesting to note that scaling holds on a much wider window than the power law expressions defining the critical exponents.

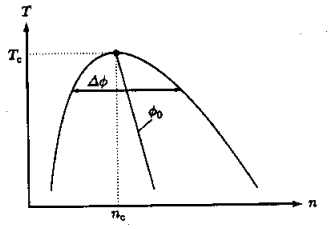

Fig. 4.4.3. Schematic phase boundary for the liquid-gas transition showing the asymmetry of the order parameter about the critical density.

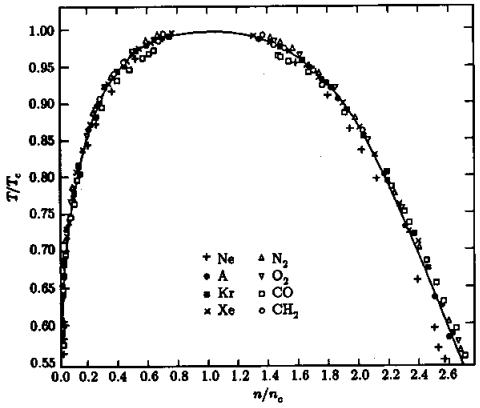

Fig. 4.4.4. Phase boundary in units of reduced temperature and density for eight different molecular fluids near their liquid-gas transitions. Note the universal behavior and the fact that the solid line is $\Delta\phi \propto (T_c - T)^{\beta}$ with $\beta = 1/3$ rather than the mean-field result $\beta = 1/2$. [E.A. Guggenheim, *J. Chem. Phys.* **13**, 253 (1945).]

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FIG. 8 – Critical scaling in gas-liquid transitions at constant pressure. At very low density and low temperature, at the left of the curve the system is a gas, at very large density and still low temperature, at the right of the curve the system is a liquid. In the region below the curve there is coexistence of gas and liquid. Above the curve the system goes continuously from a gas to a liquid when increasing the density. The critical line behaves as $|\rho_l - \rho_g| \sim |T - T_c|^{\beta}$ with $\beta \sim 0.327$ close to the maximum. Note that scaling holds as far as $T/T_c \sim 0.55$!

Scale invariance

Kadanoff proposed that this quite incredible feature could be explained assuming that near a critical point a system looks the same at all length scales. This is called *scale*

invariance. More precisely, he showed that a diverging correlation length *implies* (under some more or less mild assumptions) the scaling hypothesis, the ensuing scaling laws postulated by Widom and the relations between critical exponents.

The idea is the following : take an Ising model in equilibrium at temperature T. Since the system has a correlation length $\xi(T)$, spins lying on a region of linear size $\ell a \ll \xi$ are strongly correlated and, basically, act as a single unit. One can then define $N' = N\ell^{-d}$ *block spins*,

$$s_I \equiv |m_\ell|^{-1}\ell^{-d}\sum_{i\in B_I} s_i \ , \qquad m_\ell \equiv \ell^{-d}\sum_{i\in B_I}\langle\, s_i\,\rangle \ , \tag{2.97}$$

and these lie on a lattice with lattice spacing $a' = a\ell$. Kadanoff then *assumed* that the original Hamiltonian when written in terms of block spins keeps the same functional form though with modified coupling constants

$$-\beta H_\ell \equiv K_\ell \sum_{\langle\, IJ\,\rangle} s_I s_J + h_\ell \sum_I s_I \tag{2.98}$$

with $K \equiv \beta J$ and $h = \beta H$ (an assumption that is correct for the chain – see below – but is incorrect in general). This means that the coupling constants vary with the observation scale.

The correlation length in absolute units clearly remains unchanged under the change of variables. However, if one measures it in units of the lattice spacing, it turns out that the one for the block spin system is significantly reduced with respect to the original one :

$$\xi = \xi_\ell(\ell a) = \xi_1 a \ , \qquad \Rightarrow \qquad \xi_\ell = \xi_1\ell^{-1} < \xi_1 \ . \tag{2.99}$$

Thus, one can interpret the block spin system as being farther away from criticality and at a new reduced temperature t_ℓ. A simple calculation shows that the magnetic field transforms as $h_\ell = hm_\ell\ell^d$.

Equation (2.98) implies the following relation between the total free-enegies of the block spin and original systems :

$$F(t_\ell, h_\ell) = N\ell^{-d} f(t_\ell, h_\ell) = F(t, h) = N f(t, h) \ . \tag{2.100}$$

Within this approach we still do not know how the reduced temperature and external field transform. If one now *assumes* a power law dependence on the scale :

$$t_\ell = t\ell^{y_t} \ , \qquad h_\ell = h\ell^{y_h} \ , \tag{2.101}$$

with $y_t > 0$ and $y_h > 0$ (the renormalization group does indeed allow one to compute this changes) then

$$f(t, h) = \ell^{-d} f(t\ell^{y_t}, h\ell^{y_h}) \ . \tag{2.102}$$

Upto now nothing fixes the block scale ℓ and we can then choose it at will ; taking $\ell = |t|^{-1/y_t}$ and defining $\Delta = y_h/y_t$ and $2 - \alpha \equiv d/y_t$, one is simply left with

$$f(t, h) = |t|^{2-\alpha} F_f(h/|t|^\Delta) \ . \tag{2.103}$$

From this scaling form of the free-energy density one can derive the scaling relations and the relations between the exponents characterizing the thermodynamic observables and correlation functions.

This argument justifies the scaling relations but it has one flaw, the fact that one can easily verify that the assumption in (2.98) does not hold in general, and a deficiency, that is that the method does not provide a way to calculate the critical exponents or justify universality. These two problems are solved by the renormalization group.

An example : the Ising chain

Before introducing the renormalization group, let us discuss one example where the coarse-graining procedure can be done exactly, again the one dimensional Ising model with N (even) spins in the absence of an applied field. The partition function reads

$$Z(N,J) = \sum_{s_i=\pm 1} e^{\beta J \sum_{i=1}^{N-1} s_i s_{i+1}} \tag{2.104}$$

We shall call $K \equiv \beta J$. The sum in the exponential is

$$s_1 s_2 + s_2 s_3 + s_3 s_4 + s_4 s_5 + \dots \tag{2.105}$$

It is clear that s_2 enters only in the first two terms, s_4 enters only on the third and forth term and so on and so forth. One can then sum over all configurations of the spins with an even label. For example, the sum over $s_2 = \pm 1$ yields

$$e^{K(s_1+s_3)} + e^{-K(s_1+s_3)} \ . \tag{2.106}$$

One then obtains :

$$Z(N,K) = \sum_{s_i=\pm 1; i\ odd} \prod_{i=1}^{N-1} [e^{K(s_i+s_{i+2})} + e^{-K(s_i+s_{i+2})}] \tag{2.107}$$

If we find a function $\kappa(K)$ and a new coupling constant K' such that each of these terms can be written as

$$e^{K(s_i+s_{i+2})} + e^{-K(s_i+s_{i+2})} = \kappa(K) e^{K' s_i s_{i+2}} \ , \tag{2.108}$$

the right-hand-side in eq. (2.107) would be proportional to the partition function of another one dimensional Ising model with $N/2$ spins and a different coupling constant K' :

$$Z(N,K) = \kappa(K)^{N/2} Z(N/2, K') \ . \tag{2.109}$$

Indeed, the solution to (2.108) can be easily found ; it is enough to consider all the cases $s_i = \pm 1$ and $s_{i+2} = \pm 1$ to obtain :

$$K' = \frac{1}{2} \ln \cosh(2K) \ , \tag{2.110}$$

$$\kappa(K) = 2 \cosh^{1/2}(2K) \ . \tag{2.111}$$

Now, we know that the free-energy, and in particular $\ln Z$, should be linear in N ;

$$-\beta F(N,K) = \ln Z(N,K) = N\zeta(K) \ . \tag{2.112}$$

Thus, taking the ln of eq. (2.114) and using (2.112)

$$\ln Z(N,K) = \frac{N}{2}\ln\kappa(K) + \ln Z(N/2,K') \ , \tag{2.113}$$

$$\zeta(K) = \frac{1}{2}\ln\kappa(K) + \frac{1}{2}\zeta(K') \ . \tag{2.114}$$

or equivalently

$$\zeta(K') = -\ln[2\cosh^{1/2}(2K) + 2\zeta(K)] \tag{2.115}$$

Inserting a value of K on the right-hand-side one obtains the new coupling constant K' and the new free-energy $\zeta(K')$.

Equations (2.110) and (2.115) provide recursion relations for the coupling constant and the partition function. Note that K' is always smaller than K. One can also solve for K as a function of K' :

$$K = \frac{1}{2}\cosh^{-1}(e^{2K'}) \tag{2.116}$$

$$\zeta(K) = \frac{1}{2}\ln 2 + \frac{1}{2}K' + \frac{1}{2}\zeta(K') \ , \tag{2.117}$$

obtaining now an increasing flow $K(K')$.

One can use these results to compute the value of the partition function for any K. The argument goes as follows. For very small K', *i.e.* very high temperature, the spins are basically independent and $Z(K') \sim 2^N$ and $\zeta(K') = \ln 2$. Using then (2.116) and (2.117) one computes K and $\zeta(K)$. One then iterates using these values as starting points K' and $\zeta(K')$. The agreement between the values generated this way and the results of the exact calculation are quite amazing (see, *e.g* [21]).

The process described in the previous paragraph is a *flow* in the space of parameters. Starting from any non-zero value of the coupling constant the iteration converges to $K = 0$. There are then two *fixed points*, a *stable fixed point* at $K = 0$ or infinite temperature (to which trajectories are attracted) and an *unstable fixed point* $K \to \infty$ or zero temperature from which trajectories depart. The stable fixed point represents the high temperature paramagnetic phase while the unstable fixed point is the critical $T = 0$ point. The critical behavior can be obtained from the dependence of $\zeta(K)$ on the parameter $K - K_c$.

A similar procedure can be applied to the $d = 2$ problem. In this case, however, the *decimation* of spins cannot be done exactly and one is forced to use some approximation. There are a number of successful recipes in the literature.

2.10.3 The renormalization group

The development of the renormalization group by K. Wilson in the early 70s gave a totally new way of understanding condensed-matter and particle physics phenomena. He transformed the picture of phase transitions that developed in the 60s – with the understanding of concepts like scaling, universality and correlations – into a calculational tool and got the Nobel Prize in Physics in 1982.

The renormalization group is ingeneered in such a way to explain how short-range couplings generate a collective phenomenon observable at *all* length scales. It relates different scales making the expected scale invariance appear. The method is general and it does not rely on a special model, being thus adapted to treat very different models with similar global behaviour, the *universality* property.

The procedure

The renormalization group procedure is based on the construction of block spins. First, take the system with N spins, say a cubic lattice of linear size L, and divide it in blocks of linear size ℓ. Define $N' = N\ell^{-d}$ coarse-grained spin variables using, for example, (2.97). Rescale the distance between the coarse-grained spins, that occupy the centers of the blocks, from ℓa to a, a being the original lattice spacing.

Compute the Hamiltonian by expressing the original energy in terms of the coarse-grained variables. If new terms are generated through the coarse-graing argue that they are either irrelavant, that is to say, they become less and less important after successive iteration of the coarse-graining, or that only a few such new terms are generated. Collect all the coupling constants in $[K] = (K_1, \ldots, K_n)$ and follow their renormalization, $[K'] = R_\ell[K]$, calling R_ℓ the renormalization tranformation using a coarse-graining scale ℓ.

The new coupling constants, $[K]$, and the correlation length, ξ, become functions of the previous ones

$$[K'] = R_\ell[K] \,, \qquad \xi([K']) = \xi([K])/ell \,. \tag{2.118}$$

With each iteration we are observing the system at a new scale – the scale of the blocks instead of the original one – and we are deriving the effective energy that describes the system at this scale. The flow generated in this way – in the space of models that translates into the space of parameters once new terms in the energy are no longer generated – approaches a fixed point that represents the critical point. At the critical point the renormalization procedure must reach a stable fixed point

$$[K'^*] = R_\ell[K^*] = [K^*] \,, \qquad \xi^* \equiv \xi([K^*]) = \xi([K^*])/\ell \,. \tag{2.119}$$

The latter equation can be satisfied by

$$\xi^* = 0 \,, \qquad \text{or} \qquad \xi^* \to \infty \tag{2.120}$$

only. The former is called a *trivial* and the *latter* a critical fixed point.

Critical behaviour is given by the behaviour of the trajectories in parameter space close to the fixed points. Let us illustrate this with an example. Take a system that depends on

a single parameter, say temperature, T. Linearizing the RG transformation close to the fixed point T^* leads to

$$T' - T^* = R_\ell T - R_\ell T^* \sim \Lambda_e ll(T - T^*) + O((T - T^*)^2) \tag{2.121}$$

where

$$\Lambda_\ell \equiv \left.\frac{\partial R_\ell}{\partial T}\right|_{T^*} \tag{2.122}$$

Since one expects that the renormalization transformations compose in such a way that coarsening at distance $\ell\ell'$ can be achieved by coarsening first at distance ℓ' and then at distance ℓ, one must have $\Delta_{\ell\ell'} = \Delta_\ell \Delta_{\ell'}$ and thus $\Delta_\ell = \ell^{y_t}$. Defining the reduced temperature t as usual, $t = (T - T^*)/T^*$, (2.121) becomes $t' = t\ell^{y_t}$ and after n such iterations, $t^{(n)} = t(\ell^{y_t})^n$. Now, to make contact with the critical exponents, let us study the evolution of the correlation length :

$$\xi(t^{(n)}) = \ell^{-n}\xi(t) = \xi(t\ell^{ny_t}) \tag{2.123}$$

ℓ is still arbitrary. Choosing $\ell^n = (b/t)^{1/y_t}$ with $b \gg 1$,

$$\xi(t) = (bt^{-1})^{-1/y_t}\xi(b) \sim t^{-1/y_t} \tag{2.124}$$

If $t > 0$, $\xi(b)$ is the correlation length at very high temperature and it does take some finite small value. Since $\xi(t) \sim t^{-\nu}$, from the definition of the critical exponent ν, one has

$$\nu = 1/y_t = \ell^{-1} \ln \Lambda_\ell = \ell^{-1} \ln \left.\frac{\partial R_\ell}{\partial T}\right|_{T^*} . \tag{2.125}$$

This procedure can be applied to compute the free-energy close to the fixed point and from it other critical exponents, *etc.*

Note that the renormalization procedure reduces finite size effects since at each step of the iteration ξ is reduced while the lattice spacing is maintained.

2.10.4 Finite size effects

A real system is large but finite, $1 \ll N_A \sim 10^{23} < \infty$. Finite size effects will then play a role in the phase transition that is rounded by the fact that $N_A < \infty$. Finite size effects become important when $\xi \sim L$, the linear size of the system, say $L \sim 1$cm for an actual sample. A rough estimation of how close to T_c one needs to get to see deviations from critical scaling shows that finite size effects are quite negligible in experiments but are certainly not in numerical simulations and have to be taken into account very carefully when trying to compare numerical data to analytical predictions.

Finite size effects are taken into account by introducing correcting factors in the scaling laws, for example,

$$\chi_L \sim |t|^{-\gamma} g\left(\frac{L}{\xi}\right) \tag{2.126}$$

with $g(x \to \infty) \to 1$ and $g(x \to 0) \to x^{\gamma/\nu}$.

Note that periodic boundary conditions suppress boundary effects and then reduces finite size effects.

2.10.5 Fluctuations of macroscopic observables

A direct consequence of having a diverging correlations length is that the critical measure-to-measure fluctuationf of global observables like, for instance, the magnetization density, are not Gaussian. The reason is simple, if $L < \xi$, a global measurement is not the result of an average over many uncorrelated regions and, thus, one cannot use the central limit theorem to argue for a normal distribution of fluctuations. Recently, the study of critical fluctuations of macroscopic observables received much attention. The best adapted model for this analysis is the $2d$ XY model, that is critical on a finite interval of temperatures (and not only at a single precise value of T_c) [41]. This model, in the so-called spin-wave approximation, is mapped onto an interface model, the Edwards-Wilkinson one [**?**]

In the limit we are now interested in L is finite with respect to ξ and finite size effects are important. *Finite size scaling* implies

$$p_L(M) = L^{\beta/\nu}\, \Pi\left(ML^{\beta/\nu}, \frac{\xi}{L} \right) \ . \tag{2.127}$$

3 Statistical analysis of cosmic structures

Cosmology aims at discribing the Universe at its largest scales. As it is well-known the Universe has structures of very different types and sizes. Tools from Statistical Mechanics have been used to describe them at different levels.

A first description of this problem can be purely *statistical*, in the sense that one can be interested in performing a statistical analysis of the structures, mass distributions, observed without discussing the physical mechanisms that lead to them. This is the kind of approach followed in the description of any stochastic signal. Some questions one can then ask at this level of description are :

- What is the present mass distribution ?
- What was the mass distribution in the distant past ?

This kind of analysis turns out to be intimately related to the discussion on phase transitions presented in Sect. . Indeed, the analysis of the mass density and its fluctuations is very similar to the analysis of the order parameter. Concepts such as correlation lengths and fractals naturaly appear.

Another, perhaps more interesting, level of description is to try to understand how a self-gravitating system, with long-range interactions, can be thermodynamically stable. (This takes us back to the first Section where we discussed the statistical mechanics of systems with long-range interactions.) Another way of posing this question is

- What determines the particular configuration into which a self-gravitating system settles ?

This is the *statistical mechanics* point of view. Chadrasekhar proposed that these are simply dictated by a *maximum entropy* principle, that is to say, that they are most probable than any other configuration.

Finally, one can be interested in dynamics and wonder

- How can one obtain the present mass distribution from the evolution of an initial one ?

Choosing a 'correct' initial mass distribution one can then see the formation of structures by integrating (for example numerically) the equations of motion. However, this is not so simple conceptually since one has to be careful, in this case, and take into account *relativistic effects*. The causal limit essential to any Big Bang model implies that there is a finite horizon for causal processes i.e. light can travel only a finite distance in the time since the Big Bang. Using this limit Zeldovich [12] showed that there is a strong constraint on the power spectrum (i.e. what is usually called the structure factor in statistical physics) describing mass fluctuations. It states that if fluctuations are built, starting from a uniform distribution of matter, by causal physics (i.e. physical processes moving matter and momentum coherently up to a maximal scale), then the small k form of the power spectrum is $P(k) \propto k^4$. The importance of this argument is in its corollaries : it implies

that the spectrum considered to correctly describe the perturbations at very large scales observed [13] in the microwave background, $P(k) \sim k$, cannot be produced by causal physics acting prior to the time when radiation decouples from matter. And it is one of the motivations for and successes of the popular *inflation model* that it can produce such fluctuations (by modifying the causal structure of the Big Bang model at early times).

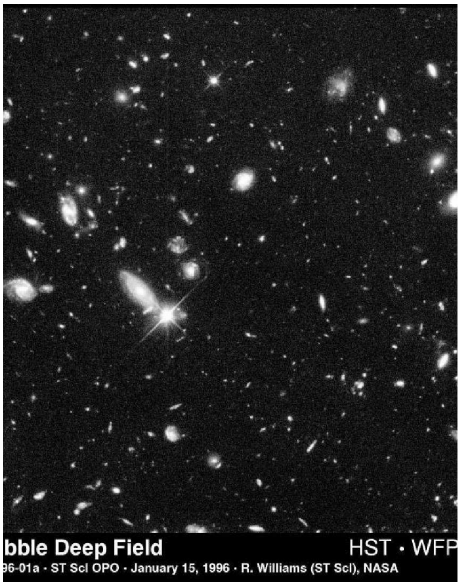

FIG. 9 – Large-scale structures in the universe as observed with the Hubble space telescope.

3.1 Statistical methods

We focus here on the first kind of description given in the introduction, the one that is borrowed from the analysis of generic stochastic signals.

We shall present two types of methods : one group are intended to describe mass distributions with small amplitude fluctuations about a finite average ; another group treats mass distributions that are extremely irregular with an average that vanishes in the infinite volume limit.

Take an electromagnetic signal with noise, the density of a fluid in thermal equilibrium, the value of an asset in the stock market, etc. All these quantities fluctuate either in space and/or in time. The average over a large spatial region or a very long time window takes a finite value that remains finite for larger and/or longer sampling. A number of statistical tools that serve to characterise such fluctuations are well documented. We shall describe here the most important ones.

Let us focus on time-independent quantities first. We distinguish different types of stochastic processes :

- *Continuous stochastic processes* such that the stochastic field is continuous on space and can take, in general positive and negative values. The density of a fluid in thermal equilibrium is an example (though positive definite).
- *A point process* such as a distribution of point mass particles. In this case the stochastic field is discontinuous. This problem can be rendered smooth by applying a coarse-graining over a length ℓ, in the manner described in Sect. 2.6.3. When $\ell \gg a$ with a the typical interparticle separation the coarse-grained field becomes continuous and of the kind introduced in the previous item.
- Point distributions giving rise to *fractal measures*. In these cases the average mass density vanishes in the infinite volume limit. The volume is asymptotically empty. Taking an arbitrary occupied point in space the averaged density decays slowly as a power of distance.

First, we review the definition of a space-dependent stochastic field (the generalization to a space and time dependent field is straightforward). Take a d-dimentional volume V and partition it into $i = 1, \ldots, N$ cells of volume dv ($V = Ndv$), that is to say, think about a d dimensional lattice. A random field $\phi(\vec{r})$ characterized by its probability density function (pdf) $P[\phi(\vec{x})]$ is such that on each cell a value of ϕ is drawn from P. The function P can be interpreted as the joint pdf of the random variables ϕ on each cell.

A random field is said to be *continuous* if

$$\lim_{\Delta \to 0} \langle\, |\phi(\vec{r} + \vec{\Delta}) - \phi(\vec{r})|^2 \,\rangle = 0 \qquad \forall \vec{r}\,. \tag{3.1}$$

The angular brackets indicate here and in the rest of this Section the average over $P[\phi(\vec{r})]$.

A *stationary, statistically translational invariant* or *statistically homogenous* stochastic field is such that its statistical properties do not depend on the spatial location studied. More precisely, taking n points $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n$, the joint probability distribution of the value of the random field at the translated points $\vec{x}_1 + \vec{\Delta}, \vec{x}_2 + \vec{\Delta}, \ldots, \vec{x}_n + \vec{\Delta}$ does not depend on the translation vectors $\vec{\Delta}$:

$$P[\phi(\vec{x}_1 + \vec{\Delta}), \phi(\vec{x}_2 + \vec{\Delta}), \ldots, \phi(\vec{x}_n + \vec{\Delta})] = P[\phi(\vec{x}_1), \phi(\vec{x}_2), \ldots, \phi(\vec{x}_n)]\,. \tag{3.2}$$

This means that it depends only on the relative distance between the selected points, $\vec{x}_1 - \vec{x}_2$, *etc.*

A *statistical rotational invariant* or *isotropic* stochastic field is such that its statistical properties do not depend on the direction observed, that is to say, $P[\phi(\vec{x})]$ is also invariant under rotations.

In the **cosmological** context the last two properties are ensured by the **cosmological principle** that states that there no preferential points or directions in the universe.

