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Advanced statistical physics

Master 2 iCFP - Soft Matter

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Prerequisites :

- equilibrium statistical physics (ensemble theory)
- probability : moments, cumulants (variance, etc), generating function, central limit theorem,...
- Gaussian integrals, saddle-point (steepest descent)

Contents

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PART 1 : Out-of-equilibrium statistical physics

0 Introduction

This first set of lectures is devoted to out-of-equilibirum statistical physics. Equilibrium statistical physics provides a well defined procedure to study the thermodynamic properties of systems with complex dynamics. The main idea is to replace the study of the complex dynamics of the system, i.e. how its state $\vec{\Gamma}(t)$ evolves in time (here $\vec{\Gamma}$ represents a point in phase space), by some statistical information, i.e. the probability $\rho(\vec{\Gamma})$ to find the system in a given state. The first approach would require to solve a macroscopic number of differential equations, while the beauty of the second approach lies on the fact that the determination of the probability density relies on very few information, what can be understood as a result of a maximum entropy principle. The choice of the distribution, microcanonical, canonical, grand canonical, etc, is driven by physical considerations or simply by convenience.

Out-of-equilibirum statistical physics requires a statistical treatment of the dynamics, which can be achieved by various approaches, phenomenoligical or microscopic. On the more phenomenological side : the Langevin equation, the master equation and the Fokker-Planck equation provide different approaches for the analysis of stochastic processes. On the more microscopic side : kinetic equations (BBGKY hierarchy, Boltzmann equation, Vlasov equation, hydrodynamic equations,...). Note that the frontier between phenomenological and microscopic is not so sharp, as we will see by deriving a Langevin equation from a microscopic model (§ f) page 43).

1 Stochastic processes (1) : the Langevin equation for a particle in a fluid

The aim of this introductory chapter is to start the discussion of stochastic processes with a concrete and simple example, and introduce several general and important ideas. Consider a particle in a fluid, submitted to a friction force. The usual *phenomenological* model is friction proportional to the velocity (Stokes regime) :

$$F_f = -\gamma\, v\,, \tag{1.1}$$

where γ is the friction coefficient. For a spherical particle of radius R, fluid mechanics gives $\gamma = 6\pi\eta\, R$ where η is the viscosity of the fluid (for example, $\eta \simeq 10^{-3}$ kg.m^{-1}.s^{-1} for water at $T = 20\,^{\circ}$C). In the absence of any other external force, the Newton equation of motion takes the form $m\,\dot{v} = -\gamma\, v$. The friction coefficient has dimension of a mass divided by a time, hence we can write

$$\gamma = \frac{m}{\tau} \tag{1.2}$$

where τ is the *relaxation time* for the velocity.

1.1 Fluctuations and Langevin force

In 1827, the scottish botanist Robert Brown observed with a microscope that pollen grains at the surface of water move erratically. [1] It was understood later that this observation supports the atomist description of matter as it is the manifestation of the *fluctuations* in the fluid (erratic motion of the molecules). A clear description of the phenomenon was given much later by Albert Einstein in 1905. If the particle (the pollen grain) is small, it is not only submitted to the friction

[1] You can find some historical perspectives in the excellent article of Bertrand Duplantier [9].

force but it is also sensitive to the *fluctuations in the fluid*, i.e. the collisions with molecules. The typical collision time between molecules in a fluid is $\tau_{\rm coll} \sim 10^{-15}$ s, thus we expect that the Brownian particle experiences collisions with the rate $1/\tau_{\rm coll}$ and which can be considered as *independent*. The friction force is due to the effect of these collisions over a much larger time scale. Additionally to the friction force, we model the frequent collisions by introducing in the Newton equation a force $\xi(t)$ fluctuating in time, called the "**Langevin force**" :

$$m\frac{{\rm d}v(t)}{{\rm d}t} = -\gamma\, v(t) + \xi(t) \tag{1.3}$$

$$\frac{{\rm d}x(t)}{{\rm d}t} = v(t) \tag{1.4}$$

Because the collisions are exerted at random along all directions, we expect that

$$\langle \xi(t) \rangle = 0 \tag{1.5}$$

where $\langle \cdots \rangle$ denotes *statistical averaging* [2] (it is also true if we consider averaging over time for a single history). As the Langevin force models the force exerted on the particle by the molecules, it is natural to assume short time correlations $\langle \xi(t)\xi(t') \rangle = \frac{C}{\tau_{\rm coll}}\, \varphi((t-t')/\tau_{\rm coll})$ where φ is normalised function of width ~ 1 centered on the origin (like $(1/2){\rm e}^{-|x|}$ or $\pi^{-1/2}{\rm e}^{-x^2}$) and C the strength of the fluctuations. As we are interested in the dynamics of the Brownian particle over time $\gg \tau_{\rm coll}$ we can simply consider

$$\big\langle \xi(t)\xi(t') \big\rangle = C\, \delta(t-t') \tag{1.6}$$

(which corresponds formally to $\tau_{\rm coll} \to 0$). A random function characterised by such local correlations is called a "*white noise*".

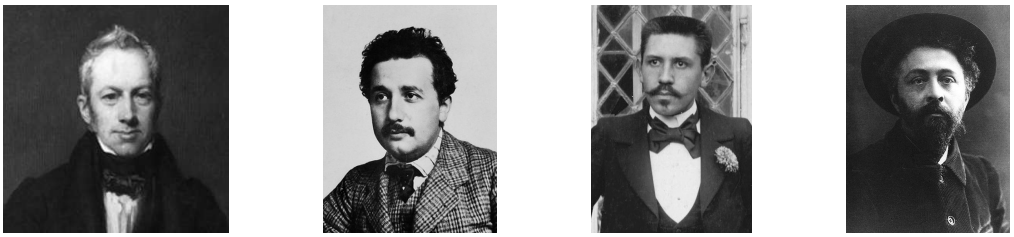


Figure 1: *Robert Brown (1773-1858), Albert Einstein (1879-1955), Paul Langevin (1872-1946) and Jean Perrin (1870-1942).*

This model was introduced by Paul Langevin [3] Why studying a model for the motion of a pollen grain at the surface of a fluid (or more generally a "colloid" in a fluid) is an important problem ? The reason is that several ideas of the Langevin model have a much broader application in out-of-equilibrium statistical physics.

We now analyse the statistical properties of the particle. Taking advantage that the equation of motion is *linear*, its integration gives

$$v(t) = v(0)\, {\rm e}^{-t/\tau} + \frac{1}{m}\int_0^t {\rm d}t'\, \xi(t')\, {\rm e}^{-(t-t')/\tau}\,. \tag{1.7}$$

[2] Statistical averaging corresponds to average over **different histories** of the particle, with same initial conditions but different realisations of the Langevin force. This is the procedure followed by Jean Perrin in his experiments [35] ; cf. Fig. 3.

[3] P. Langevin, "*