An example of the above, on which we shall focus in this section is given by a mass point distribution. The density field is defined as

$$\phi(\vec{x}) = \sum_{i=1}^{N} m_i\, \delta(\vec{x} - \vec{x}_i) \tag{3.3}$$

where the index $i = 1, \ldots, N$ labels the particles and m_i and $\vec{x}_i$ are the mass and position of the particle i. (In what follows we assume that particles are separated by a distance that is longer than an infinitesimal dx.)

Having a stochastic field defined by its pdf one can now compute all interesting averaged quantities, *e.g.* average, mean-square displacement, moments, *etc.* The *average* of a stationary stochastic field is just

$$\langle\, \phi(\vec{x})\, \rangle = \phi_0 \ . \tag{3.4}$$

ϕ_0 is independent of the position $\vec{x}$. When $\phi_0 > 0$ the field is called *homogenoeus* and all the machinery of usual studies of random variables applies. Instead, when $\phi_0 = 0$ one faces a new situation to be discussed below.

In the generic context of a space-dependent stochastic process one can define *ergodicity* as

$$\langle\, F[\phi(\vec{x}_1), \ldots, \phi(\vec{x}_n)]\, \rangle = \lim_{V\to\infty} \int_V d^d y\ F[\phi(\vec{x}_1 + \vec{y}), \ldots, \phi(\vec{x}_n + \vec{y})] \tag{3.5}$$

(to be compared with the discussion in Sect.). F is a generic functional of the random field and ϕ is almost any realization of it. Ergodicity can be proven for some continuous stochastic fields but it is not valid in full generality. Note that if the integral runs over only a subvolume then the right-hand-side is just an estimator of the left-hand-side. In **cosmological** application it is clear that one is forced to make observations over partial volumes of the universe.

The *homogeneity scale*, λ, is the length scale above which the partial space average gets sufficiently close to the 'theoretical value' for the average of the stochastic field (computed with its pdf), ϕ_0 :

$$\left| \frac{1}{v} \int_v d^3x\ \phi(\vec{x}) - \phi_0 \right| < \phi_0 \qquad \forall R > \lambda \ , \ \ \forall \vec{x} \ , \tag{3.6}$$

with $v = 4\pi R^3/3$. At smaller scales than λ the fluctuations are important and the partial average deviates substantially from ϕ_0.

3.1.1 Correlation functions and correlation length

The n-point *correlation function* is defined as

$$c_n(\vec{x}_1, \ldots, \vec{x}_n) \equiv \langle\, \phi(\vec{x}_1), \ldots, \phi(\vec{x}_n)\, \rangle \ . \tag{3.7}$$

The stationary property of the process ensures that c_n depends only on the relative distances $|\vec{x}_1 - \vec{x}_2|$, *etc.*

The *reduced* n-point *correlation function* is defined as

$$C_n(\vec{x}_1, \ldots, \vec{x}_n) \equiv \langle\, (\phi(\vec{x}_1) - \phi_0) \ldots (\phi(\vec{x}_n) - \phi_0)\, \rangle \ . \tag{3.8}$$

These correlation functions measure the spatial memory of the *fluctuations* of the random field at the scales given by the distance between the selected spatial points. For $n = 1, 2$ the reduced correlation functions coincide with the connected ones.

In the case of a stochastic field with a positive average value ϕ_0. One can render the correlation functions defined above *adimensional* by dividing by ϕ_0^n.

As in any stochastic process one can also study the *cumulant expansion*.

A *correlation length* is introduced in analogy with the concept discussed in the context of second order phase transitions (see Sect. 2.6.3). Several definitions exist and they all lead to the same qualitative behaviour. We shall adopt the following

$$\xi^2 \equiv \frac{\int d^d x \; x^2 \; |C_2(x)|}{\int d^d x \; |C_2(x)|} \; . \tag{3.9}$$

The correlation length serves to distinguish reduced correlations decaying slowly from those decaying fast with distance x :

– *Slow algebraic decay – long-range correlations :*

$$C_2(x) \sim x^{-\gamma} \qquad \text{with} \qquad 0 < \gamma < d \tag{3.10}$$

at sufficiently large x. These correlations characterize the order parameter fluctuations at second order critical points. The slow decay of the correlation at long distances implies that the correlation length defined in (3.9) diverges :

$$\xi \to \infty \; . \tag{3.11}$$

– *Exponential decay – short-range correlations :*

$$C_2(x) \sim e^{-x/x^*} \; , \tag{3.12}$$

again at sufficiently large x. This is the behaviour of the order parameter fluctuations far away from a critical point (both in the ordered and disordered phases). The correlation length is finite in this case

$$\xi \sim x^* \; . \tag{3.13}$$

A fast algebraic decay ($\gamma > d$) belongs to this class.

As in critical phenomena, the coarse-grained field over a length ℓ larger than ξ ($\ell \gg \xi$) becomes a Gaussian variable while coarse-graining over a shorter length ($\ell \ll \xi$) does not have an important effect and the coarse-grained field keeps a strong memory of its original pdf.

Note that these definitions of short and long range correlations are identical to the ones discussed in Sect. when studying short and long range interactions.

3.1.2 The power spectrum

The analysis of a stochastic process limited to the two-point correlation function (reduced or not) can be expressed in transformed Fourier space through the introduction of the *power spectrum* (PS), *structure factor*, or *Bartlett spectrum*, $S(\vec{k})$:

$$S(\vec{k}) \equiv \frac{\langle\, |\delta\phi(\vec{k})|^2 \,\rangle}{V} \tag{3.14}$$

where the angular brackets are the usual ensemble average. If the stochastic process is isotropic one has $S(\vec{k}) = S(k)$. In a stationary and ergodic stochastic process the PS is simply related to the connected correlation. Indeed, using first ergodicity and then stationarity

$$S(\vec{k}) = \frac{1}{V}\int_V d^dx \int_V d^dx' \,\langle\, \delta\phi(\vec{x})\delta\phi(\vec{x}') \,\rangle\, e^{-i\vec{k}(\vec{x}-\vec{x}')} = \int d^dx \; C_2(\vec{x})\, e^{-i\vec{k}\vec{x}} \;. \tag{3.15}$$

Conversely $C_2(\vec{x})$ is the inverse Fourier transform of $S(\vec{k})$.

Let us now focus on the isotropic case of interest in **cosmological** applications. The small k behaviour of the power spectrum is intimately related to the variance of mass fluctuations. Without presenting the explicit calculation we simply quote that for

$$P(k) = Ak^n f(k) \;, \tag{3.16}$$

with $f(k)$ a long wave-length cut-off function, for instance, $f(k) = e^{-k/k_c}$ and A a constant, one has

$$\sigma^2(R) \sim \begin{cases} R^{-(d+n)} & \text{for } -d < n < 1 \;, \\ R^{-(d+1)} \ln R & \text{for } n = 1 \;, \\ R^{-(d+1)} & \text{for } n > 1 \;. \end{cases}$$

Therefore one has Super-Poisson statistics for $-d < n < 0$, Poisson-like (k independent) for $n = 0$, sub-Poisson for $n > 0$. The latter plays an important role in cosmological applications since the so-called *Harrison-Zeldovich condition* implies $P(k) \sim k$ at short k and $\sigma^2(R) \sim R^{-4}$ in $d = 3$.

3.1.3 An example : Gaussian continuous stochastic field

The properties of Gaussian random fields have been summarized in Appendix B. These allow us to compute any n-th order correlation function. Indeed, the so-called *Wick theorem* related the expectation value of higher order correlations to sums of products of the two-point correlation functions only. The theorem is, indeed, a rather trivial property of Gaussian integrals that happens to be extremely useful in *perturbation theory* – in any conctext, field theory, equilibrium or non-equilibrium statistical mechanics, *etc.* where one separates the quadratic part of the energy or action and treats the non-quadratic parts perturbatively.

As an example, if a density is characterized by a scalar field $\phi(\vec{x})$ with a Gaussian distribution with a space-independent mean ϕ_0 and a two-point connected correlation $C_2(\vec{x},\vec{y}) = \langle\,(\phi(\vec{x})-\phi_0)(\phi(\vec{y})-\phi_0)\,\rangle$ one has

$$C_{2n}(\vec{x}_1,\vec{x}_2,\dots\vec{x}_{2n}) = \sum C_2(\vec{x}_i,\vec{x}_j)\dots C_2(\vec{x}_k,\vec{x}_l) \tag{3.17}$$

where the sum runs possible ways of linking the $2n$ spatial points in pairs ; and zero for an odd number of points. One can thus easily express all higher order correlations.

3.1.4 Another example : Poisson point process

Take a volume V and divide it into n subvolumes dv, such that $ndv = V$. Place N particles in V. The particle density over the volume V is then $\rho_0 = N/V$. If the subvolumes dv are small enough one can imagine that each of them can be either empty of occupied by a unique particle. This defines a stochastic density field $\rho(\vec{r})$:

$$\rho(\vec{r}) \;=\; \begin{cases} dv^{-1} & \text{with probability} \quad \rho_0 dv \\ 0 & \text{with probability} \quad 1-\rho_0 dv \end{cases}$$

where $\vec{r}$ is the center of the subvolume. Subcells are independent : the occupation of any of them does not influence the occupation or not of another one. In each cell the probability of occupation is given by the binomial distribution.

From the definition of the stocahstic process one now computes any correlation function. For instance

$$\langle\,\rho(\vec{r}_1)\rho(\vec{r}_2)\,\rangle = \begin{cases} \rho_0^2 & \text{if} \quad \vec{r}_1 \neq r_2 \\ \rho_0/dV & \text{if} \quad \vec{r}_1 = r_2 \end{cases}$$

The definition of the correlation length (3.9) yield $\xi = 0$, as expected for a process with no spatial correlations.

The probability of finding M particles with a volume V is the well-known Poisson distribution law

$$P(M) = \frac{\langle\,M\,\rangle^M e^{-\langle\,M\,\rangle}}{M!}\;. \tag{3.18}$$

with $\langle\,M\,\rangle = \rho_0 V$.

The structure factor is simply constant $S(\vec{k}) = \rho_0$. This is also called a *white noise* since every mode $\vec{k}$ has exactly the same weight.

3.2 Fractals

Fractals [42] are complex and irregular structures that appear :

– In termodynamical systems when the controlling parameter is fine tuned to be at the critical point. For instance, clusters of aligned spins at the critical temperature have fractal characteristics.

– In more common structures observed in nature such as coast lines. The fractal properties developed in these systems as the result of a dynamic process.

In the case of mass point distributions we are here interested in one can examine whether these present fractal characteristics too. The statistical analysis presented in the previous Subsection needs to be modified to account for this possibility.

The question then arises as to how to describe a sufficiently irregular structure such that the techinques used to study regular functions do not apply. A number of ne concepts have to be introduced.

The most intuitive way of defining a fractal is through the *mass vs. radius method*. The idea is to sit on an occupied point of the distribution and measure the mass M as a function of the linear size R of an enclosing volume. If the mass scales as

$$\lim_{R\to\infty} M(R) = R^{d_f} \tag{3.19}$$

D usually coincides with more precise definitions of the fractal dimension. One finds $d_f \leq d$, with d the dimension of space (ordinary uniform mass distribution saturate the bound). This definion can be used to study mass distributions from galaxy sureys and $d_f > d$ can be explicitly tested. Note that $M(R)$ is a *conditional probability* since one needs to see the mass distribution from an occupied point.

Since fractals have $d_f < d$ the average density on the infinite voluem limit ($V \to \infty$, $R \to \infty$) vanishes. A fractal set of points is *asymptotically empty*. Equivalently, if one takes an arbitrary point within V and computes $M(R)$ from it one finds a vanishing result ! This implies that only conditional correlation functions of the mass density of a fractal distribution may yield non-vanishing results.

Fractals are characetrised by voids and structures of any legnth scale with no upper cut-off. The mass fluctuations with respect to the mean are independent of the spatial length scale of observation.

Note that a fractal structure may have a finite length cut-off meaning that it might crossover to a homogeneous structure at longer length scales.

We shall not further develop this analysis. The interested student can look at the classical reference [42] or [25, 26] in the context of the analysis of galaxy structures.

3.3 Dynamics

A problem of current interest in this field is to generate point mass distributions that correspond, in the continuum limit, to the power-spectrum expected from cosmological observations, more precisely, $S(k) \sim k$ for small k.

Recent numerical studies use shuffled lattice initial conditions with $S(k) \sim k^2$ at small k as the initial condition of a numerical integration of the Newtonian dynamics (a method called *molecular dynamics*) of an ensemble of self-gravitating particles. One finds clustering of structures that resemble the one in cosmological observations.

Interestingly enough, researchers in this field have recently established collaborations with people interested in liquid theory, close packing problems and so on, who have good experience in generating particle configurations with strange structure factors at small k – long distance in real space.

4 Stochastic processes

Simultaneously to the development of equilibrium statistical mechanics, which assumes that systems can be described in terms of Boltzmann-Gibbs probability distributions, the question of how this equilibrium is reached was raised (in fact by Boltzmann himself), and led to the well known debate about irreversibility and the arrow of time. Although the conceptual issues are formidable, one can take a phenomenological point of view and postulate the nature of the coupling between a given system and a thermal bath such that equilibrium is, at least in principle, reached at long times. This is known as the Langevin approach, which provides a consistent description of the *dynamics* of systems subject to thermal noise, such that the stationary solution reproduces the Boltzmann-Gibbs distribution.

On can be interested in situations such that the dynamics should lead at long times to equilibrium, but the time needed to do so is either infinite or very large compared to experimental time scales.[4] These systems are usually referred to as 'glassy'. In these cases, equilibrium concepts are *a priori* useless ; the description of the system is inherently of dynamical nature. The theoretical framework available to describe the dynamics of a system subject to thermal noise is good for both cases.

Almost any physical system is subject to fluctuations that have an unknown origin and/or can only be characterized only statistically. This noise is one of the manifestations of the exchange of energy between the system and its environment ; the other accompanying feature is, as we will see in more detail below, *dissipation*. The time evolution of a system coupled to its environment can be described in two equivalent ways. One is the Langevin approach that consists in studying Newton's equations with the addition of two terms representing friction and thermal noise. The other description is probabilistic and is concerned with the evolution of the probability distribution of the relevant degrees of freedom of the system. Both approaches turn out to be very useful to understand the dynamics of model systems.

The environment is often assumed to be a heat bath in equilibrium at a given temperature. In these conditions, many systems do equilibrate with such an environment after a short transient. The dynamics of equilibrated systems has several special features that we also review in this Section. How these properties are modified in systems that never reach equilibrium is a problem of current interest in research but we shall not develop it here.

[4] There might of course be systems that never reach thermal equilibrium, such as driven dissipative systems for example.

4.1 The Langevin equation

The Langevin equation is a stochastic differential equation that describes phenomenologically a large variety of problems. It describes the time evolution of a set of slow variables coupled to a much larger set of fast variables that are usually (but not necessarily) assumed to be in thermal equilibrium at a given temperature. We first introduce it in the context of Brownian motion and later derive it in more generality.

4.1.1 Brownian motion

The Brownian motion is the erratic motion of a mesoscopic colloidal particle (in the micrometer range) immersed in an equilibrated fluid made up of much lighter molecules. The jerky motion of the colloidal particle is due to the collisions with the molecules in the liquid. Knowing that each individual collision deflects the trajectory of the particle by a tiny amount, Langevin proposed to collect the effect of all molecules in the fluid in a time-dependent random force. If the particle moves in d dimensions, has mass m, its center of mass position at time t is represented by $\vec{x} = (x_1, \ldots, x_d)$ and its velocity is $\vec{v} = \dot{\vec{x}}$, Newton's equation reads

$$m\dot{\vec{v}}(t) = \vec{F}(\vec{x}, t) + \vec{f}(t) \; . \tag{4.1}$$

The force $\vec{F}$ designates all external deterministic forces, and depends in general also on the position of the particle $\vec{x}$, while $\vec{f}$ represents the net force exerted by all the individual molecules in the fluid on the massive particle. The latter depends on the time-dependent positions of all the molecules and is a rapidly fluctuating function of time. The characteristic time for the variation of this force is related to the time interval between successive collisions, that we call τ_c, and can be estimated to be of the order of the pico-second or even shorter for a typical liquid. [5]

Due to its rapid fluctuations, the time-dependence of the force $\vec{f}$ cannot be specified. One can, instead, make reasonable assumptions about its average over a large number of identical macroscopic situations and characterize it in statistical terms. More precisely, one considers an ensemble of n systems made of one tracer particle moving in a fluid and that are prepared in identical conditions, and defines ensemble-average quantities

$$\langle\, \mathcal{O}(t) \,\rangle = \frac{1}{n} \sum_{k=1}^{n} \mathcal{O}^{(k)}_{\vec{f}}(t) \; , \tag{4.2}$$

with the label k identifying the copy in the ensemble and $\mathcal{O}$ is an observable that depends on the force $\vec{f}$. (Equivalently, one can consider a single experiment in which one uses n identical non-interacting tracer particles moving in the medium.) Equation (4.1) implies that the position and velocity of the particle are both fluctuating quantities that depend

[5] This does not mean, however, that the correlation function of this random force is short range in time. Because of momentum conservation in the surrounding fluid, there appears a now well known 'long time tail' in the force correlation function, only decaying as $t^{-3/2}$ in three dimensions.

on $\vec{f}$. The aim is then to predict the average result (and the fluctuations) over a large number of experiments performed in identical conditions, or equivalently over a large number of particles provided these are non interacting.

In the absence of external forces, the problem is fully isotropic and the ensemble-averaged velocity can only vanish. If however the particle acquires a non-vanishing velocity $\vec{v}$, then the environment will react and induce a non zero force which, by symmetry, must be in the direction of $\vec{v}$. Thus, one can propose the following decomposition :

$$\vec{f} = f_1(v)\vec{v} + \xi \ , \tag{4.3}$$

where f_1 is some function of the modulus of $\vec{v}$, and ξ is an isotropic random force, the *thermal noise*, that keeps the agitation of the particle (this name has its origin in the random noise that one can actually hear in electric circuits). ξ has vanishing ensemble-average at each instant t : $\langle\, \vec{\xi}_i(t)\,\rangle = 0$, for all i and all times. The average over different realizations of the history of the system introduced in eqn (4.2) corresponds now to an average over histories of the time-dependent random force, $\vec{\xi}$. Thus, henceforth the angular brackets represent :

$$\langle\, \mathcal{O}(t)\,\rangle = \int_{\infty}^{\infty} \prod_{j=0}^{\mathcal{N}_t} \prod_{i=1}^{d} d\xi_i(t_j)\, P[\xi_i(t_j)]\, \mathcal{O}_{\vec{\xi}}(t_j) \equiv \int \mathcal{D}\xi\, P(\vec{\xi})\, \mathcal{O}_{\vec{\xi}}(t) \ ,$$

where $P[\xi_i(t_j)]$ is the probability of occurrence of ξ_i at time $t_j = j\delta$, with $j = 1, \ldots, \mathcal{N}_t$, and δ an infinitesimal time-interval. In the second term above we wrote it explicitly, and in the third term we used a short-hand notation that we adopt hereafter. The subindex $\vec{\xi}$ in $\mathcal{O}$ indicates that it is evaluated in the solution to the Langevin equation and hence depends on the thermal noise realization.

The simplest assumption for $f_1(v)$ is that it tends to a constant for small velocities, leading to the familiar *friction force* :

$$f_1(v \to 0)\vec{v} \ = \ -\gamma\vec{v} \qquad \gamma > 0 \ , \tag{4.4}$$

that opposes the motion of the particle. The *friction coefficient*, γ, is proportional to the *shear viscosity* η of the medium[6], $\gamma = c\eta > 0$, with c a constant of geometric origin that depends on the size and shape of the colloidal particle. When the medium is a normal fluid, and the particle is a sphere of radius a that is much larger than the mean free-path of the molecules one has $c = 6\pi a$ and one recovers the *Stokes law* for a spherical particle in a viscous fluid. The friction coefficient γ is of the order of $n_p \ell \tau_c T$ with n_p the density of particles in the fluid, ℓ the mean free path, τ_c the average time between collisions, the temperature T is measured in units of the Boltzmann's constant k_B. For a typical liquid,

[6]The shear viscosity of a system measures its resistance to flow. A flow field can be established by placing the system between two plates and pulling them apart in opposite directions creating a *shear force*. The rate at which the plates are pulled apart is called the *shear rate*. Other geometries are also possible.

like water in normal conditions, the viscosity is of the order of 0.01 Poise.[7] With the choice (4.4) eqn (4.1) becomes

$$m\dot{\vec{v}}(t) = -\gamma\vec{v}(t) + \vec{F}(\vec{x},t) + \vec{\xi}(t)\ . \tag{4.5}$$

So far we have characterized the random force exerted by the fluid by giving its average value, the friction force. In order characterize more completely the motion of the particle, one also needs to know how the random force fluctuates in time. This information is (in part) contained in its *correlation function*, defined by comparing the thermal noise at two subsequent times t and t', with $t = t' + \tau$. Since collisions are very irregular, one can assume that the forces at two different times are statistically independent for long enough time-separations period (but see footnote 5), i.e.

$$\langle\, \xi_i(t)\xi_j(t')\,\rangle = \langle\, \xi_i(t)\,\rangle\langle\, \xi_j(t')\,\rangle = 0 \quad \text{if } \tau \equiv t - t' \gg \tau_c \quad \forall\, i,j,= 1,\ldots,d\ .$$

The correlation between the same component of the random force evaluated at different times is, by definition, a symmetric function of times, $\langle\, \xi_i(t)\xi_i(t')\,\rangle = \langle\, \xi_i(t')\xi_i(t)\,\rangle$. In addition, one assumes that the correlation between the same component of the force at two different times is *stationary*, that is to say, that it only depends on the time-difference τ. This is a property of the reservoir (the fluid in our case) in thermal equilibrium. Finally, since we assume that all directions of space are equivalent, the components of the random force in different directions are uncorrelated (even at time-differences that are shorter than τ_c) :

$$\langle\, \xi_i(t)\xi_j(t')\,\rangle \;\; = \;\; \delta_{ij}\, g(|\tau|)\ , \qquad \forall\, i,j = 1,\ldots,d\ . \tag{4.6}$$

This comes from the fact that δ_{ij} is the only rotationally invariant tensor. In the above equation, $\langle\xi_i^2(t')\rangle = g(0) > 0$ and $g(|\tau|)$ sharply peaked around $\tau = 0$ with a support of the order of τ_c. At macroscopic time-scales, τ is actually much longer than τ_c, and one can approximate $g(|\tau|)$ by a delta function of weight $2A$

$$\langle\, \xi_i(t)\xi_j(t')\,\rangle = 2A\delta_{ij}\,\delta(\tau)\ , \qquad \forall\, i,j = 1,\ldots,d\ . \tag{4.7}$$

The Fourier transform of the stationary correlation of the noise defines its *spectral density*, $S(\omega)$. In this case, $S(\omega)$ is independent of the frequency ω, defining a *white noise*.

Two-time correlations do not characterize time-dependent random variables completely. This is achieved either by giving all higher-order correlations or, equivalently, by specifying its full multivariate probability distribution function. The simplest choice is a multivariate Gaussian distribution compatible with the above two-time correlation. In discrete time, we write :

$$P(\vec{\xi}) = \frac{1}{\mathcal{N}}\,\exp\left(-\frac{1}{4A}\sum_{j=0}^{\mathcal{N}_t}\sum_{i=1}^{d}\xi_i^2(t_j)\right)\ , \tag{4.8}$$

[7] The friction coefficient and the viscosity are measured in units of [mass]/[time] and Poise≡ [energy×time]/[volume] in the CGS system, respectively.

with $\mathcal{N}$ the normalization constant. The Gaussian hypothesis is based on the central limit theorem. Indeed, if one observes the thermal force acting on a sufficiently large particle, with a time-grid that is much larger that τ_c, $\vec{\xi}$ is the result of a large number of random forces with finite average and variance, all sharing the same distribution law. However, one could imagine 'sporadic' thermal baths that would lead to deviations from a Gaussian distribution of random forces, in particular in the tails.

The Gaussian hypothesis implies that all higher-order correlations can be expressed as functions of the two-time correlation (4.6). This is the content of Wick's theorem, which states that :

$$\langle\, \xi_{i_{2n}}(t_{2n}) \dots \xi_{i_1}(t_1) \,\rangle = \sum_{pairs} \langle\, \xi_{i_{2n}}(t_{2n}) \xi_{i_{2n-1}}(t_{2n-1}) \,\rangle \dots \langle\, \xi_{i_2}(t_2) \xi_{i_1}(t_1) \,\rangle \;,$$

with the sum running over all the different ways of separating the product of $2n$ variables into n pairs. The average of a product of an odd number of noise factors vanishes identically since the thermal noise has zero-average (remember that the average of the random force, namely the friction force, has been subtracted off). So far the variance, $2A$, is a free parameter. We shall see later on that if the environment is assumed to be in equilibrium at a temperature T, then A must in fact relate to γ and T.

Irreversibility and dissipation.

The friction force $-\gamma\vec{v}$ in the Langevin equation (4.5) explicitly breaks the time-reversal ($t \to -t$) invariance, a property that has to be respected by any set of microscopic dynamic equations. This is the well known paradox raised by the irreversibility of thermodynamics. However, the Langevin equation is an effective equation that only describes the particle and *not* the individual motion of the molecules of the surrounding fluid. Of course, Newton's equation describing the whole system, the particle and all the molecules of the fluid, must be time reversal invariant. However, time-reversal can be broken in the *reduced* equation, where the ability of the thermal bath to reach equilibrium is assumed from the start. The Langevin approach is a clever way to hide the irreversibility problem under the rug (by transferring the conceptual difficulties to the reservoir) and allows to investigate in a phenomelogical way the dynamics of the particle alone. In Sect. **??** we shall study a simple model where the assumptions behind Langevin's equation can be made more transparent.

Note that the energy of the particle is not conserved and, in general, flows to the bath leading to *dissipation*. At very long times however, the particle may reach a stationary regime in which the exchange of energy becomes symmetric on average : the particle gives and receives energy from the bath at equal rate.

Generation of memory.

The Langevin equation (4.5) is a first order differential equation on the velocity. The full dynamics of the particle is determined by this equation together with $\vec{v}(t) = \dot{\vec{x}}(t)$ which is also a first-order differential equation.

These features imply that the pair velocity-position of the particle at time $t + \delta$, with δ an infinitesimal time-step, depends on the pair velocity-position at time t and the value

of the noise at time t. Thus, the full set of equations defines a *Markov process*, that is a stochastic process that depends on its history only through its very last step. Notice, however, that the pair of first order differential equations could also be described by a single second-order differential equation :

$$m\ddot{\vec{x}}(t) + \gamma\dot{\vec{x}}(t) = \vec{F}(\vec{x},t) + \vec{\xi}(t) \; . \tag{4.9}$$

Having replaced the velocity by its definition in terms of the position the Markov character of the process is lost. This is a very general feature : by integrating away some degrees of freedom one generates memory in the evolution. Generalizations of the Langevin equation, such as the one that we present in Sect. 2.10.5, and the ones that will be generated to describe the slow evolution of super-cooled liquids and glasses, do have memory.

Fluctuation – dissipation relation of the second kind.

In the heuristic derivation of the Langevin equation that we presented above the constant A is not fixed. The simplest way of fixing the value of this parameter is to study the velocity fluctuations of a Brownian particle in a constant external force. The time-dependent velocity follows from the integration over time of eqn (4.5)

$$\vec{v}(t) = \vec{v}_0 e^{-\frac{\gamma}{m}t} + \frac{1}{m}\int_0^t dt' \; e^{-\frac{\gamma}{m}(t-t')} \; [\, \vec{F} + \vec{\xi}(t') \,] \; ,$$

with $\vec{v}_0$ the initial velocity at $t = 0$. Using the fact that the noise has zero average one finds

$$\langle\, \vec{v}(t) \,\rangle = \vec{v}_0 e^{-\frac{\gamma}{m}t} + \frac{\vec{F}}{\gamma}\left(1 - e^{-\frac{\gamma}{m}t}\right) \;\; \rightarrow \;\; \frac{\vec{F}}{\gamma} \quad \text{when} \;\; t \gg t_c^v \equiv \frac{m}{\gamma} \; .$$

Using the noise-noise auto-correlation in eqn (4.7), and setting $\vec{v}_0 = \vec{0}$ for simplicity, one readily calculates the mean-square displacement of the velocity in each direction of space, $\sigma^2_{v_i}(t) \equiv \langle\, (v_i(t) - \langle v_i(t) \rangle)^2 \,\rangle$,

$$\sigma^2_{v_i}(t) = \frac{1}{m^2}\int_0^t dt' \int_0^t dt'' \; e^{-\frac{\gamma}{m}(2t-t'-t'')} \; \langle\, \xi_i(t')\xi_i(t'') \,\rangle = \frac{A}{\gamma m}\left(1 - e^{-\frac{2\gamma}{m}t}\right) \; .$$

Since the Langevin equation is a phenomenological description of the approach to thermal equilibrium, we must impose for consistency that the above quantity saturates to the expected value calculated with the canonical distribution at temperature T. Thus,

$$\lim_{t \gg t_c^v} \sigma^2_{v_i}(t) = \frac{A}{\gamma m} = \langle\, (v_i - \langle\, v_i \,\rangle)^2 \rangle_{eq} = \frac{T}{m} \; ,$$

where $\langle \quad \rangle_{eq}$ denotes an average taken with Maxwell's velocity distribution. For this equality to hold one enforces that :

$$A = \gamma T \; . \tag{4.10}$$

This relation is known under the name of fluctuation–dissipation theorem (FDT) of the 'second kind' in Kubo's nomenclature. (The 'first kind' will be discussed below; these names are here a little unfortunate).

It is important to note that this FDT characterizes the surrounding fluid and not the particle, since it relates the noise-noise correlation to the friction coefficient. In the case of the Brownian particle this relation ensures that after a transient of the order of t_c, the bath maintains the mean kinetic energy of the particle constant and equal to its equilibrium value. The Gaussian distribution of the noise and the linear relation linking it to the velocity imply that the velocity of the particle is indeed distributed according to Maxwell's distribution. We shall see later that even when the environment satisfies a fluctuation – dissipation relation (FDR) the system in contact with it does not necessarily follow and satisfy an FDR itself. This is one of the main characteristics of non-equilibrium systems in contact with equilibrated environments.

Diffusion in velocity space.

For the sake of simplicity let us focus in this section on a one dimensional problem. The two-time velocity-velocity 'variogram', defined as : $\Delta_{vv}(t,t') \equiv \langle\, (v(t)-v(t'))^2 \,\rangle = C_{vv}(t,t) + C_{vv}(t',t') - 2C_{vv}(t,t')$ is a simple function of the two-time correlation of the velocity $C_{vv}(t,t') = \langle\, v(t)v(t') \,\rangle$ that itself is easily calculated to be :

$$C_{vv}(t,t') = v_0^2\, e^{-\frac{\gamma}{m}(t+t')} + \frac{T}{m}\left(e^{-\frac{\gamma}{m}|t-t'|} - e^{-\frac{\gamma}{m}(t+t')}\right) . \tag{4.11}$$

The first term comes from the initial condition and the second term sometimes goes under the name of *Dirichlet correlator*. When $t+t' \gg t_c$ the initial condition is forgotten, the last term vanishes, and the correlation and displacement become functions of $|t-t'|$ only, as expected in equilibrium (see Sect. 4.3.1). The variogram crosses over from a diffusive regime to saturation at the characteristic time t_c^v :

$$\Delta_{vv}(t,t') \;\sim\; \begin{cases} 2D_v|t-t'| & \text{when } |t-t'| \ll t_c^v \text{ with } D_v \equiv \dfrac{T\gamma}{m^2} , \\ \dfrac{4T}{m} & \text{when } |t-t'| \gg t_c^v . \end{cases}$$

The coefficient D_v of the linear regime is called the *velocity diffusion coefficient*.

Diffusion in position space.

The position-position variogram is similarly defined as $\Delta_{xx}(t,t') \equiv \langle\, (x(t)-x(t'))^2 \,\rangle$ and measures the square of the typical displacement of the particle between t and t'. Choosing $x_0 = v_0 = 0$ one finds :

$$\Delta_{xx}(t,t') = \frac{2D_v m^2}{\gamma^2}\left[|t-t'| + \frac{2m}{\gamma}\left(e^{-\frac{\gamma}{m}|t-t'|}-1\right) - \frac{m}{2\gamma}\left(e^{-\frac{2\gamma}{m}|t-t'|}-1\right)\right] ,$$

and there is also a change in behavior at time-differences of the order of t_c^v :

$$\Delta_{xx}(t,t') \sim \begin{cases} \frac{2D_v}{3}|t-t'|^3 & \text{when } |t-t'| \ll t_c^v \ , \\ 2D_x|t-t'| & \text{when } |t-t'| \gg t_c^v \text{ with } D_x \equiv \frac{T}{\gamma} \ . \end{cases}$$

At small times, the particle is subject to a random acceleration ; its velocity is thus of the order of $\sqrt{|t-t'|}$, leading to a typical displacement of the order of $|t-t'|^{3/2}$. For times larger than t_c^v, the velocity saturates under the effect of friction, and normal diffusion sets in, with a typical displacement given by $\sqrt{D_x|t-t'|}$.

Einstein relation.

The *mobility* of the particle is defined as

$$\mu \equiv \lim_{F\to 0}\lim_{t\to\infty} \frac{\langle\, v(t)\,\rangle}{F}. \tag{4.12}$$

Using the above result on D_x, we find :

$$\mu = \frac{1}{\gamma} \equiv \frac{D_x}{T} \text{ when } |t-t'| \gg t_c^v \ , \tag{4.13}$$

This identity between μ and D_x is known as the *Einstein relation* between the transport properties of the particle, its diffusion in real space, and the temperature of the surroundings. It expresses the *fluctuation–dissipation theorem of the first kind*, to be distinguished from the one of the second kind by the fact that it now describes a dynamic property of the particle induced by those of the bath.

Stokes-Einstein relation.

We have mentioned that in a normal fluid the viscosity and friction coefficient of the frictional force exerted on an spherical particle of radious a are related by the Stokes law $\gamma = 6\pi a\eta$. This relation, combined with (4.13) implies the *Stokes-Einstein* relation

$$6\pi a\eta = \frac{T}{D_x}$$

linking the viscosity to the temperature and spatial diffusion constant. This prediction first obtained by Einstein and then confirmed by Langevin was experimentally verified by Perrin. Much more recently, though, it has been noticed that in liquids that are supercooled this relation ceases to be valid.

Smoluchowski (strong overdamped) limit.

In many situations in which friction is very strong the inertial term $m\dot{\vec{v}}$ can be dropped from eqn (4.5) :

$$\gamma\dot{\vec{x}}(t) = \vec{F}(\vec{x},t) + \vec{\xi}(t) \ . \tag{4.14}$$

This limit is acceptable when the observation times are much longer than the characteristic time for relaxation $t_c^v = m/\gamma$, such that the mean-squared displacement of the velocity saturates and the position diffuses. The range of validity of this approximation can be easily put to test in the example of a particle moving in a harmonic potential.

In the white-noise case the friction coefficient can be eliminated from the Langevin equation in the Smoluchowski limit and the noise-noise correlation with the rescaling of time : $\tau \equiv t\gamma^{-1}$, $\tilde{x}(\tau) \equiv x(t\gamma^{-1})$.

4.1.2 Generalized Langevin equations

Langevin-like equations are used to describe the dynamics of a much more general microscopic or macroscopic systems coupled to environments. The applications in physics, chemistry and engineering are numerous. One can cite, for instance, the description of the dynamics of macromolecules in solution, with the analysis of the electrophoresis technique as a particular case. The time required to dissociate molecules or the transition rate between molecular configurations are subjects of great interest in chemistry that have been attacked with the Langevin approach. Stochastic equations with damping and white noise are also used to describe noisy electric circuits. To treat glassy problems that are typically macroscopic systems constituted by particles (colloids, atoms, molecules, spins...) in contact with an environment (the solution, phonons...) that is described statistically we need to justify them beyond the simple Brownian motion problem.

Langevin equations with multiplicative noise.

So far the random force appeared as a separate term in the Langevin equation. Extensions of the Langevin approach with *multiplicative noise* lead to the so-called *non-linear Langevin equations* [30] in which the usually delta-correlated Gaussian noise $\vec{\xi}$ multiplies a certain function $e(\vec{x}, t)$ of the stochastic variable $\vec{x}$ itself :

$$m\ddot{\vec{x}} + \gamma\dot{\vec{x}} = -\vec{F}(\vec{x}, t) + e(\vec{x}, t)\vec{\xi}(t) \; . \tag{4.15}$$

However, as written, this equation is at best ambiguous. A proper prescription in a discrete time setting must be specified. This is a very important point that we shall not discuss here. It leads to what is called Ito and Stratonovich calculus, basically different prescriptions as to how to interpret the continuous differential equation and how to discretize the time-derivative.

Langevin equations with memory.

A derivation of a generalized linear Langevin equation with memory is very simple. In general, one studies the coupled (closed) system made by the actual system of interest in interaction with an environment. The description of the bath and of its interaction with the system depends on the problem at hand. The simplest choice is that of an independent ensemble of harmonic oscillators that couple linearly to each coordinate-like degree of freedom in the system. This choice allows one to solve the dynamic equations for the bath variables analytically. After introducing their solution in the dynamic equations

for the system, one thus obtains the dynamics of the *reduced* system. Until this point the dynamics of the system remains deterministic and is completely determined by its initial conditions as well as those of the reservoir variables. The statistical element comes in when one proposes that the initial coordinates and momenta of the oscillators in the bath are distributed according to an equilibrium measure. This induces randomness and friction in the dynamics of the reduced system. After performing explicitly these calculations one ends up with the generalized Langevin equation :

$$m\dot{\vec{v}}(t) = \vec{F}(\vec{x},t) + \vec{\xi}(t) - \int_0^t dt'\,\gamma(t-t')\dot{\vec{x}}(t')\ . \tag{4.16}$$

with the Gaussian thermal noise characterized by

$$\langle \xi_i(t)\rangle = 0\ , \qquad \forall\, i \ \text{ and } \ \forall\, t\ , \tag{4.17}$$

$$\langle \xi_i(t)\xi_j(t')\rangle = T\,\delta_{ij}\gamma(t-t')\ , \tag{4.18}$$

and $\gamma(t-t')$ a *retarded friction*. A multiplicative retarded noise arises from a model in which one couples the coordinates of the oscillators to a generic function of the coordinates of the system.

Different oscillator reservoirs are characterized by different kernels $\gamma(t-t')$. The spectral function of the colored bath is usually assumed to have the form

$$S(\omega) = T\tilde{\gamma}(\omega) = 2T\gamma\left(\frac{|\omega|}{\tilde{\omega}}\right)^{\delta-1} f_c\left(\frac{|\omega|}{\Lambda}\right)\ . \tag{4.19}$$

The function $f_c(x)$ is a high-frequency cut-off of typical width Λ and is usually chosen to be an exponential. The frequency $\tilde{\omega} \ll \Lambda$ is a reference frequency that allows one to have a coupling strength γ with the dimensions of a viscosity. If $\delta = 1$, the friction is said to be *Ohmic*, $S(\omega)$ is constant when $|\omega| \ll \Lambda$ and one recovers a white noise. When $\delta > 1$ ($\delta < 1$) the bath is *superOhmic* (*subOhmic*). The exponent δ is taken to vary in the interval $[0,2]$ to avoid divergencies.

Time-dependent, $\vec{f}(t)$, and constant non-potential forces, $\vec{f}^{np}$, as the ones applied to granular matter and in rheological measurements, respectively, are simply included in the right-hand-side (RHS) as part of the deterministic force. When the force derives from a potential, $F_i(t) = -\partial_{x_i}V(\vec{x}(t))$.

In so far we have discussed systems with position and momentum degrees of freedom. Other variables might be of interest to describe the dynamics of different kind of systems. In particular, a continuous Langevin equation for classical spins can also be used if one replaces the hard Ising constraint, $s_i = \pm 1$, by a soft one implemented with a potential term of the form $V(s_i) = u(s_i^2-1)^2$ with u a coupling strength (that one eventually takes to infinity to recover a hard constraint). The soft spins are continuous unbounded variables, $s_i \in (-\infty,\infty)$, but the potential energy favors the configurations with s_i close to ± 1. Even simpler models are constructed with spherical spins, that are also continuous unbounded variables globally constrained to satisfy $\sum_{i=1}^N s_i^2 = N$.

4.2 Averages, correlations and responses

In Sect. 2.10.5 we analyzed several averaged properties of Brownian motion. In this Section we introduce the averaged observables on which we shall focus in the rest of the book. We use a vector $\vec{x}$ to encode all dynamic degrees of freedom in the system. These can be position and momenta for a particle system, spins for a magnetic sample, or even a field such as the local and time-dependent density.

4.2.1 One-time functions

The simplest dynamic observables depend only on one time and are defined by

$$\langle\, A(\vec{x},t)\,\rangle = \int \mathcal{D}\vec{\xi}\, P(\vec{\xi})\, A(\vec{x}_\xi,t)\ , \tag{4.20}$$

where $\vec{\xi}$ symbolically denotes the noise at all times. The integral indicates a sum over all possible noise history realizations, each counted with its weight $P(\xi)$. This is a *path-integral* and we shall not discuss it here. Even if A can in principle be any complicated functional of the system's degrees of freedom, in most cases of interest it is a simple scalar function of these variables. Typical examples we shall examine later are the energy density, the magnetization density in a magnetic system, the particle density in a liquid or a glass, etc.

4.2.2 The correlation functions

Given any two functionals of $\vec{x}$, say $A(\vec{x},t)$ and $B(\vec{x},t)$, one defines the *correlation function* between A and B at two subsequent times t and t' as

$$C_{AB}(t,t') \equiv \langle\, A(\vec{x},t)B(\vec{x},t')\,\rangle = \int \mathcal{D}\vec{\xi}\, P(\vec{\xi})\, A(\vec{x}_\xi,t)B(\vec{x}_\xi,t')\ .$$

Note that the *auto-correlations* are, by definition, symmetric under exchanges of t and t', $C_{AA}(t,t') = C_{AA}(t',t)$.

In a generic situation $C_{AB}(t,t')$ is a function of *both* times t and t'. We shall see that when the system reaches a steady state, and in particular the equilibrium measure, $C_{AB}(t,t')$ becomes stationary and a function of time-differences only $C_{AB}(t,t') = C^{st}_{AB}(t-t') = C^{st}_{AB}(\tau)$ with $\tau \equiv t-t'$. In complete generality we write the two-time correlator as $C_{AB}(t,t') = \mathcal{C}_{AB}(\tau,t')$ and we define Fourier transforms with respect to the time difference τ :

$$\tilde{\mathcal{C}}_{AB}(\omega,t') \equiv \int_{-\infty}^{\infty} d\tau\, \mathcal{C}_{AB}(\tau,t')\, e^{i\omega\tau}$$

with the inverse Fourier transform given by

$$\mathcal{C}_{AB}(\tau,t') = \int \frac{d\omega}{2\pi}\, \tilde{\mathcal{C}}_{AB}(\omega,t')\, e^{-i\omega\tau}\ .$$

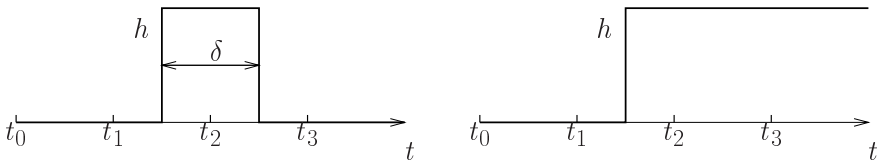

FIG. 10 – Sketch of perturbations of strength h; a kick (left) and a step (right).

In the stationary limit these become the usual expressions

$$\tilde{\mathcal{C}}_{AB}(\omega) \equiv \int_{-\infty}^{\infty} d\tau \; C^{st}_{AB}(\tau)\, e^{i\omega\tau} \;, \qquad C^{st}_{AB}(\tau) \equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \; \tilde{\mathcal{C}}_{AB}(\omega)\, e^{-i\omega\tau} \;,$$

and $\tilde{\mathcal{C}}_{AA}(\omega)$ is the spectral density of A.

Sometimes it is useful to calculate the *connected correlation* functions in which one correlates the fluctuations of A and B about their averages :

$$C^{c}_{AB}(t,t') \equiv \langle \left(A(\vec{x},t) - \langle A(\vec{x},t)\rangle\right) \left(B(\vec{x},t') - \langle B(\vec{x},t')\rangle\right) \rangle \;.$$

Other important *two-time quantities* in the analysis of dynamical problems with diffusion are the *displacement between observables* :

$$\Delta^{(1)}_{AB}(t,t') \equiv \left\langle \left(A(\vec{x},t) - B(\vec{x},t')\right)^2 \right\rangle = C_{AB}(t,t) + C_{AB}(t',t') - 2\, C_{AB}(t,t') \;,$$

and the *displacement between the fluctuations* of these observables,

$$\begin{aligned} \Delta^{(2)}_{AB}(t,t') &\equiv \left\langle \left(A(\vec{x},t) - \langle A(\vec{x},t)\rangle - B(\vec{x},t') + \langle B(\vec{x},t')\rangle\right)^2 \right\rangle \\ &= C^{c}_{AB}(t,t) + C^{c}_{AB}(t',t') - 2\, C^{c}_{AB}(t,t') \;. \end{aligned}$$

4.2.3 The linear response

The application of an infinitesimal external force of strength h, possibly time-dependent, that couples linearly to a generic function B of the system's degrees of freedom, modifies the Hamiltonian according to

$$H \to H - h(t) B(\vec{x},t) \;.$$

We represent the instantaneous infinitesimal perturbation $h(t)$ as the kick between $t_2 - \delta/2$ and $t_2 + \delta/2$ in Fig. 10-left and a step-like perturbation that is continuously applied after time t_2 in the right panel of the same figure.

The variation of the average of another generic function A evaluated at time t, due to the applied force is

$$\delta\langle\, A(\vec{x},t)\,\rangle = \int_0^{\infty} dt' \; R_{AB}(t,t')\; \delta h(t') \;. \tag{4.21}$$

This relation defines the *instantaneous linear response* $R_{AB}(t,t')$.

It is important to notice that the perturbation can modify the particle's position only at future times. This is the reason why the integration in (4.21) can only span the time interval going from the initial time $t'=0$ to the measuring time $t'=t$. Otherwise stated, the instantaneous linear response is *causal* and hence proportional to the Heavide theta function :

$$R_{AB}(t,t') \equiv \left.\frac{\delta\langle A(t)\rangle}{\delta h(t')}\right|_{h=0} = r_{AB}(t,t')\,\theta(\tau) \qquad \tau \equiv t-t' \ . \tag{4.22}$$

Equation (4.21) then means that the change in the averaged function A due to the coupling of B to the force h exerted during a finite time-interval is a linear superposition of the changes due to spike-like perturbations applied at each instant in the same time-interval.

A very useful expression for the linear response of a Langevin process with additive noise is a consequence of Novikov's formula, which applies to general functions of Gaussian random variables with zero mean and states that

$$\langle\, x(t)\xi(t')\,\rangle = \int_0^\infty dt''\, \langle\, \xi(t'')\xi(t')\,\rangle \, \left\langle \frac{\delta x(t)}{\delta\xi(t'')} \right\rangle \ . \tag{4.23}$$

Using the noise-noise correlation (4.18) and the fact that the second factor in the integrand equals the linear response one finds

$$\langle\, x(t)\xi(t')\,\rangle = T\int_0^\infty dt''\, \gamma(t',t'')\, R(t,t'') \ . \tag{4.24}$$

For a white noise $\gamma(t',t'') = 2\gamma\delta(t'-t'')$ and the relation becomes : $2\gamma T R(t,t') = \langle\, x(t)\xi(t')\,\rangle$. The Itô convention assumes that the noise term $\xi(t)$ has a strictly zero correlation time and is always slightly posterior to (and therefore independent of) any function $G(x,t)$, possibly determined by all previous values of $\xi(t')$, $t'<t$. Therefore, $\langle\, \xi(t)x(t)\,\rangle$ vanishes. The Stratonovich rule, on the other hand, assumes that the noise term $\xi(t)$ has a very small, but non zero correlation time, which is taken to zero *after* the continuous time limit of the Langevin equation has been taken. This implies that the linear responses take the boundary values :

$$\begin{array}{rll} \text{Stratonovich} & R(t,t) = 1/2\gamma \ , & R(t,t^-) = 1/\gamma \ , \\ \text{Itô} & R(t,t) = 0 \ , & R(t,t^-) = 1/\gamma \ . \end{array}$$

A function that we shall explore in great detail in future chapters is the *integrated linear response*

$$\chi_{AB}(t,t_w) \equiv \int_{t_w}^t dt''\, R_{AB}(t,t'') \ . \tag{4.25}$$

It represents the influence on the observable A of a perturbation applied at the *waiting-time* t_w and held constant until the measuring time t, as the one sketch in Fig. 10-right, normalized by the strength of the applied field.

The Fourier transform with respect to the time-difference τ of the response function at fixed time t' reads

$$\tilde{\chi}_{AB}(\omega, t') \equiv \int_{-\infty}^{\infty} d\tau \, r_{AB}(t'+\tau, t') \, \theta(\tau) \, e^{i\omega\tau} \; , \tag{4.26}$$

and defines a *generalized ac-susceptibility*. The real and imaginary parts of $\tilde{\chi}_{AB}$, are called χ'_{AB} and χ''_{AB}, respectively. The generalized ac-susceptibility satisfies $\tilde{\chi}^*_{AB}(\omega, t') = -\tilde{\chi}_{AB}(-\omega, t')$ and χ'_{AB} and χ''_{AB} are, respectively, even and odd functions of ω :

$$\chi'_{AB}(\omega, t') = \chi'_{AB}(-\omega, t') \; , \qquad \chi''_{AB}(\omega, t') = -\chi''_{AB}(-\omega, t') \; .$$

In equilibrium $\tilde{\chi}_{AB}(\omega, t') \to \tilde{\chi}_{AB}(\omega)$ since $\chi_{AB}(t, t') \to \chi^{st}_{AB}(\tau)$ for all observables A and B.

4.3 Probabilistic formalism

In this Section we recall some features of the alternative approach to stochastic processes that consists in studying the evolution of the time-dependent probability distribution of the system's degrees of freedom, instead of writing a stochastic evolution equation for their dynamics.

4.3.1 Time-dependent probabilities

Let us consider a stochastic processes characterized by a dynamic variable $\vec{x}$. For simplicity we use a notation in which we encode all dynamic variables in a single vectorial degree of freedom $\vec{x} = (x_1, x_2, \ldots, x_d)$. Later we shall make explicit the case in which one has position-like and momentum-like variables. The time-dependence of $\vec{x}$ can be dictated by a Langevin equation of the kind discussed in the previous Sections or it can be determined by other stochastic dynamic rules. Since its evolution is not deterministic, it can be known only in probabilistic sense. The knowledge of the joint time-dependent probability density

$$P(\vec{x}_n, t_n; \vec{x}_{n-1}, t_{n-1}; \ldots; \vec{x}_0, t_0) \; ,$$

characterizes the process completely (we use a discretized description of all times, $t_0 \leq t_1 \leq \ldots \leq t_n$, t_n being the total time). In **??** we shall use a short-hand notation denoting $\vec{X}$ the complete trajectory of the process, $\vec{X} \equiv (\vec{x}_n, t_n; \ldots; \vec{x}_0, t_0)$.

The conditional probability density

$$\begin{aligned} P(\vec{x}_n, t_n; \vec{x}_{n-1}, t_{n-1}; \ldots; \vec{x}_{k+1}, t_{k+1} | \vec{x}_k, t_k; \vec{x}_{k-1}, t_{k-1}; \ldots \vec{x}_0, t_0) \\ = \frac{P(\vec{x}_n, t_n; \vec{x}_{n-1}, t_{n-1}; \ldots; \vec{x}_{k+1}, t_{k+1})}{P(\vec{x}_k, t_k; \vec{x}_{k-1}, t_{k-1}; \ldots; \vec{x}_0, t_0)} \end{aligned} \tag{4.1}$$

allows one to know the probability of finding future configurations given that the process took some specified previous values.

One can distinguish between processes for which their full history is needed to predict their future (in a probabilistic sense) and processes for which the knowledge of the present

is enough to do so. The former are called *non-Markov* while the latter are *Markov*. The standard example of a Markov chain is a random walk on a d-dimensional square lattice : at each time-step the walker can jump to any of its $2d$ neighboring sites with equal probability $1/(2d)$ that is totally independent of how the walker got to its present position. A self-avoiding random walk on the same lattice is instead a non-Markovian stochastic process : since the chain cannot cross on the lattice one needs to know the positions the walker occupied at all previous times.[8] In more technical terms, a Markov process is such that

$$P(\vec{x}_n, t_n; \ldots; \vec{x}_{k+1}, t_{k+1} | \vec{x}_k, t_k; \ldots \vec{x}_0, t_0) = P(\vec{x}_n, t_n; \ldots; \vec{x}_{k+1}, t_{k+1} | \vec{x}_k, t_k) \ .$$

This property implies that any joint probability density can be expressed in terms of conditional probabilities that depend only on the present and immediately subsequent configurations, called *transition probabilities*,

$$T(\vec{x}_k, t_k | \vec{x}_{k-1}, t_{k-1}) \equiv P(\vec{x}_k, t_k | \vec{x}_{k-1}, t_{k-1}) \ .$$

Hence,

$$P(\vec{x}_n, t_n; \ldots; \vec{x}_0, t_0) = T(\vec{x}_n, t_n | \vec{x}_{n-1}, t_{n-1}) \ldots T(\vec{x}_1, t_1 | \vec{x}_0, t_0) P(\vec{x}_0, t_0) \ .$$

Clearly, the transition probabilities satisfy

$$\int d\vec{x}_k \ T(\vec{x}_k, t_k | \vec{x}_{k-1}, t_{k-1}) = 1 \ , \qquad T(\vec{x}_k, t_k | \vec{x}_{k-1}, t_{k-1}) \geq 0 \ .$$

Chapman-Kolmogorov integral equations.

The probability density P of a generic (and not necessarily Markov) stochastic process evaluated at t_2 is related to the one at t_1 by the integral equation

$$P(\vec{x}_2, t_2) = \int d\vec{x}_1 \ P(\vec{x}_2, t_2; \vec{x}_1, t_1) = \int d\vec{x}_1 \ P(\vec{x}_2, t_2 | \vec{x}_1, t_1) P(\vec{x}_1, t_1)$$

where the integration runs over all possible values of $\vec{x}_1$. Note that t_1 and t_2 are not necessarily infinitesimally close to each other.

The conditional probabilities satisfy a similar integral equation. Indeed,

$$\begin{aligned} P(\vec{x}_3, t_3; \vec{x}_1, t_1) &= P(\vec{x}_3, t_3 | \vec{x}_1, t_1) \, P(\vec{x}_1, t_1) = \int d\vec{x}_2 \, P(\vec{x}_3, t_3; \vec{x}_2, t_2; \vec{x}_1, t_1) \\ &= \int d\vec{x}_2 \ P(\vec{x}_3, t_3 | \vec{x}_2, t_2; \vec{x}_1, t_1) P(\vec{x}_2, t_2; \vec{x}_1, t_1) \\ &= \int d\vec{x}_2 \, P(\vec{x}_3, t_3 | \vec{x}_2, t_2; \vec{x}_1, t_1) P(\vec{x}_2, t_2 | \vec{x}_1, t_1) P(\vec{x}_1, t_1) \ , \end{aligned} \tag{4.2}$$

[8] Note however that we refer here to dynamically generated self-avoiding walks, which does not define the same statistical ensemble as that relevant for polymers in thermal equilibrium. On this point, see [**?**].

from where we get

$$T(\vec{x}_3, t_3|\vec{x}_1, t_1) = \int d\vec{x}_2 \; T(\vec{x}_3, t_3|\vec{x}_2, t_2) T(\vec{x}_2, t_2|\vec{x}_1, t_1) \; , \tag{4.3}$$

if the process is Markov. This is the *Chapman-Kolmogorov* equation that links the transition probabilities.

Generation and elimination of memory.

Two points about the differences between Markov and non-Markov processes are worth discussing before going on.

First, the minimum time-separation, $\delta = t_{k+1} - t_k$, that is physically observable may play a role in the classification of a process as Markov or non-Markov. In most realistic situations, if one investigated the dynamics with a sufficiently fine time grid, non-Markov effects would be observable. However, for many practical purposes one can assume that these fine details are overlooked by a sparse time-grid that is longer than the characteristic memory time. Thus, the processes can be considered to be effectively Markov, in the same way as the noise-noise correlations in the Langevin approach can usually be taken to be delta functions (in time).

Besides, as we have already noticed when we rewrote the Langevin equation for the Brownian particle as a function of the coordinate only, the elimination of some degrees of freedom in the system, by integrating their dynamic equations and replacing the result in the remaining ones, may transform a Markov process into a non-Markov one. The same can occur at the level of the probabilistic description that we are discussing in this Section.

Thus, we conclude that the Markov or non-Markov character of a process may depend on the level of description we want to obtain and on the approach we adopt.

Stationarity and ergodicity.

A stochastic process is *stationary* when the joint-probability distribution is *invariant under translations of time* (TTI) :

$$P(\vec{x}_n, t_n; \ldots; \vec{x}_0, t_0) = P(\vec{x}_n, t_n + \Delta; \ldots; \vec{x}_0, t_0 + \Delta) \; . \tag{4.4}$$

In particular, this implies that the one-time probability is independent of time, $P(\vec{x}, t) = P_{st}(\vec{x})$, and the two-time joint probability depends on the time-difference only, $P(\vec{x}_1, t_1; \vec{x}_2, t_2) = P_{st}(\vec{x}_1, t_1 - t_2; \vec{x}_2, 0)$. This immediately implies that the conditional probabilities are also functions of the time-difference only : $P(\vec{x}_1, t_1|\vec{x}_2, t_2) = P_{st}(\vec{x}_1, t_1 - t_2|\vec{x}_2, 0)$. For a Markov process the latter properties are sufficient to determine the stationary character of the process since all joint probabilities can be expressed in terms of one-time and transition probabilities only.

Property (4.4) immediately implies that in a stationary process the the correlation between any number of observables, $A_1, \ldots, A_n$, evaluated at different times $t_1 \leq \ldots \leq t_n$, is invariant under translations of time, irrespective of the values of the time differences

$t_2 - t_1, \ldots, t_n - t_{n-1}$,

$$C_{A_n A_{n-1} \ldots A_1}(t_n + \Delta, \ldots, t_1 + \Delta) = C_{A_n A_{n-1} \ldots A_1}(t_n, \ldots, t_1) \ .$$

In particular, one has $C_{AB}(t, t') = C^{st}_{AB}(t - t')$. Similarly, one proves that the multi-time linear responses are also stationary when (4.4) holds.

An *ergodic* Markov chain is such that all possible configuration, *i.e.* all possible values of $\vec{x}$, are accessible from any initial condition.

4.3.2 The master equation

Let us now focus on a Markov chain. The evolution of the conditional probability density $P(\vec{x}, t_k | \vec{x}', t_0)$ on the time sequence $t_0, \ldots, t_n$, is determined by the *master equation*

$$\begin{aligned} P(\vec{x}, t_{k+1} | \vec{x}'', t_0) - P(\vec{x}, t_k | \vec{x}'', t_0) = & - \sum_{\vec{x}'} T(\vec{x}', t_{k+1} | \vec{x}, t_k) P(\vec{x}, t_k | \vec{x}'', t_0) \\ & + \sum_{\vec{x}'} T(\vec{x}, t_{k+1} | \vec{x}', t_k) P(\vec{x}', t_k | \vec{x}'', t_0) \ . \end{aligned} \tag{4.5}$$

Sometimes, one simplifies the notation and writes $P(\vec{x}, t)$ for the unknown in this equation, with the initial condition $P(\vec{x}, t_0)$ kept implicit. The LHS is the definition of the change in the probability dentisty between the subsequent times t_k and t_{k+1}. The RHS has two contributions : the first (negative) term represents the process of leaving the configuration $\vec{x}$, the second (positive) term represents the process of reaching the configuration $\vec{x}$.

The master equation (4.5) can be written in a *matricial* form. Indeed, one recasts it as

$$P(\vec{x}, t_{k+1} | \vec{x}'', t_0) = \sum_{\vec{x}'} W(\vec{x}, t_{k+1} | \vec{x}', t_k) P(\vec{x}', t_k | \vec{x}'', t_0) \tag{4.6}$$

with the matrix W written in terms of the transition probabilities, T.

Balance and detailed balance.

Any stationary solution to the master equation satisfies

$$\sum_{\vec{x}'} T(\vec{x}', t_{k+1} | \vec{x}, t_k) P_{st}(\vec{x}) = \sum_{\vec{x}'} T(\vec{x}, t_{k+1} | \vec{x}', t_k) P_{st}(\vec{x}') \qquad \forall \ \vec{x}. \tag{4.7}$$

This equation is called *balance* and it is a necessary condition to allow for a steady state. The balance condition may admit many solutions. *Detailed balance* is a restatement of the invariance of the dynamics under time-reversal in a probabilistic sense. It states that, in the steady state, any transition is balanced by its time-reversed,

$$T(\vec{x}', \delta | \vec{x}, 0) P_{st}(\vec{x}) \ = \ T(\vec{x}^R, \delta | \vec{x}'^R, 0) P_{st}(\vec{x}'^R) \ , \tag{4.8}$$

and the stationary measure is also invariant under time-reversal,

$$P_{st}(\vec{x}) \ = \ P_{st}(\vec{x}^R) \ . \tag{4.9}$$

We classified the stochastic variables of a system depending on their parity properties under time-reversal

$$x_i^R(t) \equiv x_i(-t) = \epsilon_i x_i(t) \quad \text{with} \;\; \epsilon_i = \pm 1 \; ,$$

for even and odd variables, respectively. One can check that detailed balance implies balance.

When the number of possible 'microstates' $\vec{x}$ is finite, detailed balance is sufficient (though not necessary) to ensure that the stochastic process approaches its stationary distribution function for long times.

As an example let us consider a particle system characterized by the positions and momenta of each particle. A transition corresponds to modifying the position and momentum of one particle from $(\vec{r}, \vec{v})$ to $(\vec{r}', \vec{v}')$. Since the backwards motion from $\vec{r}'$ to $\vec{r}$ occurs in the opposite direction, the reversed transition corresponds to modifying $(\vec{r}', -\vec{v}')$ into $(\vec{r}, -\vec{v})$. Detailed balance requires that these two processes be equiprobable when the system attained its stationary state, *i.e.*

$$\begin{aligned} P_{st}(\vec{r}', \vec{v}', \delta; \vec{r}, \vec{v}, 0) &= P_{st}(\vec{r}, -\vec{v}, \delta; \vec{r}', -\vec{v}', 0) \\ T(\vec{r}', \vec{v}', \delta | \vec{r}, \vec{v}, 0) P_{st}(\vec{r}, \vec{v}) &= T(\vec{r}, -\vec{v}, \delta | \vec{r}', -\vec{v}', 0) P_{st}(\vec{r}', -\vec{v}') \; . \end{aligned} \tag{4.10}$$

Note that these conditions ensure that the master equation admits a stationary solution. We still do not know if this solution is the only one or whether the process converges, asymptotically, to it. We shall discuss these two questions in Sect. 4.3.3. Furthermore, we have to determine, in as much generality as possible, when the stationary solution coincides with the equilibrium measure $P_{st}(\vec{x}) = P_{eq}(\vec{x})$. We shall come back to these very important issues later. Finally, we have not discussed here the effect of external fields on the time-reversal properties of a stochastic process. The external fields should also be time-reversed in the RHS of the generalized (4.8).

4.3.3 The Fokker-Planck equation

The integral Chapman-Kolmogorov equation can be transformed into a differential equation under certain assumptions. Several textbooks describe this derivation [28]. Here we summarize some of the forms that this equation can take.

Kramers-Moyal expansion.

Starting from the Chapman-Kolmogorov equation, Kramers and Moyal derived a general differential equation for the conditional probabilities. This equation involves a series in which the coefficients are related to the momenta of the conditional probability. For non-Markov systems these coefficients depend on the full history of the process. For Markov processes the differential equation is local in time but it might involve an infinite number of terms. When the Kramers-Moyal expansion stops after the second term, as happens for Langevin processes with additive noise, we are left with a *Fokker-Planck equation* (see

also below). In the case where the process does not 'jump', *i.e.* all displacements become small in the limit $\delta \to 0$, one can write [28] :

$$\frac{\partial P(\vec{x},t|\vec{x}',t')}{\partial t} = -\frac{\partial}{\partial x_i}\left[D_i^{(1)}(\vec{x},t)P(\vec{x},t|\vec{x}',t')\right] + \frac{\partial^2}{\partial x_i \partial x_j}\left[D_{ij}^{(2)}(\vec{x},t)P(\vec{x},t|\vec{x}',t')\right] \tag{4.11}$$

The *drift* $D_i^{(1)}(\vec{x},t)$ and the *diffusion constants* $D_{ij}^{(2)}(\vec{x},t)$ are given by :

$$\begin{aligned} D_i^{(1)}(\vec{x},t) &= \lim_{\delta\to 0}\frac{1}{\delta}\int d\vec{x}'\,(x'-x)_i T(\vec{x}',t_{k+1}|\vec{x},t_k) \\ D_{ij}^{(2)}(\vec{x},t) &= \lim_{\delta\to 0}\frac{1}{2!\delta}\int d\vec{x}'\,(x'-x)_i(x'-x)_j T(\vec{x}',t_{k+1}|\vec{x},t_k). \end{aligned} \tag{4.12}$$

The names given to these coefficients reflect their underlying physical nature, as will be clear below. The above Fokker-Planck equation describes a Brownian motion process with a local and time dependent drift and diffusion constants. There are however a much wider class of processes that admit a continuous time limit, although they lose the property of being continuous (in $\vec{x}$). Suppose that the process can make jumps of non vanishing amplitude, but more and more as $\delta \to 0$, such that the contribution to the transition probabilities $T(\vec{x}',t_{k+1}|\vec{x},t_k)$ corresponding to these jumps are proportional to δ. In this case, the Kramers-Moyal expansion must contain non local spatial terms, corresponding to these jumps, and reads

$$\begin{aligned} \frac{\partial P(\vec{x},t|\vec{x}',t')}{\partial t} &= -\frac{\partial}{\partial x_i}\left[D_i^{(1)}(\vec{x},t)P(\vec{x},t|\vec{x}',t')\right] + \frac{\partial^2}{\partial x_i \partial x_j}\left[D_{ij}^{(2)}(\vec{x},t)P(\vec{x},t|\vec{x}',t')\right] \\ &+ \int d\vec{x}''\left[\frac{\hat{T}(\vec{x},t+\delta|\vec{x}'',t)}{\delta}P(\vec{x}'',t|\vec{x}',t') - \frac{\hat{T}(\vec{x}'',t+\delta|\vec{x},t)}{\delta}P(\vec{x},t|\vec{x}',t')\right], \end{aligned} \tag{4.13}$$

where the last term describes the jumps in the trajectories of the stochastic process, and $\hat{T}$ the corresponding transition probabilities. That the above decomposition between a (continuous) Brownian diffusion component and a jump component is unique in the continuous time limit is the content of the work of P. Lévy on infinitely divisible processes, and is called the *Lévy decomposition*. In some cases, the jump component admits a fractional derivative representation, generalizing the second order diffusion term. This corresponds to what is known as *Lévy flight processes* [39].

When the jump processes vanish, the Fokker-Planck equation can be recast in the form of a *local conservation law*. Indeed, defining the *probability current*

$$J_i(\vec{x},t|\vec{x}',t') \equiv D_i^{(1)}(\vec{x},t)P(\vec{x},t|\vec{x}',t') - \sum_j \frac{\partial}{\partial x_j}D_{ij}^{(2)}(\vec{x},t)P(\vec{x},t|\vec{x}',t')\,,$$

it becomes

$$\frac{\partial P(\vec{x},t|\vec{x}',t')}{\partial t} = -\sum_i \frac{\partial J_i(\vec{x},t|\vec{x}',t')}{\partial x_i}\,.$$

Two special cases : Kramers and Smoluchowski.

The Kramers and Smoluchowski equations are particular cases that hold exactly for a linear Langevin process with white additive noise. The probability distribution of the thermal noise, $P(\xi)$, induces a time-dependent probability distribution of the dynamic variables $\vec{x}$ and $\vec{v}$:

$$P(\vec{x},\vec{v},t) \equiv \int \mathcal{D}\xi\, P(\xi)\, \delta\left(\vec{x}-\vec{x}_\xi(t)\right) \delta\left(\vec{v}-\vec{v}_\xi(t)\right) \ , \tag{4.14}$$

where we adopted the short-hand notation $P(\vec{x},\vec{v},t)$ for the conditional probability $P(\vec{x},\vec{v},t|\vec{x}',\vec{v}',t')$.

In the overdamped limit, the velocity $\vec{v}$ is slaved to the local force and $P(\vec{x},\vec{v},t)$ is replaced by an exclusive function of $\vec{x}$:

$$P(\vec{x},t) \equiv \int \mathcal{D}\xi\, P(\xi)\, \delta\left(\vec{x}-\vec{x}_\xi(t)\right) \tag{4.15}$$

that is determined by the following Fokker-Planck equation (also called *Smoluchowski equation* in this context) :

$$\gamma \frac{\partial P(\vec{x},t)}{\partial t} = \frac{\partial}{\partial x_i}\left[P(\vec{x},t)\,\frac{\partial V(\vec{x})}{\partial x_i}\right] + T\frac{\partial^2}{\partial x_i^2} P(\vec{x},t) \ , \tag{4.16}$$

with the initial condition $P(\vec{x}_0,t_0)$. [Note that this equation actually applies to the conditional probability $P(\vec{x},t|\vec{x}_0,t_0)$.]

In the case where inertia cannot be neglected, and noise is additive, one can establish that the probability density $P(\vec{x},\vec{v},t)$ satisfies a first order differential *Kramers equation* :

$$\begin{aligned} \frac{\partial P(\vec{x},\vec{v},t)}{\partial t} &= -\frac{\partial}{\partial x_i}\left(v_i P(\vec{x},\vec{v},t)\right) \\ &\quad + \frac{1}{m}\frac{\partial}{\partial v_i}\left[\left(\gamma v_i + \frac{\partial V(x)}{\partial x_i} + \frac{\gamma T}{m}\frac{\partial}{\partial v_i}\right) P(\vec{x},\vec{v},t)\right] \end{aligned} \tag{4.17}$$

with the initial condition $P(\vec{x}_0,\vec{v}_0,t_0)$.

It is very important to note that the balancing of factors on the RHS of the Kramers and Smoluchowski equations is a direct consequence of the equilibration of the noise (see Sect. 4.1.2) when the equations derive from a Langevin process. It is totally equivalent to the relation (4.10) between the strength of the noise-noise correlator and the friction coefficient. More generally, it is a particular case of the detailed-balance condition (4.8), that calling $H_{fp}(\vec{x})$ the operator acting on $P(\vec{x},t)$ in the RHS of the Fokker-Planck equation, reads

$$H_{fp}(\vec{x}) P_{st}(\vec{x}) = P_{st}(\{\epsilon_i x_i\}) H_{fp}^\dagger(\{\epsilon_i x_i\}) \ . \tag{4.18}$$

The Fokker-Planck equation for a stochastic field.

A Fokker-Planck equation can also be deduced for a stochastic variable that is actually a d-dimensional field, $\vec{\phi}(\vec{x},t) = (\phi_1(\vec{x},t),\ldots,\phi_d(\vec{x},t)$. It the natural generalization of the equations presented in the previous section. In the Smoluchowski limit, and for additive noise it reads

$$\frac{\partial P(\vec{\phi},t)}{\partial t} = \frac{\delta}{\delta\phi_a(\vec{x},t)}\left[P(\vec{\phi},t)\frac{\delta V[\phi]}{\delta\phi_a(\vec{x},t)}\right] + T\frac{\delta}{\delta\phi_a^2}P(\vec{\phi},t)\ .$$

Approach to stationarity.

Under rather mild conditions one can prove that if a stochastic process governed by a generic master equation admits a stationary state asymptotically, this one is unique. We present a proof of this statement below. A very simple exception to this rule is given by "decomposable" systems made of two or more non-interacting systems in which case one can construct several stationary asymptotic solutions given by linear superpositions with arbitrary coefficients of the stationary solution for each subsystem. Another case of exceptions is given by certain problems with a continuous set of possible states. We shall not discuss these special cases here but focus on the more generic situation.

Possibly, the simplest way to test under which conditions the time-dependent solution to the Fokker-Planck equation approaches a stationary form asymptotically is to use the "$\mathcal{H}$-theorem' [31, 30]'. The $\mathcal{H}$-functional or Lyapunov-functional

$$\mathcal{H}_{P_1,P_2}(t) \equiv \int d\vec{x}\, C\left(\frac{P_1(\vec{x},t)}{P_2(\vec{x},t)}\right)\, P_2(\vec{x},t)\ , \tag{4.19}$$

measures a "distance" between the (normalised) PDFs, P_1 and P_2. $C(y)$ is any strictly convex function, i.e., it satisfies $\sum_i C(\omega_i y_i) > \sum_i C(y_i)\omega_i$ for $\sum_i \omega_i = 1$ and $\omega_i \geq 0$. Customarily one uses $C(x) = x\ln x$ which suggests to relate $\mathcal{H}$ to a non-equilibrium extension of the entropy concept via $S(t) = S_o - \mathcal{H}(t)$ with S_o the thermodynamic entropy.

Now, $\mathcal{H}_{P_1,P_2}(t)$ is bounded from below and it is a monotonic decreasing function of time when (a) the diffusion matrix $D^{(2)}_{ij}$ is positive definite[9], (b) the drift matrix does not have singularities (that correspond to infinite high barriers that render the problem decomposable) and (c) P_1 and P_2 are different from zero away from infinity. Thus, the distance between any two normalized solutions vanishes asymptotically.

When the drift and diffusion matrices do not depend on time, the Fokker-Planck equation may admit a stationary solution. Based on the above argument, any other normalized solution necessarily approaches the stationary one in the long-time limit. Two types of stationary solution can be identified. The simpler ones have constant current $J_i(\vec{x}) = J_i$ fixed by the boundary conditions. Natural boundary conditions demand $J_i = 0$, when $x_j \to \infty$ for all j, thus, $J_i = 0$ everywhere in space, in which case the stationary solution

[9]The argument needs to be slightly modified for the Kramers equation given that its diffusion matrix is not positive definite; still, one also proves that the asymptotic solution is unique in this case [30].

takes the *potential form*

$$P_{st}(\vec{x}) \propto e^{-\phi(\vec{x})} , \qquad \phi(\vec{x}) = -\int_{\vec{x}} dx'_k \left[{D^{(2)}_{ki}}^{-1}(\vec{x}') \left(D^{(1)}_i(\vec{x}') - \frac{\partial D^{(2)}_{ij}(\vec{x}')}{\partial {x_j}'} \right) \right]$$

where a sum over repeated indices is assumed. In the simple case $D^{(1)}_i(\vec{x}) = -\partial_{x_i} V(\vec{x})$ and $D^{(2)}_{ij}(\vec{x}) = T\delta_{ij}$ one easily checks that this expression becomes the Boltzmann factor. The question then arises as to whether an explicit solution is possible when the drift term is not of a potential form.

Another family of solution correspond to non-equilibrium steady states (NESS) with a divergenceless, time-independent current that is not necessarily constant in space. When the drift term itself is divergenceless and $D^{(2)}$ is constant – corresponding for example to tracer particles advected by a incompressible convection flow and subject to molecular diffusion – then the NESS is trivial and is given by $P_{st}(\vec{x}) = 1/V$, where V is the total volume accessible to the particle. The local current is then given by $J_i = D^{(1)}_i(\vec{x})/V$ and is by construction divergenceless. Another case that can be solved in full generality is when the drift term is the sum of a potential part and a divergenceless part that are everywhere orthogonal to each other. Then, the divergenless part simply advects the particles along equi-potential lines and does not modify the standard equilibrium Boltzmann factor. In the completely general case of an arbitrary drift and diffusion structure, there are in general no explicit construction of the NESS.

Approach to equilibrium.

Whether a stochastic process approaches equilibrium asymptotically depends on the nature of the forces applied, the boundary conditions, etc. In the following we shall focus on Fokker-Planck processes with no jumps. Among these, a subclass admit a spectral representation of the Fokker-Plank operator with generic complex eigenvalues. The asymptotic analysis has to be performed on a case-by-case basis.

A more restrictive class of systems are represented by self-adjoint FP operators. The potential case, $D^{(2)}_{ij} = T\delta_{ij}$ and $D^{(1)}_i = -\partial_{x_i} V$, is a special problem in this class and one proves that the process does indeed approach a stationary solution that is given by the canonical equilibrium measure.

An easy and elegant proof of this statement, for a Smoluchowski potential problem relies on a mapping of the Fokker-Planck equation to the Schrödinger equation [**?**]. Introducing

$$P(\vec{x}, t) \equiv c\, e^{-\frac{\beta}{2} V(\vec{x})}\, p(\vec{x}, t) \tag{4.20}$$

with c a positive constant the Fokker-Planck equation becomes

$$\begin{aligned} \frac{\partial p(\vec{x}, t)}{\partial t} &= \left[T \frac{\partial^2}{\partial x_i^2} - \left(-\frac{1}{2} \frac{\partial^2 V(\vec{x})}{\partial x_i^2} + \frac{\beta}{4} \left(\frac{\partial V(\vec{x})}{\partial x_i} \right)^2 \right) \right] p(\vec{x}, t) \\ &= -L_s p(\vec{x}, t) . \end{aligned} \tag{4.21}$$

This is a Schrödinger equation in imaginary time. The potential energy term, say V_s, is a function of the original potential V. $p(\vec{x},t)$ is related to the probability density and plays the role of a wave function, while in true quantum mechanics it is the modulus squared of the wave function which has a probability interpretation. The operator L_s admits a spectral representation in terms of its eigenvalues λ_n and its eigenvectors ψ_n. Since the potential V_s is independent of time, the eigenvectors, ψ_n, are time-independent, $\psi_n(\vec{x})$. If the potential V_s grows to infinity sufficiently fast when $x_i \to \pm\infty$, for all i, the spectrum is discrete and there is gap between the lowest eigenvalue, λ_0, and the first excited state, λ_1. The ground state wavevector is everywhere positive and can hence describe a probability. One can also show that the operator L_s can be written as the square of a certain operator, and is thus positive semi-definite in a Hilbert space[10] and the eigenvalues, λ_n, are real and satisfy $\lambda_n \leq 0$.

The solution to eqn (4.21) can be expressed as the series

$$p(\vec{x},t) = \sum_n c_n \psi_n(\vec{x}) e^{-\lambda_n t} \,, \tag{4.22}$$

with c_n arbitrary numerical constants. When a stationary solution exists, the operator has a vanishing eigenvalue, $\lambda_0 = 0$, that, if the conditions mentioned in the previous subsection are satisfied, is not degenerate. One has $p_{st}(\vec{x}) = c_0\psi_0(\vec{x})$. The eigenstates associated to non-zero eigenvalue can be degenerate in which case one needs a more refined notation to distinguish their associated eigenvectors. We skip this detail and we continue to use the simplified notation above. If there is a gap in the spectrum, $\lambda_1 > 0$, in the long-time limit only the contribution of the zero eigenvalue survives and $p(\vec{x},t) \to p_{st}(\vec{x}) = c_0\psi_0(\vec{x})$. The constant c_0 is fixed to one by the normalization of the probability. Indeed, $c_0 = \int d\vec{x}\psi_0(\vec{x})p(\vec{x},0) = \int d\vec{x}P(\vec{x},0) = 1$.

Going back to the original PDF, $P(\vec{x},t)$, one has

$$\lim_{t\to\infty} P(\vec{x},t) = \psi_0^2(\vec{x}) = c^2 e^{-\beta V(\vec{x})} = \frac{e^{-\beta V(\vec{x})}}{\int d\vec{x}\, e^{-\beta V(\vec{x})}}$$

where we used the conservation of probability to compute c^{-2}. Thus P_{eq} is indeed the asymptotic solution to the Fokker-Planck equation.

Note that this argument assumes that a sufficiently long t ($t > t_{eq}$) is reached such that only the $\lambda_0 = 0$ term survives in the sum. This hypothesis does not hold in the asymptotic analysis for the relaxing models we analyze in the next Sections. If the next eigenvalue λ_1 does not vanish, its inverse is the time-scale needed to equilibrate the model. If however, there is no gap in the spectrum, one does not have a simple argument to estimate how long one should wait until the asymptotic limit is reached. This is a question that will be raised regularly in the treatment of glassy dynamics. Moreover, when non-potential or time-dependent forces are exerted on the system the transformation (4.20) is not sufficient to deal with their effect and equilibrium cannot be established.

[10]This space is defined via the scalar product $(f,g) \equiv \int d\vec{x} f(\vec{x})g(\vec{x})/P_{st}(\vec{x})$ and an operator $\mathcal{L}$ is self-adjoint if $(f,\mathcal{L}g) = (\mathcal{L}f,g)$.

Since the eigenvectors corresponding to excited states are not everywhere positive, one cannot interpret $\psi_0\psi_n$ directly as a probability. Interestingly however, one can construct linear combination of these that can be interpreted as *metastable states*, that can be defined as states with lifetimes longer than a certain fixed but long time-scale.

4.4 Montecarlo

This is a numerical technique to simulate the temporal evolution of a system including the stochastic effect of its coupling to a heat bath. It was introduced by Metropolis, Rosenbluth, Rosenbluth, Teller and Teller in 1953 [J. Chem. Phys. **21**, 1087 (1953)]

One uses a master equation with transition probabilities that satisfy detail balance. At each step a spin in the sample, say s_i, is chosen at random. It is then turned with probability

$$W_i = \begin{cases} e^{-\Delta E_i/T} & \Delta E_i \geq 0 \,, \\ 1 & \Delta E_i < 0 \,, \end{cases} \tag{4.23}$$

where $\Delta E_i = E(-s_i) - E(s_i)$ where E is the energy of the system and $-s_i$ is the reversed value of the spin s_i. The spin flips whether W_i exceeds a random number taken from a uniform distribution between 0 and 1. This rule implies that all updates that are favourable in energy ($\Delta E_i < 0$) are accepted while some updates that increase the energy of the system are also acceped [with probability (4.23)]. These *a priori* unfavourable moves might help the system get out of metastable configurations and reach equilibrium. The unit of time is defined as a Montecarlo sweep, that is to say, N attemps to flip a spin (note that due to the random choice of spins, some will appear more than once and others will not appear within the N chosen ones).

If the system at hand is such that the equilibration time is relatively short at the working temperature, T, after a short transient the configurations obtained with the Montecarlo sampling are typical of the the equilibrium measure at T. This means the Montecarlo code generates configurations with probability the Gibbs-Boltzmann probability density. This remark allow one to compute *equilibrium averages* using *temporal averages* :

$$\langle \mathcal{O} \rangle_{eq} \approx \frac{1}{\Delta t} \sum_{k=1}^{\Delta t} \mathcal{O}_k \tag{4.24}$$

where k labels the Montecarlo steps, Δt is a sufficiently long Montecarlo time-interval (after equilibration) and $\mathcal{O}$ is a generic observable. The average on the left is the theoretical equilibrium one.

The equilibrium Montecarlo method is an *importance sampling* one in the sense that instead of averaging over all the possible configurations of the system (of the order of $2^N = e^{N \ln 2}$ in an Ising spin system, where N is the number of spins in the sample) one just averages over a much smaller number of configurations (typically of the order of N

instead of the order of an exponential of N) obtaining still results that estimate rather accurately the exact value.

The convergence of the Montecarlo method to the equilibrium measure is ensured by the considerations presented in the previous Subsections (note that the dynamics satisfies detailed balance). In some cases (glassy systems) the Montecarlo time needed to reach the equilibrium measure can be a very rapidly growing function of the number of variables in the problem and equilibration can fall beyond the reachable time-window. In these cases it becomes interesting to study the dynamics of the system.

4.5 Lattice field theory

The definition of quantum gaude theories on an Euclidean space-time lattice was proposed by K. Wilson in 1974. The lattice spacing provides a natural short length-scale cut-off and the ultraviolet diverges are regularized. In this way the theory can be studied both in the weak and strong coupling limits. This method is thus specially suited to treat problems where perturbation techniques fail, such as QCD. In particular, essentially strong-coupling phenomena like quark confinement can be searched and found in lattice QCD.

Still, a difficult problem remains to be solved before achieving full success with this approach : the lattice spacing has to be eventually sent to zero. In this process the *bare* coupling constants, say g_0, get renormalized (in complete analogy to the renormalization group calculations of statistical models, such as the Ising chain discussed in Sect. 2.6.3). In other words, a relation between a and g develops : g depends on the observation scale. The continuum limit is well behaved only if the running coupling constants reach a stable fixed point. This statement is rather difficult to prove analytically for generic theories – including those of interest in particle physics. One then resorts to an alternative route, computer simulations.

Indeed, having defined the theory on a lattice the similarity with statistical mechanics and condensed matter problems becomes apparent. The lattice gauge theories can then be studied with numerical simulations and, in particular, Montecarlo thechniques.

Let us sketch how a lattice gaude theory is defined. For concreteness we use again (*cfr.* Sect. 2.6.3) a scalar (mass) field ϕ coupled to a gauge field A.

- Time is Wick rotated to construct an Euclidean $1+d$ dimensional space-time.
- One identifies the Euclidean action $S_E(\phi, A)$ that also depends on the coupling constants (mass, coupling strength, *etc.*)
- The path-integral expression for the average of any observable $\mathcal{O}(\phi, A)$ reads

$$\langle\, \mathcal{O}\, \rangle \;=\; Z^{-1} \int \mathcal{D}\phi \mathcal{D}A\; \mathcal{O}(\phi, A)\, e^{-\frac{1}{\hbar} S_E[\phi, A]}\;, \tag{4.25}$$

$$Z \;=\; \int \mathcal{D}\phi\phi \mathcal{D}A\; e^{-\frac{1}{\hbar} S_E[\phi, A]}\;, \tag{4.26}$$

cfr. eq. 2.66. The quantity Z is called *vacuum-to-vacuum permanence amplitude* in the quantum field theoretical context and it is just the *partition function* in the

statistical sense.
- If one is interested in Minkowski space-time results the averages in (4.25) should be continued back.
- Let us now define the theory on the lattice. We first focus on a purely scalar field theory (ignoring, for the moment, the gauge field A). Space-time is defined as a typically hypercubic lattice with lattice spacing a and *finite* volume V. The field is defined on the *vertices of lattice* : $\phi(\vec{x}) \to \phi_i$ where i labels the lattice sites. The derivatives in S_E are replaced by finite differences. The functional integrals become ordinary integrals.
- Without entering into the details, it turns out that to respect gauge invariance, one is forced to define the gauge fields on the *plaquettes* (and not on the sites).

4.6 Stochastic quantization

The basic idea of the method of stochastic quantization is to interpret the factor

$$\frac{e^{-\frac{1}{\hbar}S_E[\phi]}}{\int \mathcal{D}\phi e^{-\frac{1}{\hbar}S_E[\phi]}} \ . \tag{4.27}$$

as the stationary distribution of a stochastic process running on a *fictitious time*. The steps to follow are then
- $1+d$-dimensional Euclidean space is enlarged to include a new coordinate t.
- The system of interest is assumed to be in contact with a (classical) heat bath at temperature $T = \hbar/k_B$.
- The most natural stochastic evolution ensuring (for sufficiently well-behaved S_E) the approach to the equilibrium measure (4.27) is a Langevin equation

$$\partial_t \phi(\vec{x},t) = -\frac{\delta S_E[\phi]}{\delta\phi(\vec{x},t)} + \eta(\vec{x},t) \ . \tag{4.28}$$

  S_E a generalization of the original Euclidean action that includes an integration over the fictitious time t :

$$S_E = \int dt \int d^{1+d}x \ \mathcal{L}[\phi(\vec{x},t), \vec{\nabla}_x \phi(\vec{x},t)] \ . \tag{4.29}$$

  η is a white Gaussian noise with zero mean and variance proportional to $k_B T$.
- Correlations are now defined by performing the averages over the thermal noise. For well-behaved S_E that ensure the approach to equilibrium one then has

$$\lim_{t\to\infty} \langle\, \phi(\vec{x}_1,t) \dots \phi(\vec{x}_n,t) \,\rangle = \langle\, \phi(\vec{x}_1) \dots \phi(\vec{x}_n) \,\rangle \tag{4.30}$$

  where the right-hand-side is the expectation value of the n-point correlation function in the quantum field theory. This result is just a consequence of the discussion in this Section.

Extensions of this approach to **Abelian and non-Abelian gauge field theories**, **fermionic field theories**, **supersymmetric field theories**, field theories defined in **Minkowski space**, *etc.* exist and have been discussed in [**?**, 33]. An advantage of stochastic quantization with respect to other methods is that it is not necessary to fix the gauge in a gaude field theory : the stochastic averages of gauge-invariant observables do converge while non-invariant Green functions do not have an equilibrium limit. The equilibrium expressions of the stochastic averages have always been found to agree with the ones computed using ordinary gauge-fixed perturbation theory.

5 Dynamics of phase transitions

An interface is a frontier separating two regions of space occupied by different phases. It could be the border between water and oil in a liquid mixture, the border between regions with positive and negative magnetization in a magnet, the limit of a fluid invading porous media, *etc.* The static and dynamic properties of interfaces have many points in common with the ones of (sometimes directed) manifolds with d internal dimensions embedded in $N + d$ dimensional spaces with N the dimension of the transverse space, see eq. (**??**). In this way, one includes cases such as directed lines ($d = 1$) that mimic vortex lines in $N+d = 3$ dimensional high-T_c superconductors, polymers in ($N+d = 2$ or 3-dimensional) random media, *etc.*

A slighly different situation is the one of *growth* phenomena, as for instance, the burning front in a forrest, the advance of a crack in a rock, fluid invation in porous media, the growth of semiconductors *via* epitaxial beam, or even the growth of bacterial colony.

As a physicist one would like to characterize the static and dynamic properties of these interfaces and surfaces. The analysis os the static properties of domain walls and interfaces corresponds, typically, to determining their equilibrium conformations (geometric properties, numbers, degeneracies, etc.) The study of the dynamic properties of domain walls and interfaces includes the analysis of their relaxation to equilibrium, response to external driving forces, creep motion and the depinning transition.

Domain growth and interface frowth in the presence of quenched disorder is sometimes considered to be a 'baby' spin-glass problem due to the presence of frustration given by the competition between the elastic energy that tends to reduce the deformations and quenched disorder that tends to distort the structure.

5.1 Scale invariance

In general, the morphology of an interface depends on the length scale of observation : the Alps look rough on Earth but they look smooth seen from the Moon. However, a number of surfaces called *self-similar* do not depend on the scale of observation ; they are characterized by the absence of a characteristic scale. Such scale-invariance is ubiquotous in nature, with the classical example of critical phenomena, and it is characterized by the existence of power laws that characterize many quantities over many orders of magnitude.

5.2 Domain growth

Take a magnetic system, such as the ubiquitous Ising model, and quench it into the low temperate phase starting from a random initial condition. In the course of time neighbouring spins realize that their preferred configuration is an ordered one and domains of the two ordered phases form and grow. At any finite time the configuration is such that

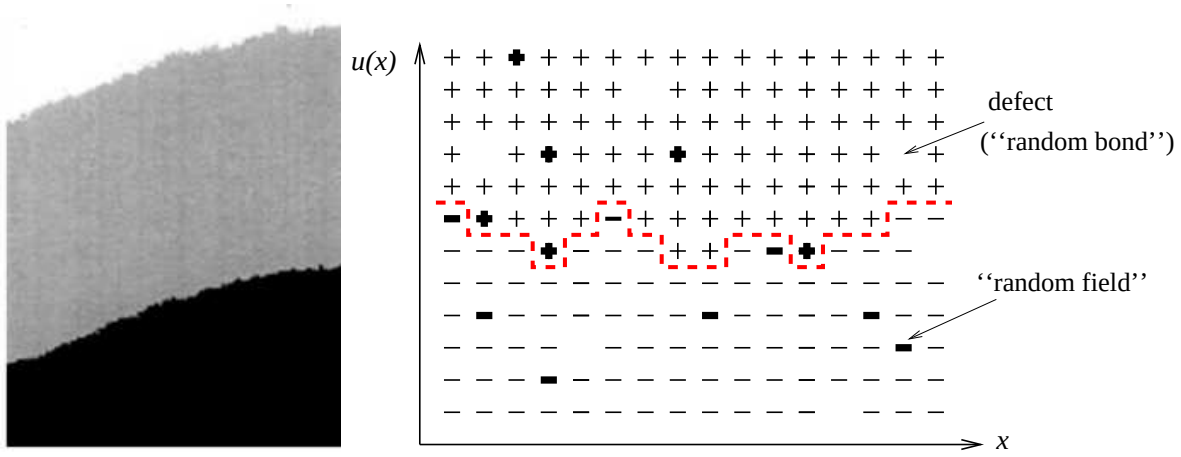

FIG. 11 – Left : an experimental view of a domain wall. Right : a sketch of a domain wall in a $2d$ Ising magnet.

both types of domains exist. The magnetization is zeroupto corrections in the inverse system size.

The domain growth kinetics in systems undergoing an ordering process after a quench is an important problem for material science applications but also for our understanding of pattern formation in nonequilibrium systems. The late stage dynamics is believed to be governed by a few properties of the systems whereas material details should be irrelevant. Among these relevant properties one may expect to find the number of degenerate gound states, the nature of the conservation laws and the hardness or softness of the domain walls. Thus, classes akin to the universality classes of critical phenomena have been identified.

5.2.1 Discrete models

The dynamics of discrete spin models is defined via a stochastic rule, of the type introduced in Sects. **??** and **??**. Time-dependent macroscopic observables are then expressed in terms of the values of the spins at each time-step. For instace, the magnetization density and its two-time self correlation function are defined as

$$m(t) \equiv N^{-1} \sum_{i=1}^{N} \langle\, s_i(t) \,\rangle \;, \qquad C(t,t_w) \equiv N^{-1} \sum_{i=1}^{N} \langle\, s_i(t) s_i(t_w) \,\rangle \tag{5.1}$$

where the angular brackets indicate an average over many independent runs of the dynamic rule starting from identical initial conditions. Averages over different initial conditions can also be taken.

This formulation of the domain growth process is very convenient to for computer simulations.

5.2.2 Continuous models

Coarsening occurs in lattice models with a phase transition from a disordered to an ordered phase. The Ising model is an example. In order to describe this process theoretically it is convenient to introduce a coarse-grained description in terms of an order parameter, the magnetization density,

$$\phi(\vec{x},t) \equiv \frac{1}{V}\sum_{i\in V_{\vec{x}}} s_i(t) \ . \tag{5.2}$$

For simplicity, we consider a scalar field ϕ but cases in which vectorial or even tensorial order parameters are also of experimental relevance.

The Landau-Ginzburg free-energy functional that characterizes equilibrium is

$$F[\phi] = \int d^dx \ \left\{ \frac{c}{2}\left[\nabla\phi(\vec{x},t)\right]^2 + V[\phi(\vec{x})] \right\} \tag{5.3}$$

with

$$V(\phi) = (\phi_0^2 - \phi^2)^2 \ . \tag{5.4}$$

The first term in (5.3) represents the energy cost to create a domain wall. It represents the elasticity of the interface, see the discussion leading to eq. (**??**). The second term has a double well structure with two minima, at $\phi = \pm\phi_0$, that correspond to the equilibrium states at low temperatures.

In most cases, the domain wall and interface dynamics is *overdamped*. It is then given by the *time-dependent Ginzburg-Landau* equation or *model A* in the classification of Hohenberg-Halperin :

$$\frac{\partial\phi}{\partial t} = -\frac{\delta F}{\delta\phi} + \xi \ . \tag{5.5}$$

This equation does not conserve the order parameter ($\langle\phi(\vec{x},t)\rangle$ is not constant but decays as a function of time for generic initial conditions). ξ is a thermal noise usually taken to be Gaussian distributed with zero mean and correlations

$$\langle\, \xi(\vec{x},t)\xi(\vec{x}',t')\,\rangle = 2k_BT\delta^d(\vec{x}-\vec{x}')\delta(t-t') \ . \tag{5.6}$$

Initial conditions are usually taken to be random with short-range correlations or simply

$$[\,\phi(\vec{x},0)\phi(\vec{x}',0)\,] = \Delta\delta(\vec{x}-\vec{x}') \ . \tag{5.7}$$

5.2.3 Scaling hypothesis

The scaling hypothesis states that at late times and in the scaling limit

$$r \gg \xi \ , \qquad R \gg \xi \ , \qquad \text{with} \qquad r/R \ \text{ arbitrary} \ , \tag{5.8}$$

and r a distance between two points in the sample, $r \equiv |\vec{x}-\vec{x}'|$, there exists a *single characteristic length*, $R(t)$, such that the domain structure is, in the statistical sense,

independent of time when lengths are scaled by $R(t)$. This hypothesis has been proved analytically in very simple models only, such as the one dimensional Ising chain with Glauber dynamics or the $O(N)$ model in the large N limit.

Let us explain what the scaling hypothesis means in practice using the coarse-grained notation. The two-time and two-point dependent order-parameter correlation function is

$$C(\vec{x},t;\vec{x}',t') = C(\vec{r};t,t') = \langle \phi(\vec{x},t)\phi(\vec{x}',t')\rangle \tag{5.9}$$

where $\vec{r} \equiv \vec{x} - \vec{x}'$ and we assumed that there is translational invariance in space. The times t and t' are measured from an origin that corresponds to the sample preparation done, usually, with a quench from high temperature. Its Fourier transform is

$$S(\vec{k};t,t') = \langle \phi(\vec{k},t)\phi(-\vec{k},t')\rangle \ . \tag{5.10}$$

In the late stages of the coarsening process the spherically averaged structure factor $S(k,t)$ at equal times $t = t'$ can be measured experimentally with small-angle scattering of neutrons, x-rays or light. In the limits given in (5.8) it has been found to satisfy scaling :

$$S(k,t) \sim m_{eq}^2(T)\ R^d(t)\, G[kR(t)] \ , \tag{5.11}$$

with $m_{eq}(T)$ the equilibrium magnetization density. Correspondingly the real-space correlation function is expected to behave as

$$C(r,t) \sim m_{eq}^2(T)\ F[r/R(t)] \ . \tag{5.12}$$

G is the Fourier transform of F. Similarly, the two-times pair correlation function satisfies

$$C(r;t,t') \sim f\left(\frac{r}{R(t)}, \frac{R(t)}{R(t')}\right) \tag{5.13}$$

As for the strictly local correlation one can argue that in the long waiting-time limit $t' \gg t_0$, it actually separates in two additive terms

$$C(t,t') \sim C_{st}(t-t') + \mathcal{C}(t,t') \tag{5.14}$$

with the first one describing thermal fluctuations within the domains,

$$C_{st}(t-t') \ = \ \left\{ \begin{array}{ll} 1 - q_{ea}(T) = 1 - m_{eq}^2(T) \ , & t - t' = 0 \ , \\ 0 \ , & t - t' \to \infty \ , \end{array} \right. \tag{5.15}$$

and the second one describing the motion of domain walls

$$\mathcal{C}(t,t') \ = \ f_C\left(\frac{R(t)}{R(t')}\right) = \left\{ \begin{array}{ll} q_{ea}(T) = m_{eq}^2(T) \ , & t' \to t \ , \\ 0 \ , & t - t' \to \infty \ . \end{array} \right. \tag{5.16}$$

Note that adding the two contributions one recovers $C(t,t) = 1$ as expected and $C(t,t') \to 0$ when $t \gg t'$.

5.2.4 The averaged domain length

Due to the scaling hypothesis, all information about the system dynamics can be obtained from the knowledge of the time-dependent domain structure. Ideally, one would like to know their size distribution, $\rho(R,t)$, their geometric properties as given by their radious of gyration, surface length, *etc.* These can only be obtained with numerical simulations in generic d in some particular one-dimensional models. Still, it is very difficult to extract detailed meaning information about all domains.

The average domain size $R(t)$ entering the scaling forms is usually determined using several indirect criteria the most common ones being :

– The 'inverse perimeter density'

$$R(t) = -E_{eq}/[U(t) - U_{eq}] \ , \tag{5.17}$$

where $U(t)$ is the averaged energy at time t and U_{eq} is the equilibrium energy, both measured at the working temperature T.

– The fluctuations of the order parameter in an N-spin system

$$R(t) = N \left\langle \left(N^{-1} \sum_{i=1}^{N} s_i \right)^2 \right\rangle \ . \tag{5.18}$$

– The check of the scaling hypothesis.

These quantities are computed with numerical simulations of lattice models or the numerical integration of the continuous partial differential equation for the evolution of the order parameter. In order to avoid finite-size effects, a rule-of-thumb states that the growth has to be stopped when R reaches 0.4 L, with L the linear size of the system. Another limitation is given by the fact that the true asymptotic behaviour may be veiled by crossover effects.

5.2.5 The curvature argument

The time-dependent Ginzburg-Landau model allows us to gain some insight about the mechanism driving the domain growth and the direct computation of the averaged domain length.

Take a domain wall separating regions where the configuration is the one of the two equilibrium states :

$$\phi(\vec{x},t) = \pm\phi_0 + \delta\phi(\vec{x},t) \tag{5.19}$$

Linearizing eq. (5.5) around $\pm\phi_0$ one finds

$$\delta\phi(\vec{x},t) \sim e^{-\sqrt{V''(\phi_0)}n} \tag{5.20}$$

where n is the distance along the normal to the surface. The order parameter appraoches the asymptotic values very rapidly. This means that the free-energy of a configuration

with an interface is concentrated in very narrow region close to it. In consequence, the curvature is the driving force for domain growth in clean systems as this one. The evolution is such that domain walls are render flatter and eventually disappear as time evolves.

The free-energy, $F[\phi]$, of a flat equilibrium interface can be simply evaluated. Its configuration is obtained from eq. (5.5) with $\partial\phi/\partial t = 0$ with border conditions $\phi(\vec{x} \to \infty) = +\pm\phi_0$. It reads $(d\phi/dn)^2 = 2V(\phi)$. Thus, the free-energy per unit area, or surface tension, is

$$\sigma = \int_{-\infty}^{\infty} dn\ (d\phi/dn)^2 = \int_{-\phi_0}^{\phi_0} d\phi\ \sqrt{2V(\phi)}\ . \tag{5.21}$$

The growth law in clean systems with non-conserved order parameter dynamics can be obtained using an argument that is similar to the one leading to the excess pressure inside a bubble. Take a spherical domain of the equilibrium phase $-\phi_0$ inside the other one ϕ_0. Due to the surface tension, there is a force per unit area acting on the domain wall that we call F. The total force on the spherical wall is then FA_d where A_d is its surface. The work done by this force when the radious of the domain goes from R to $R + dR$ is $dW = FA_d dR$. The decrease in surface energy is $dE = E(R + dR) - E(R) = E'(R)dR$ and this can be expressed in terms of the surface tension using $E(R) = \sigma A_d$ and then $E'(R) = \sigma A'_d(R)$. One finds $dE = \sigma A'_d(R)dR$. Thus

$$dW = -dE\ , \qquad \Rightarrow \qquad F = \sigma \frac{\ln dA_d}{dR} \tag{5.22}$$

Now, assuming a compact domain surface, $A_d = \Omega_d R^{d-1}$ with Ω_d and angular factor, and the

$$F = (d-1)\,\sigma\ R^{-1}\ . \tag{5.23}$$

Note that the force is proportional to the curvature of the wall. This force will drive the walls. If the viscosity is η, neglecting the inertia, at zero temperature one has

$$\eta \frac{dR}{dt} = (d-1)\,\sigma\ R^{-1} \tag{5.24}$$

that leads to

$$R(t) \sim t^{\frac{1}{2}}\ . \tag{5.25}$$

Note that the motion of the wall is determined by the local curvature only. The potential is important to determine the two equilibrium states but not to select the velocity of the domain walls.

*** PROVE $\eta = \sigma$ ***

Let us show another way of obtaining the same result. In polar coordinates the equation of motion reads

$$\frac{\partial\phi}{\partial t} = \frac{\partial^2\phi}{\partial r^2} + \frac{d-1}{r}\frac{\partial\phi}{\partial r} - V'(\phi) \tag{5.26}$$

where r is a coordinate along the radious of the spherical domain ($T = 0$). If we introduce the configuration $\phi(r,t) = f(r - R(t))$ in the dynamic equation we find

$$0 = f'' + [(d-1)/r + dR/dt]\ f' - V'(f) \tag{5.27}$$

Multiplying by f' and integrating over r yields

$$R^2(t) = R^2(0) - 2(d-1)t \tag{5.28}$$

This result is the same as the one above provided $\eta = \sigma$.

Summary of growth laws in clean systems

In pure and isotropic systems the domain growth is characterized by a power law

$$R(t) = At^{\phi} \tag{5.29}$$

with ϕ the *growth exponent*.

The averaged radious of the magnetic domains in clean ferromagnetic models has been determined using computer simulation studies of Ising (and Potts) models and with field-theoretical Langevin-like effective equations (the argument above). One finds the so-called *Lifshitz-Allen-Cahn* growth law

$$R(t) = At^{1/2} \tag{5.30}$$

with A a weakly temperature dependent coefficient, independently of the number of equilibrium states (Ising or Potts models). The domain walls are sharp. The domains and their surface are compact (*i.e.* they have dimension d and $d-1$, respectively).

For systems with continuous variables, such as rotors or XY models, and no conserved order parameter, a number of computer simulations have shown that the growth law is

$$R(t) \sim t^{1/4} \, . \tag{5.31}$$

These models support the formation of wider domain walls. This result was hardly debated during some years, since several authors claimed that (5.31) was just a crossover towards the asymptotic regime (5.30), at least at non-zero temperature.

Another question one may would be interested in is characterizing the distribution of the sizes of these domains and its evolution. This is known in $d = 1$ but much less can be said about the higher dimensional problem.

A different type of dynamics occurs in the case of phase separation (the water and oil mixture). In this case, the material is locally conserved, *i.e.* water does not transform into oil but they just separate. Determining the growth and geometrical properties of the domains is already much harder in this case. After some discussion, it was established, as late as in the early 90s, that for systems with *conserved order parameter* as the example at hand, the growth is given by

$$R(t) \sim t^{1/3} \, . \tag{5.32}$$

5.2.6 Role of disorder : the activation argument

The situation becomes much less clear when there is quenched disorder in the form of non-magnetic impurities in a magnetic sample, lattice dislocations, residual stress, etc.

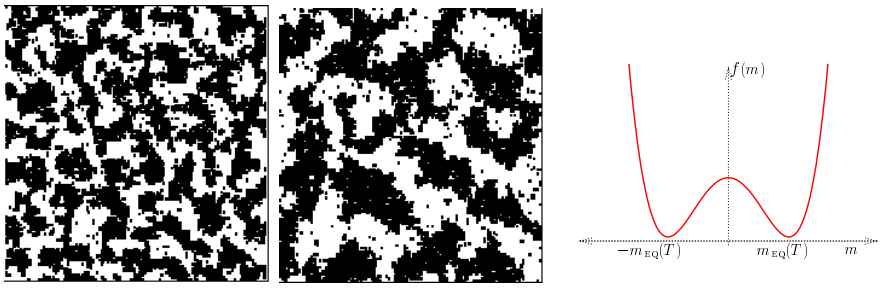

FIG. 12 – Time evolution of a spin configuration ; two snapshots of a $2d$ slice in a $3d$ Ising model on a cubic lattice at $t_w = 1000$, $t_w = 10000$ MC steps in a simulation.

Qualitatively, the dynamics is expected to be slower than in the pure cases. In general, based on the Larkin argument explained in Sect. **??**, one expects that in $d < 4$ the late epochs and large scale evolutions is no longer curvature driven but that disorder controls it. Indeed, disorder generates metastable states that trap the system in its evolution and thus render its relaxation slower. Determining the precise growth law becomes a difficult task.

A hand-waving argument to estimate the growth law in dirty systems is the following. Take a system in one equilibrium state with a domain of the opposite equilibrium state within it. One can mimic this configuration as corresponding to an excited state with respect to the fully ordered one with absolute minimum free-energy. Call $B(R)$ the free-energy barrier between the excited and complete equilibrium states. An Arrhenius argument implies that the time scale for the activated process corresponding to the decay of the excited state (*i.e.* erasing the domain wall) is given by the Arrhenius law

$$\tau \sim \tau_0 e^{B(R)/(k_B T)} \tag{5.33}$$

If

$$B(R) \sim \Upsilon(T) R^{\psi} \tag{5.34}$$

for large R then after a time t one should find domains with an averaged – and typical – size

$$R(t) \sim \left(\frac{k_B T}{\Upsilon(T)} \ \ln t/\tau_0 \right)^{1/\psi} . \tag{5.35}$$

All smaller fluctuation would have disappeared at t while typically one would find this size. The exponent ψ is expected to depend on the dimensionality of space but not on temperature. In 'normal' systems it is expected to just $d-1$ – the surface of the domain – but in spin-glass problems, it might be smaller than $d-1$ due to the assumed fractal nature of the walls. The prefactor Υ is expected to be weakly temperature dependent.

The same argument applies to the reconformations of a portion of any domain wall or interface where R is the observation scale.

However, already for the (relatively easy) random ferromagnet there is no consensus about the actual growth law. In these problems there is a competition between the 'pure' part of the Hamiltonian, that tries to minimize the total $(d-1)$ dimensional area of the domain wall, and the 'impurity' part that makes the wall deviate from flatness and pass through the locations of lowest local energy (think of $J_{ij} = J + \delta J_{ij}$ with J and δJ_{ij} contributing to the pure and impurity parts of the Hamiltonian, respectively). The activation argument in eq. (**??**) together with the power-lwa growth of barriers in eq. (5.34) implies a logarithmic growth of $R(t)$. Simulations, instead, suggest a power law with a temperature dependent exponent. Whether the latter is a pre-asymptotic result and the trully asymptotic one is hidden by the premature pinning of domain walls or it is a genuine behaviour invalidating (5.34) or even eq. (5.33) is still an open problem.

In the $3d$ RFIM the curvature-driven growth mechanism that leads to (5.30) is impeded by the random field roughening of the domain walls. Indeeed, one observes that after a quench to low temperature the spins rapidly coalesce and form small domains, these domains expand and compact at the expense of their smaller neighbours but their growth is partially stopped by the random fields that pin the interfaces. Much longer time scales are needed to surmount the (free) energy barriers introduced by the local fluctuations in the fields, and eventually reach the long-range order. Comparing to the pure Ising model one notices that the initial growth follows a very similar time-dependence in the two cases but the subsequent coarsening is much slower in the presence of random fields. The precise behaviour of the growth law depends on time, temperature and the strength of the random field. In the early stages of growth, one expects the zero-field result to hold with a reduction in the amplitude

$$R(t) \sim (A - Bh^2)\, t^{1/2} \,. \tag{5.36}$$

The time-window over which this law is observed numerically is smaller, the larger the field strength. In the late time regime, where pinning is effective Villain deduced a logarithmic growth

$$R(t) \sim \frac{T}{h^2} \ln t \tag{5.37}$$

by estimating the maximum barrier height encountered by the domain wall and using the Arrhenius law to derive the associated time-scale.

In the case of spin-glasses, if the mean-field picture with a large number of equilibrium states is realized in finite dimensional models, the dynamics would be one in which all these states grow in competition. If, instead, the droplet model applies, there would be two types of domains growing and this phenomenological theory predicts that these will have an average radious growing as

$$R(t) = (\ln t)^{1/\psi} \,, \tag{5.38}$$

with the exponent ψ satisfying $0 \leq \psi \leq d-1$. Some refined arguments that we shall not discuss here indicate that the dimension of the bulk of these domains should be compact but their surface should be a rough with fractal dimension $d_s > d-1$.

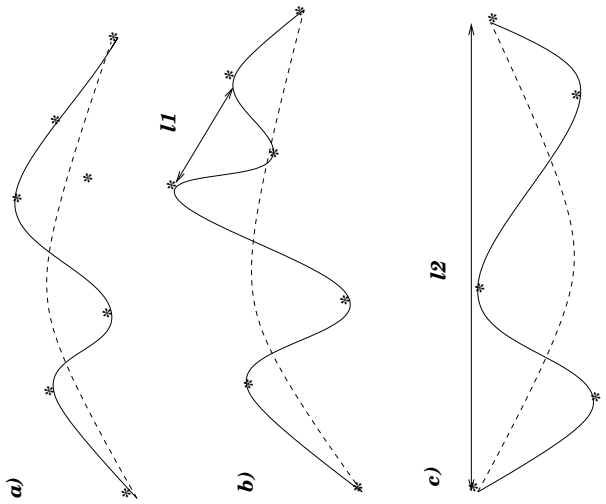

FIG. 13 – Schematic evolution of a pinned object on well separated time scales. On scale $t(\ell_1)$, the object reconforms by flipping a small portion of size ℓ_1 from one favourable configuration to another (a $\rightarrow$ b). On a much longer time scale $t(\ell_2) \gg t(\ell_1)$, the conformation on scale ℓ_2 (dotted lines) has evolved (b $\rightarrow$ c). The dynamics of the short wavelengths happens on a time scale such that long wavelengths are effectively frozen.

Note that if one starts such a dynamics in a very large ($L \gg a$) system with no biasing magnetic field the system will never magnetize in finite times with respect to L. More explicitly, if the growth law is the power law (5.30) one needs times of the order of L^2 to grow a domain of the size of the system. For any shorter time, domains of the two types exist and the system is *out of equilibrium*. This systems constitutes a first example of a problem with *slow dynamics*. Whether all systems with slow dynamics, in particular structural and spin glasses, undergo some kind of simple though slow domain growth is an open question.

Another implication of the slow dynamics is that if one observes the decay of a correlation function, as for instance the one in eq. (**??**), the contribution of the term $\mathcal{C}$ will be very important even at long times t' and t.

5.2.7 Separation of time-scales

The equation (**??**) also allows one to define a very important quantity which we call, by analogy with the glass temperature T_g, the 'glass length' ℓ_g, through $\Upsilon(T)\ell_g^{\psi} = \mathcal{A}T$, introduced in this context in [**?**, **?**, **?**]. The factor $\mathcal{A}$ is rather arbitrary ; the choice $\mathcal{A} = 35$ corresponds to a time of 1000 seconds if $\tau_0 = 10^{-12}$ seconds. In analogy with the glass temperature T_g, one sees that length scales larger than ℓ_g cannot be equilibrated on reasonable time scales, while length scales smaller than ℓ_g are fully equilibrated. Qualitatively speaking, the equilibrated modes contribute to the stationary part of the correlation and/or

response function, while the glassy modes $\ell > \ell_g$ contribute to the aging part. Therefore, the strong hierarchy of time scales induced by the exponential activation law allows equilibrated modes and aging modes to coexist.

Finally, it is easy to understand that the logarithmic growth law, Eq. (**??**), leads to a strong *cooling rate* dependence of the typical size of the domains [**?**] : since the growth law is essentially that of pure systems as long as $\xi \ll \ell_g(T)$, a longer time spent at higher temperatures (where ℓ_g is large) obviously allows the domains to grow larger before getting pinned at lower temperatures.

5.2.8 The large N approximation

Let us study try to find a solution to eq. (5.5) with the Landau-Ginzburg free-energy (5.3) and the double-well potential (5.4). It turns out that temperature does not play a very important role in the domain-growth process, it just adds some thermal fluctuations within the domains, as long as it is smaller than T_c. Therefore, we shall first set it to zero and only later discuss its effect.

In the absence of temperature, eq. (5.5) is just a gradient descent in the energy landscape F. Two terms contribute to F : the bulk-energy term that is minimized by $\phi = \pm\phi_0$ and the elastic energy $(\nabla\phi)^2$ which is minimized by flat configurations. As a consequence the system evolves with growing regions of constant field, $\phi(\vec{x}, t) = \pm\phi_0$, separated by flatter and flatter walls.

Even if the qualitative behaviour of the solution to eq. (5.5) is easy to grasp, it is still too difficult ot solve analytically. A very useful approximation is to upgrade the scalar field to a vectorial one with N components

$$\phi(\vec{x}, t) \to \vec{\phi}(\vec{x}, t) = (\phi_1(\vec{x}, t), \ldots, \phi_N(\vec{x}, t)) \; . \tag{5.39}$$

and modify the free-energy

$$F = \int d^d x \left[\frac{1}{2} (\nabla\vec{\phi})^2 + (\phi_0^2 - N^{-1}\phi^2)^2 \right] \; , \tag{5.40}$$

with $\phi^2 = \sum_\alpha \phi_\alpha^2$, the dynamic equation becomes

$$\partial_t \phi_\alpha(\vec{x}, t) = \nabla^2 \phi_\alpha(\vec{x}, t) - \frac{4}{N} \phi_\alpha(\vec{x}, t) \left[\phi_0^2 - N^{-1}\phi^2(\vec{x}, t) \right] . \tag{5.41}$$

In this way one makes contact with the random manifold problem defined in (**??**) though the manifold is here in the presence of a 'deterministic' potential. Now, if one considers the limit $N \to \infty$ while keeping the dimension of real space fixed to d, the cubic term in the right-hand-side can be replaced by

$$-\phi_\alpha(\vec{x}, t) N^{-1} \phi^2(\vec{x}, t) \to -\phi_\alpha(\vec{x}, t) N^{-1} [\, \phi^2(\vec{x}, t) \,]_{ic} \equiv -\phi_\alpha(\vec{x}, t)\, z(t) \tag{5.42}$$

since $N^{-1}\phi^2(\vec{x},t)$ does not fluctuate, it is equal to its average over the initial conditions and it is therefore not expected to depend on the spatial position if the initial conditions are chosen from a distribution that is statistically translational invariant. If one keeps the scalar notation the replacement (5.42) is just an approximation and it usually called the *Hartree approximation*. The dynamic equation now becomes *linear* in the field $\phi_\alpha(\vec{x},t)$:

$$\partial_t\phi(\vec{x},t) = [\nabla^2 + a(t)]\phi(\vec{x},t) \;, \tag{5.43}$$

where $a(t) = \phi_0^2 - [\phi^2(\vec{x},t)]_{ic}$ has to be determined self-consistently. Equation (5.43) can be integrated in Fourier space :

$$\phi(\vec{k},t) = \phi(\vec{k},0)\exp\left(-k^2t + \int_0^t a(t')dt'\right) \tag{5.44}$$

and the self-consistency equation on $a(t)$ reads :

$$a(t) = \phi_0^2 - \Delta\int\frac{d^dk}{(2\pi)^3}\exp\left(-2k^2t + 2\int_0^t a(t')dt'\right) \;, \tag{5.45}$$

where one used a delta-correlated Gaussian distribution of initial conditions with strength Δ. (Equation (5.45) is not singular at $t = 0$ since there is an underlying cut-off in the integration over k corresponding to the inverse of the lattice spacing.) In the large times limit in which the system tends to decrease its elastic and potential energies

$$[\,\phi^2(\vec{x},t)\,]_{ic} = \Delta\int\frac{d\mathbf{k}}{(2\pi)^3}\exp\left(-2k^2t + 2\int_0^t a(t')dt'\right) \tag{5.46}$$

must converge to ϕ_0^2 and this imposes

$$2\int_0^t dt'\,a(t') \simeq 3/2\log(t/t_0) \qquad \text{with} \qquad t_0 = (\Delta\phi_0^2)^{2/3}/8\pi \tag{5.47}$$

at large times, *i.e.*

$$a(t) \simeq \frac{3}{4t} \qquad \text{for} \qquad t \gg 1 \;. \tag{5.48}$$

Knowing the long-time behaviour of a we can compute asymptotic behaviour of the space time correlation function :

$$[\,\phi(\vec{x},t)\phi(\vec{x}',t')\,]_{ic} = \phi_0^2\left(\frac{4tt'}{(t+t')^2}\right)^{3/4}\exp\left(-\frac{(\vec{x}-\vec{x}')^2}{4(t+t')}\right) \;, \tag{5.49}$$

for $t \geq t'$. This expression captures the main features of the domain growth process :

– For any finite and fixed $(\vec{x}-\vec{x}')$, in the long $t' \leq t$ limit the exponential factor approaches one and one obtaines a function of t'/t only.

- For any finite and fixed $(\vec{x} - \vec{x}')$, in the long t' and t limit such that $t'/t \to 1$ the time dependence disappears and the correlation between two points converges to ϕ_0^2. This holds for any two points in space and time *provided that their distance in space and time is kept fixed when the large time limit is taken.* This means that, typically, if one looks at a finite spatial region on a finite time-scale this region will be on one of the two state $\pm\phi_0$.
- Due to the exponential factor, for fixed but very large time t and t' the magnetization density correlation falls to zero over distance $|\vec{x} - \vec{x}'| \propto \sqrt{t + t'}$. This means that, at time t, the typical size of the regions in the states $\pm\phi_0$ is $R(t) \propto \sqrt{t}$.
- For fixed $|\vec{x} - \vec{x}'|$, the magnetization density correlation always falls to zero over a time separation $t - t'$ *which is larger than* t'. This means that the time it takes to the system to decorrelate from its configuration at time t' is of the order of t' itself. The age of the system is the characteristic time-scale for the dynamical evolution : the older is the system, the slower is its dynamics. If one waits a time of the order of the age of the system a point $\vec{x}$ has been swept by different domain walls and thus the magnetic correlation has been lost.

$$J = 1 \ . \tag{.50}$$

A Additivity in the fully-connected Ising model

This fact is shown by, for example, the fully-connected Ising model :

$$E = -\frac{J}{N} \sum_{i \neq j} s_i s_j \tag{A.51}$$

where the spins s_i, $i = 1, \ldots, N$, take values ± 1, J is a finite coupling strength and the sum runs over *all pairs* of spins in the ensemble. Let us explore the additivity property of the energy for a simple configuration that corresponds to all spins pointing in the same direction, $s_i = 1$ for all i, *i.e.* the perfectly magnetized 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 $E_1 = -J(N-2)/4$ and $E_2 = -J(N-2)/4$ and one notices that $E \neq E_1 + E_2$. More precisely, $E_I \equiv E - (E_1 + E_2) = -JN/2$, still a macroscopic quantity. One has

$$E \sim E_1 \sim E_I \sim -JN \tag{A.52}$$

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

B Some useful formulæ

B.1 Stirling

Stirling formula for the factorial of a large number reads :

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

B.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,

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

B.3 Gaussian integrals

The Gaussian integral is

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

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

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

From (B.3) one has

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

The generalization to N variables

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

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

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

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 (B.6) becomes

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

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

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

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

$$\vec{x} \equiv (x_1, \ldots, x_N) \to \phi(\vec{x}) \tag{B.10}$$

and

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

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

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

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

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

B.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

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

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

$$\langle\, e^{hx} \,\rangle = e^{\frac{h^2\sigma^2}{2} + h\mu} \tag{B.15}$$

and then

$$\langle\, x^k \,\rangle = \frac{\partial^k}{\partial h^k} \; e^{\frac{h^2\sigma^2}{2} + \mu h} \Big|_{h=0} \tag{B.16}$$

from where

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

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 (B.15) becomes

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

and the generalization of (B.16) leads to

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

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

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

etc.

B.5 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 $\delta F = \int d^dx\ \alpha(\vec{x})\delta h(\vec{x}) + \frac{1}{2}\int d^dx d^dy\ \beta(\vec{x},\vec{y})\,\delta h(\vec{x})\delta h(\vec{y}) + \ldots$ and one defines the functional derivative of F with respect to h evaluated at the spatial point $\vec{x}$ as

$$\frac{\delta F}{\delta h(\vec{x})} = \alpha(\vec{x})\ , \qquad \frac{\delta^2 F}{\delta h(\vec{x})\delta h(\vec{y})} = \beta(\vec{x},\vec{y}) \tag{B.20}$$

etc. All usual properties of partial derivatives apply.

B.6 Fourier transform

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

$$\tilde{f}(\vec{k}) = \int_V d^dx\ f(\vec{x})\, e^{-i\vec{k}\vec{x}} \tag{B.21}$$

This implies

$$f(\vec{x}) = \frac{1}{V}\sum_{\vec{k}} \tilde{f}(\vec{k})\, e^{i\vec{k}\vec{x}} \tag{B.22}$$

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

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

$$\tilde{f}(\vec{x}) = \int_V \frac{d^d k}{(2\pi)^d} \; f(\vec{k})\, e^{i\vec{k}\vec{x}} \tag{B.24}$$

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

C The saddle-point method

Imagine one has to compute the following integral

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

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

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

and obtains

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

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.

D TD 1 : Notions de base

Le but de ce TD est de faire un rappel des notions de base en mécanique statistique discutées dans le cours.

1. On étudiera la propriété d'additivité de l'énergie d'un modèle typique des magnétiques, le modèle d'Ising.

   Si le modèle est complètement connecté son énergie totale est définie comme

   $$E = -\frac{J}{N}\sum_{i\neq j} s_i s_j \tag{1}$$

   où les spins s_i, $i = 1, \ldots, N$, sont des variables bimodales, $s_i = \pm 1$, J est une constante de couplage finie, et la somme porte sur *toutes les paires de spins* de l'échantillon (il y a ordre N^2 termes dans la somme).

   On explorera la propriété d'additivité de l'énergie pour une configuration simple, où tous les spins pointent dans la même direction, $s_i = 1$ pour tous les i (c'est-à-dire un état complètement aimanté).

   (a) Calculer l'énergie totale.

   (b) Imaginer le système total comme s'il était formé par deux sous-systèmes avec $N/2$ spins chaqun. Distinguer les contributions à l'énergie totale de chaque sous-système avec $N/2$ spins et de l'« interface » entre les deux. Discuter les ordres de grandeurs des contributions.

   (c) Discuter les résultats.

   Si le modèle est défini sur un réseau carré avec des interactions entre plus proches voisins seulement

   $$E = -J\sum_{\langle ij\rangle} s_i s_j \tag{2}$$

   avec J fini, que peut-on dire de la propriété d'additivité de l'énergie dans la limite $N \gg 1$?

2. *Le théorème de fluctuation-dissipation statique*

   Prenons un système caractérisé par une énergie E en équilibre thermique avec un reservoir à température T (ensemble canonique).

   Montrer la relation

   $$C_V = k_B\beta^2\left(\langle\, E^2\,\rangle - \langle\, E\,\rangle^2\right) \tag{3}$$

   où $C_V = -k_B\beta^2\partial_\beta\langle\, E\,\rangle$ est la chaleur spécifique à volume constant.

   Ces résultats ne dépendent pas du système consideré. Ils sont différentes expressions de ce qu'on appele le théoreme de fluctuation-dissipation.

3. Étudier les propriétés thermodynamiques du gaz parfait classique dans l'ensemble canonique.
   (a) Calculer la fonction de partition.
   (b) Calculer l'énergie libre.
   (c) Calculer l'énergie interne et la chaleur spécifique C_V. Quel est C_V dans l'ensemble microcanonique ?
   (d) Comparer au comportement du gaz auto-gravitant.

E TD 2 : L'approximation de champ moyen

On étudiera ce qu'on a appelé dans le cours l'approximation de champ moyen naïve du modèle d'Ising en présence d'un champ magnétique externe et uniforme h. Le modèle est défini sur un réseau carré de dimension d. On prend un système de N spins d'Ising, on suppose qu'ils sont indépendants, et on caractérise sa distribution de probabilité jointe par le simple produit des distributions de probabilité pour chaque spin. On prend

$$P(s) = \frac{1+m}{2}\delta_{s,1} + \frac{1-m}{2}\delta_{s,-1} \tag{1}$$

où δ_{xy} est la fonction delta de Kronecker et m est un parametre $|m| \leq 1$.

1. Montrer que $P(s)$ peut être une distribution de probabilité ; c'est-à-dire, qu'elle est une fonction définie positive et normalisée.
2. Calculer la moyenne du spin s.
3. Calculer l'énergie interne moyenne, $U \equiv \langle H \rangle$.
4. Calculer l'entropie.
5. Donner l'énergie libre par dégré de liberté en fonction de m.
6. Trouver l'équation pour m.
7. Discuter ses solutions.

F TD 3 : Analyse de champs aléatoires

Le but de ce TD est de se familiariser avec les propriétés statistiques des processus stochastiques discret, continus et surtout avec les théorie de champs.

1. Prenons un champ scalaire $\rho(\vec{x})$ distribué selon la loi Gaussienne

$$P[\rho] \propto e^{-\frac{1}{2}\int d^d x \int d^d y\, [\rho(\vec{x})-\mu(\vec{x})]\, A^{-1}(\vec{x},\vec{y})\, [\rho(\vec{y})-\mu(\vec{y})]} \tag{1}$$

   (a) Quelle est la moyenne du champ ρ au point spatial $\vec{z}$?

   (b) Calculer la fonction de correlation $C(\vec{u},\vec{v}) = \langle\, \rho(\vec{u})\rho(\vec{v})\, \rangle$.

   (c) Calculer la fonction de correlation reduite $C(\vec{u},\vec{v}) = \langle\, (\rho(\vec{u}) - \mu(\vec{u}))(\rho(\vec{v}) - \mu(\vec{v}))\, \rangle$.

   (d) Calculer la fonction de correlation à 'trois points' $C(\vec{u}_1,\vec{u}_2,\vec{u}_3) = \langle\, \rho(\vec{u}_1)\rho(\vec{u}_2)\rho(\vec{u}_3)\, \rangle$.

   (e) Exprimer le théorème de Wick.

2. Prenons un variable aléatoire discrete, $x = 0, 1, 2, \ldots$, distribuée selon la loi de Poisson

$$p(x) = \frac{\mu^x e^{-\mu}}{x!} \tag{2}$$

   (a) Calculer la moyenne et la variance.

   (b) Prenez un gaz de N particles dans un volume V avec densité $\rho_0 = N/V$ finie. Divisez le volume en sousvolumes de la même taille v avec $v \ll V$. Calculer la distribution de probabilité du nombre de particules dans chaque sous volume v. Comparer le résultat à la lois de Poisson.

G TD 4 : Dynamique stochastique

Nous allons travailler, par souci de simplicité, en dimension $d = 1$. La généralisation au cas d dimensionnel est immédiate. Dans cette section nous étudierons quelques équations de Langevin pour le mouvement d'une particule sur un axe sous l'effet d'un bain thermique.

1. Transformation de l'équation de Langevin.
   La forme générique de l'équation de Langevin est

$$\gamma \frac{dx}{dt} = F + \xi \,, \tag{1}$$

   où ξ répresente un bruit thermique qu'on prend, typiquement, Gaussien et blanc :

$$\langle\, \xi(t) \,\rangle = 0 \,, \qquad \langle\, \xi(t)\xi(t') \,\rangle = 2k_B T\gamma\, \delta(t - t') \,, \tag{2}$$

   pout tous les temps t et t'. F est la force totale appliquée sur la particule.
   Montrer qu'avec une transformation du temps, $\tau \equiv g(t)$, l'équation dévient

$$\frac{dx}{dt} = F + \eta \,, \tag{3}$$

   avec η un bruit blanc Gaussienne avec moyenne et corrélation :

$$\langle\, \eta(\tau) \,\rangle = 0 \,, \qquad \langle\, \eta(\tau)\eta(\tau') \,\rangle = 2k_B T\, \delta(\tau - \tau') \,. \tag{4}$$

   Trouver $g(t)$ et η.
2. Le mouvement Brownien forcé.
   Dans plusieurs application d'intérêt on 'tire' de la particule avec un force constante ; un exemple est l'électrophorèse où l'on fait avancer des particules chargées (typiquement de l'ADN) sous l'effet d'un champ électrique.
   (a) Trouver la solution de l'équation stochastique

$$\frac{dx}{dt} = \xi + f \tag{5}$$

   ou ξ est un bruit blanc et f est une force qu'on prendra constante, $f(t) = f$. On prend comme condition initielle $x(0) = x_0$.
   (b) Calculer la position moyenne de la particule $\langle\, x(t) \,\rangle$. Discuter la perte de mémoire de la condition initielle.

(c) Calculer le déplacement moyen quadratique $\Delta^2(t,t') \equiv \langle\,(x(t)-x(t'))^2\,\rangle$.
Avez vous trouvé un résulat stationnaire ? Dans quelle limite ?
Comparer le résultat à la forme diffusive normale. Peut-on identifier une constante de diffusion ?

3. L'oscillateur harmonique.
On considère une particule en contacte avec un bruit blanc et sous l'effet d'une force harmonique :

$$\frac{dx}{dt} = -kx + \xi \tag{6}$$

(a) Calculer la position moyenne $\langle\,x(t)\,\rangle$.

(b) Calculer le déplacement moyen quadratique $\Delta^2(t,t') \equiv \langle\,(x(t)-x(t'))^2\,\rangle$.
Avez vous trouvé un résulat stationnaire ?
Comparer le résultat à la forme diffusive normale. Peut-on identifier une constante de diffusion ? Discuter la limite $k \to 0$.

H Consignes pour l'ećriture du rapport

Le rapport sera écrit en **5 pages maximum**.

Il doit avoir la structure d'un article scientifique ; il avoir :

– un titre,
– un auteur,
– un résumé (6 lignes maximum),
– un corps qui peut être séparé en sections,
– une conclusion,
– une bibliographie.

Bien évidement, le rapport ne doit pas être une traduction de l'article choisi. Le texte doit montrer que l'étudiant a fait un travail de réflexion pour situer le problème étudié dans le contexte du cours et dans une problématique générale. Il doit montrer également que étudiant s'est posé et a donné réponse à la question "pour quoi on étudie ce problème", autrement dit, "pour quoi ce problème est intéressant".

En ce qui concerne les développements analytiques présentés ou mentionnés dans les articles, il n'est pas nécessaire de les reproduire dans le rapport ; il faut, pourtant, donner les idées générales qui sont derrière les résultats obtenus.

Il est conseillé d'approfondir l'étude en consultant les références cités dans l'article choisi où bien en cherchant des articles reliés.

Papers

1. Inequivalence of ensembles in systems with long range interactions

Julien Barré, David Mukamel, Stefano Ruffo, *Inequivalence of ensembles in a system with long range interactions*, cond-mat/0102036, Phys. Rev. Lett. **87**, 030601 (2001).

We study the global phase diagram of the infinite range Blume-Emery-Griffiths model both in the canonical and in the microcanonical ensembles. The canonical phase diagram is known to exhibit first order and continuous transition lines separated by a tricritical point. We find that below the tricritical point, when the canonical transition is first order, the phase diagrams of the two ensembles disagree. In this region the microcanonical ensemble exhibits energy ranges with negative specific heat and temperature jumps at transition energies. These results can be extended to weakly decaying nonintegrable interactions.

D. Mukamel, S. Ruffo, N. Schreiber, *Breaking of ergodicity and long relaxation times in systems with long-range interactions*, cond-mat/0508604.

The thermodynamic and dynamical properties of an Ising model with both short range and long range, mean field like, interactions are studied within the microcanonical ensemble. It is found that the relaxation time of thermodynamically unstable states diverges logarithmically with system size. This is in contrast with the case of short range interactions where this time is finite. Moreover, at sufficiently low energies, gaps in the magnetization interval may develop to which no microscopic configuration corresponds. As a result, in local microcanonical dynamics the system cannot move across the gap, leading to breaking of ergodicity even in finite systems. These are general features of systems with long range interactions and are expected to be valid even when the interaction is slowly decaying with distance.

Alessandro Campa, Andrea Giansanti, David Mukamel, Stefano Ruffo *Dynamics and thermodynamics of rotators interacting with both long and short range couplings*, cond-mat/0510508.

The effect of nearest-neighbor coupling on the thermodynamic and dynamical properties of the ferromagnetic Hamiltonian Mean Field model (HMF) is studied. For a range of antiferromagnetic nearest-neighbor coupling, a canonical first order transition is observed, and the canonical and microcanonical ensembles are non-equivalent. In studying the relaxation time of non-equilibrium states it is found that as in the HMF model, a class of non-magnetic states is quasi-stationary, with an algebraic divergence of their lifetime with the number of degrees of freedom N. The lifetime of metastable states is found to increase exponentially with N as expected.

Takayuki Tatekawa, Freddy Bouchet, Thierry Dauxois, Stefano Ruffo, *Thermodynamics*

of the self-gravitating ring model, Phys. Rev. E **71** (2005) 056111, cond-mat/0501583.

We present the phase diagram, in both the microcanonical and the canonical ensemble, of the Self-Gravitating-Ring (SGR) model, which describes the motion of equal point masses constrained on a ring and subject to 3D gravitational attraction. If the interaction is regularized at short distances by the introduction of a softening parameter, a global entropy maximum always exists, and thermodynamics is well defined in the mean-field limit. However, ensembles are not equivalent and a phase of negative specific heat in the microcanonical ensemble appears in a wide intermediate energy region, if the softening parameter is small enough. The phase transition changes from second to first order at a tricritical point, whose location is not the same in the two ensembles. All these features make of the SGR model the best prototype of a self-gravitating system in one dimension. In order to obtain the stable stationary mass distribution, we apply a new iterative method, inspired by a previous one used in 2D turbulence, which ensures entropy increase and, hence, convergence towards an equilibrium state.

2. Equilibrium phase transitions

G. Fletcher, *A mechanical analog of first- and second-order phase transitions*, Am. J. Phys. **65**, 74 (1997).

A mechanical model that exhibits first- and second-order phase transitions is analyzed. The possible configurations are found first by using Newtonian mechanics and second by determining the minimum of the effective potential energy taken from the Lagrangian. A comparison is made between the effective potential energy method and the Landau theory of phase transitions. Phase diagrams are obtained for the mechanical system and are compared with those of a ferromagnet.

D. Boyanovsky, H. J. de Vega, D. J. Schwarz, *Phase transitions in the early and the present Universe*, to appear in Ann. Rev. Nucl. Part. Sci 2006, hep-ph/0602002.

The evolution of the Universe is the ultimate laboratory to study fundamental physics across energy scales that span about 25 orders of magnitude : from the grand unification scale through particle and nuclear physics scales down to the scale of atomic physics. The standard models of cosmology and particle physics provide the basic understanding of the early and present Universe and predict a series of phase transitions that occurred in succession during the expansion and cooling history of the Universe. We survey these phase transitions, highlighting the equilibrium and non-equilibrium effects as well as their observational and cosmological consequences. We discuss the current theoretical and experimental programs to study phase transitions in QCD and nuclear matter in accelerators along with the new results on novel states of matter as well as on multi- fragmentation in nuclear matter. A critical assessment of similarities and differences between the conditions in the early universe and those in ultra- relativistic heavy ion collisions is

presented. Cosmological observations and accelerator experiments are converging towards an unprecedented understanding of the early and present Universe.

An improved apparatus for demonstrating first- and second-order phase transitions : Ball bearings on a rotating hoop, Richard V. Mancuso and Guy A. Schreiber, Am. J. Phys. 73, 366 (2005)

A working mechanical model for first- and second-order phase transitions and the cusp catastrophe, Richard V. Mancuso Am. J. Phys. 68, 271 (2000).

We have modified a toy to demonstrate first- and second-order phase transitions. The toy consists of a ball constrained to move on a rotating hoop. Analysis of the equilibrium positions of the ball as a function of the angular velocity and location of the axis of rotation shows that this system contains a cusp catastrophe.

On water, steam, and string theory, Christof Schmidhuber Am. J. Phys. 65, 1042 (1997)

At a pressure of 220 atm and a temperature of 374 C there is a second-order phase transition between water and steam. Understanding it requires a key concept of both condensed matter and elementary particle physics : the renormalization group. Its basic ideas are explained with images from computer simulations of the lattice gas model. Then I briefly review how the renormalization group is used to compute critical coefficients for the water ?steam phase transition. The results of this calculation are in good agreement with experiment. Finally, some applications in particle physics and string theory are mentioned.

A hand-held demonstration of cosmological phase transitions, David Lange, Marc Sher, Joel Sivillo, and Robert Welsh, Am. J. Phys. 61, 1049 (1993).

Illustrating phase transitions with soap films, David R. Lovett and John Tilley, Am. J. Phys. 59, 415 (1991).

First-order and second-order phase transitions are demonstrated using soap-film models. The models consist of two-dimensional parallel plates or three-dimensional frameworks in which film patterns are maintained. By making the sizes of the frameworks variable, it is possible to induce switching between film patterns analogous to transitions between phases. These phase changes are discussed thermodynamically and using a catastrophe theory model.

A simple geometrical model of spontaneous symmetry breaking, P. K. Aravind, Am. J. Phys. 55, 437 (1987).

A common, everyday phenomenon has a geometrical aspect that, in some respects, is analogous to a second-order phase transition. Concepts such as spontaneous symmetry breaking, order parameter, critical point, and critical exponent can thus be exhibited in a

purely geometrical context. The purpose of the model, which is entirely pedagogical, is to illustrate in an elementary and amusing way some of the concepts associated with phase transition theory.

3. Statistical analysis of cosmological structures

Dynamics

T. Baertschiger, M. Joyce, A. Gabrielli, F. Sylos Labini *Gravitational Dynamics of an Infinite Shuffled Lattice of Particles*, cond-mat/0607396.

We study, using numerical simulations, the dynamical evolution of self-gravitating point particles in static euclidean space, starting from a simple class of infinite "shuffled lattice" initial conditions. These are obtained by applying independently to each particle on an infinite perfect lattice a small random displacement, and are characterized by a power spectrum (structure factor) of density fluctuations which is quadratic in the wave number k, at small k. For a specified form of the probability distribution function of the "shuffling" applied to each particle, and zero initial velocities, these initial configurations are characterized by a single relevant parameter : the variance δ^2 of the "shuffling" normalized in units of the lattice spacing ℓ. The clustering, which develops in time starting from scales around ℓ, is qualitatively very similar to that seen in cosmological simulations, which begin from lattices with applied correlated displacements and incorporate an expanding spatial background. From very soon after the formation of the first non-linear structures, a spatio-temporal scaling relation describes well the evolution of the two-point correlations. At larger times the dynamics of these correlations converges to what is termed "self-similar" evolution in cosmology, in which the time dependence in the scaling relation is specified entirely by that of the linearized fluid theory. Comparing simulations with different δ, different resolution, but identical large scale fluctuations, we are able to identify and study features of the dynamics of the system in the transient phase leading to this behavior. In this phase, the discrete nature of the system explicitly plays an essential role.

M. Joyce, D. Levesque, B. Marcos, *A method of generating initial conditions for cosmological N body simulations*, Phys. Rev. D **72** (2005) 103509, astro-ph/0411607.

We investigate the possibility of generating initial conditions for cosmological N-body simulations by simulating a system whose correlations at thermal equilibrium approximate well those of cosmological density perturbations. The system is an appropriately modified version of the standard "one component plasma" (OCP). We show first how a well-known semi-analytic method can be used to determine the potential required to produce the desired correlations, and then verify our results for some cosmological type spectra with simulations of the full molecular dynamics. The advantage of the method, compared to

the standard one, is that it gives by construction an accurate representation of both the real and reciprocal space correlation properties of the theoretical model. Furthermore the distributions are also statistically homogeneous and isotropic. We discuss briefly the modifications needed to implement the method to produce configurations appropriate for large N-body simulations in cosmology, and also the generation of initial velocities in this context.

A. Gabrielli, M. Joyce, B. Marcos, P. Viot, *Causality constraints on fluctuations in cosmology : a study with exactly solvable one dimensional models*, Europhys. Lett. astro-ph/0303169

A well known argument in cosmology gives that the power spectrum (or structure function) $P(k)$ of mass density fluctuations produced from a uniform initial state by physics which is causal (i.e. moves matter and momentum only up to a finite scale) has the behaviour $P(k) \propto k^4$ at small k. Noting the assumption of analyticity at $k = 0$ of $P(k)$ in the standard derivation of this result, we introduce a class of solvable one dimensional models which allows us to study the relation between the behaviour of $P(k)$ at small k and the properties of the probability distribution $f(l)$ for the spatial extent l of mass and momentum conserving fluctuations. We find that the k^4 behaviour is obtained in the case that the first *six* moments of $f(l)$ are finite. Interestingly the condition that the fluctuations be localised - taken to correspond to the convergence of the first two moments of $f(l)$ - imposes only the weaker constraint $P(k) \propto k^n$ with n anywhere in the range $0 < n \leq 4$. We interpret this result to suggest that the causality bound will be loosened in this way if quantum fluctuations are permitted.

A. Gabrielli, B. Jancovici, M. Joyce, J. L. Lebowitz, L. Pietronero, F. Sylos Labini, *Generation of Primordial Cosmological Perturbations from Statistical Mechanical Models*, Phys.Rev. D 67 (2003) 043506, astro-ph/0210033.

The initial conditions describing seed fluctuations for the formation of structure in standard cosmological models, i.e.the Harrison-Zeldovich distribution, have very characteristic "super-homogeneous" properties : they are statistically translation invariant, isotropic, and the variance of the mass fluctuations in a region of volume V grows slower than V. We discuss the geometrical construction of distributions of points in $\mathbf{R}^3$ with similar properties encountered in tiling and in statistical physics, e.g. the Gibbs distribution of a one-component system of charged particles in a uniform background (OCP). Modifications of the OCP can produce equilibrium correlations of the kind assumed in the cosmological context. We then describe how such systems can be used for the generation of initial conditions in gravitational N-body simulations.

Force distributions

A. Gabrielli, T. Baertschiger, M. Joyce, B. Marcos, F. Sylos Labini, *Force distribution*

in a randomly perturbed lattice of identical particles with $1/r^2$ *pair interaction*, cond-mat/0603124.

We study the statistics of the force felt by a particle in the class of spatially correlated distribution of identical point-like particles, interacting via a $1/r^2$ pair force (i.e. gravitational or Coulomb), and obtained by randomly perturbing an infinite perfect lattice. In the first part we specify the conditions under which the force on a particle is a well defined stochastic quantity. We then study the small displacements approximation, giving both the limitations of its validity, and, when it is valid, an expression for the force variance. In the second part of the paper we extend to this class of particle distributions the method introduced by Chandrasekhar to study the force probability density function in the homogeneous Poisson particle distribution. In this way we can derive an approximate expression for the probability distribution of the force over the full range of perturbations of the lattice, i.e., from very small (compared to the lattice spacing) to very large where the Poisson limit is recovered. We show in particular the qualitative change in the large-force tail of the force distribution between these two limits. Excellent accuracy of our analytic results is found on detailed comparison with results from numerical simulations. These results provide basic statistical information about the fluctuations of the interactions (i) of the masses in self-gravitating systems like those encountered in the context of cosmological N-body simulations, and (ii) of the charges in the ordered phase of the One Component Plasma.

Statistical mechanics

H. J. de Vega, N. G. Sanchez, *Statistical Mechanics of the Self-Gravitating Gas : Thermodynamic Limit, Unstabilities and Phase Diagrams*, Comptes Rendus Physique 7 (2006) 391-397, astro-ph/0601600.

We show that the self-gravitating gas at thermal equilibrium has an infinite volume limit in the three ensembles (GCE, CE, MCE) when $(N, V) \to \infty$, keeping $N/V^{1/3}$ fixed, that is, with $\eta = Gm^2N/[V^{1/3}T]$ fixed. We develop MonteCarlo simulations, analytic mean field methods (MF) and low density expansions. We compute the equation of state and find it to be locally $p(r) = Trho_V(r)$, that is a local ideal gas equation of state. The system is in a gaseous phase for $\eta < \eta_T = 1.51024...$ and collapses into a very dense object for $\eta > \eta_T$ in the CE with the pressure becoming large and negative. The isothermal compressibility diverges at $\eta = \eta_T$. We compute the fluctuations around mean field for the three ensembles. We show that the particle distribution can be described by a Haussdorf dimension $1 < D < 3$.

H. J. de Vega, N. Sanchez, *Statistical Mechanics of the self-gravitating gas : thermodynamic limit, phase diagrams and fractal structures*, Lecture given at the 7th. Paris Cosmology Colloquium, Observatoire de Paris, June 11-15, 2002 and at the 9 th Course of the International School of Astrophysics 'Daniel Chalonge', Palermo, Italy, 7-18 Sep-

tember 2002, NATO ASI, astro-ph/0505561.

We provide a complete picture to the self-gravitating non-relativistic gas at thermal equilibrium using Monte Carlo simulations, analytic mean field methods (MF) and low density expansions. The system is shown to possess an infinite volume limit in the grand canonical (GCE), canonical (CE) and microcanonical (MCE) ensembles when $(N, V) - > \infty$, keeping $N/V^{1/3}$ fixed. We compute the equation of state (we do not assume it as is customary in hydrodynamics), as well as the energy, free energy, entropy, chemical potential, specific heats, compressibilities and speed of sound ; we analyze their properties, signs and singularities. All physical quantities turn out to depend on a single variable $\eta = Gm^2N/[V^{1/3}T]$ that is kept fixed in the $N - > \infty$ and $V - > \infty$ limit. The system is in a gaseous phase for $\eta < \eta_T$ and collapses into a dense object for $\eta > \eta_T$ in the CE with the pressure becoming large and negative. At $\eta \simeq \eta_T$ the isothermal compressibility diverges and the gas collapses. Our Monte Carlo simulations yield $\eta_T \simeq 1.515$. We find that $PV/[NT] = f(\eta)$. The function $f(\eta)$ has a second Riemann sheet which is only physically realized in the MCE. In the MCE, the collapse phase transition takes place in this second sheet near $\eta_{MC} = 1.26$ and the pressure and temperature are larger in the collapsed phase than in the gaseous phase. Both collapse phase transitions (in the CE and in the MCE) are of zeroth order since the Gibbs free energy has a jump at the transitions.

H. J. de Vega, N. Sanchez, *The Cluster Expansion for the Self-Gravitating gas and the Thermodynamic Limit*, Nucl. Phys. B 711 (2005) 604-620, astro-ph/0307318.

We develop the cluster expansion and the Mayer expansion for the self-gravitating thermal gas and prove the existence and stability of the thermodynamic limit N, V to infty with $N/V^{1/3}$ fixed. The essential (dimensionless) variable is here $\eta = [Gm^2N]/[V^{1/3}T]$ (which is kept fixed in the thermodynamic limit). We succeed in this way to obtain the expansion of the grand canonical partition function in powers of the fugacity. The corresponding cluster coefficients behave in the thermodynamic limit as $[\eta/N]^{j-1}c_j$ where c_j are pure numbers. They are expressed as integrals associated to tree cluster diagrams. A bilinear recurrence relation for the coefficients c_j is obtained from the mean field equations in the Abel form. In this way the large j behaviour of the c_j is calculated. This large j behaviour provides the position of the nearest singularity which corresponds to the critical point (collapse) of the self-gravitating gas in the grand canonical ensemble. Finally, we discuss why other attempts to define a thermodynamic limit for the self-gravitating gas fail.

H. J. de Vega, J. A. Siebert, *The Self-Gravitating Gas in the Presence of Dark Energy : Monte-Carlo Simulations and Stability Analysis*, Nucl. Phys. B 726 (2005) 464-480, astro-ph/0410147.

The self-gravitating gas in the presence of a positive cosmological constant Lambda is studied in thermal equilibrium by Monte Carlo simulations and by the mean field ap-

proach. We find excellent agreement between both approaches already for $N = 1000$ particles on a volume V [The mean field is exact in the infinite N limit]. The domain of stability of the gas is found to increase when the cosmological constant increases. The particle density is shown to be an increasing (decreasing) function of the distance when the dark energy dominates over self-gravity (and vice-versa).We confirm the validity of the thermodynamic limit : N, $V- > \infty$ with $N/V^{1/3}$ and $\Lambda V^{2/3}$ fixed. In such dilute limit extensive thermodynamic quantities like energy, free energy, entropy turn to be proportional to N. We find that the gas is stable till the isothermal compressibility diverges. Beyond this point the gas becomes a extremely dense object whose properties are studied by Monte Carlo.

4. Monte carlo methods

A new approach to Monte Carlo simulations in statistical physics : Wang-Landau sampling, D. P. Landau, Shan-Ho Tsai, and M. Exler, Am. J. Phys. 72, 1294 (2004).

We describe a Monte Carlo algorithm for doing simulations in classical statistical physics in a different way. Instead of sampling the probability distribution at a fixed temperature, a random walk is performed in energy space to extract an estimate for the density of states. The probability can be computed at any temperature by weighting the density of states by the appropriate Boltzmann factor. Thermodynamic properties can be determined from suitable derivatives of the partition function and, unlike "standard" methods, the free energy and entropy can also be computed directly. To demonstrate the simplicity and power of the algorithm, we apply it to models exhibiting first-order or second-order phase transitions.

Monte Carlo Calculations as an Aid in Teaching Statistical Mechanics, D. P. Landau, R. Alben

A simple Monte Carlo sampling method is used to illustrate the principles of statistical mechanics as applied to a simple magnetic system. The concepts of ensembles, statistical averages, and responses are clarified particularly with respect to the role of statistical fluctuations. The basic properties of magnetic phase transitions are also demonstrated using small systems of interacting moments.

A simple algorithm for the transport of gamma rays in a medium, F. Arqueros and G. D. Montesinos, Am. J. of Phys. 71 38-45 (2003).

A simple Monte Carlo algorithm for the simulation of the passage of gamma rays of about 1 MeV in a medium is presented. In this energy range the only relevant processes are Compton scattering and photoelectric absorption. The algorithm allows the visualization of the photon tracks as well as the calculation of many quantities of interest. Several

problems for a layer and a cylinder are proposed. In particular, the energy transferred to electrons in a water cylinder as a function of depth and the line shape of a NaI scintillator is calculated.

Study of radiation-matter interaction processes below 1 MeV from simulated data, Fernando Arqueros and Sergio Martinez, American Journal of Physics 60, 232-238 (1992).

The passage of 1-MeV photons through thin and thick foils of Al and Pb has been simulated. The results have been used to show the basic properties of the dominant effects in radiation-matter interaction processes at energies just below 1 MeV. For the interpretation of the data it is necessary to handle total and differential cross sections of the involved processes, as well as the conservation laws, mainly of the Compton effect, whose phenomenology is studied in depth. In particular, the effect of multiple interactions in thick foils is studied and some results of the simulation are compared with suggested theoretical approaches.

Interdisciplinary applications of computational statistical physics, Dietrich Stauffer, Am. J. of Phys. 67, 1207-1211 (1999).

Biological and financial applications of computational methods in statistical physics are discussed. Examples are given of evolutionary models of sexual reproduction and stock markets.

Monte Carlo estimations of e, P. Mohazzabi, Am. J. of Physics 66, 138-14 (1998).

Three physical processes and the corresponding Monte Carlo algorithms are outlined, in which the number e, the base of the natural logarithm, can be obtained. The value of e is estimated in each case, and the three algorithms are compared.

Updating Monte Carlo algorithms, J. R. Drugowich de Felcio, Valter L. Lbero, Am. J. Phys, 64, 1281-1285 (1996).

Using the long-range Ising model, we present modern Monte Carlo techniques2014single and multiple histogram and entropic sampling2014which permit increasing the amount of information obtained from a simulation. Numerical results for the density of states, mean energy and specific heat are compared with exact calculations, easily handled in this case. As a consequence of the simplicity of the model, the ability of those methods to generate continuous plots of thermodynamical quantities can be appreciated even by students taking basic courses of statistical physics.

Compton scattering, the electron mass, and relativity : A laboratory experiment, P. L. Jolivette and N. Rouze, American Journal of Physics 62, 266-271 (1994).

Compton scattering in a semiconductor detector is used to "discover" the relativistic relation between energy and momentum and to demonstrate the dependence of p, E

and gamma on beta. The motivation is to measure the (rest) mass of the electron, and this can be done to within 1 keV with a commonly available set of gamma ray sources. To determine precisely where the Compton edge occurs in a spectrum, a Monte Carlo calculation of detector response is described which also helps the student to understand the physics of the detection process.

5. Relativistic Brownian motion

Jörn Dunkel, Peter Hänggi, *One-dimensional nonrelativistic and relativistic Brownian motions : A microscopic collision model* Physica A (to appear), cond-mat/0606487.

We study a simple microscopic model for the one-dimensional stochastic motion of a (non)relativistic Brownian particle, embedded into a heat bath consisting of (non)relativistic particles. The stationary momentum distributions are identified self-consistently (for both Brownian and heat bath particles) by means of two coupled integral criteria. The latter follow directly from the kinematic conservation laws for the microscopic collision processes, provided one additionally assumes probabilistic independence of the initial momenta. It is shown that, in the nonrelativistic case, the integral criteria do correctly identify the Maxwellian momentum distributions as stationary (invariant) solutions. Subsequently, we apply the same criteria to the relativistic case. Surprisingly, we find here that the stationary momentum distributions differ slightly from the standard Jüttner distribution by an additional prefactor proportional to the inverse relativistic kinetic energy.

Jörn Dunkel, Peter Hänggi, *Relativistic Brownian motion : From a microscopic binary collision model to the Langevin equation* Phys. Rev. E (to appear), cond-mat/0607082.

The Langevin equation (LE) for the one-dimensional relativistic Brownian motion is derived from a microscopic collision model. The model assumes that a heavy point-like Brownian particle interacts with the lighter heat bath particles via elastic hard-core collisions. First, the commonly known, non-relativistic LE is deduced from this model, by taking into account the non-relativistic conservation laws for momentum and kinetic energy. Subsequently, this procedure is generalized to the relativistic case. There, it is found that the relativistic stochastic force is still δ-correlated (white noise) but does *no* longer correspond to a Gaussian white noise process. Explicit results for the friction and momentum-space diffusion coefficients are presented and discussed.

6. Domain growth

J. M. Kim, A. J. Bray, M. A. Moore, *Domain growth, directed polymer and self-organized criticality*, Phys. Rev. A **45**, 8546 (1992).

The nature of the roughness of the growing surface modeled by the Kardar-Parisi-Zhang (KPZ) equation has been further studied by defining a 'domain' structure for it. This was

done by mapping the height $h(x,t)$ of the surface onto a 'spin' $S(x,t) = sgn[h(x,t) - \langle h(t)\rangle]$, where $\langle h(t)\rangle$ is the mean height of the growing surface at time (t). It was then found that the growth of the surface has useful analogies with the domain-coarsening process in nonequilibrium systems quenched into an ordered phase. Thus, in $d = 1 + 1$, the average size $\langle l\rangle$ of spin domains grows as $t^{1/3}$ and the domain-size distribution $P(l,t)$ is consistent with $l^{-3/2} f(l/t^{2/3})$. We find that the autocorrelation function $A(t) = \langle S(x,t)S(x,0)\rangle$ decays as $t^{-}\alpha$, with $\alpha(d = 1 + 1) = 1.00.08$ and $\alpha(d = 2 + 1) = 1.50.1$. The form of $P(l,t)$ in higher dimensions and the connection between the spin autocorrelation function and the height autocorrelation function are discussed. For computational convenience, the KPZ equation was studied by transforming it to the problem of directed polymers in a random potential.

B. Derrida, C. Godrèche, I. Yekutieli, *Scale invariant regimes in one dimensional models of growing and coalescent droplets*, Phys. Rev. A **44**, 6241 (1991).

We consider several simplified models of breath figures in one dimension. For all these models, the combined effects of growth and of coalescence of droplets lead to a scale-invariant regime with a stable distribution of the distances between droplets. We show that at the mean-field level there exist one-parameter families of such stable distributions, each distribution being characterized by its decay at infinity. We explain how the mean-field theory can be improved by taking into account the effect of pair or higher correlations. For some models one can check that the pair and higher correlations are factorized, meaning that correlations are absent and that therefore the mean-field theory is exact. Finally, we show that a very simple model of domain growth related to spinodal decomposition, the one-dimensional Potts model in the limit of an infinite number of states, also possesses a one-parameter family of stable distributions analogous to what we obtained for breath figures.

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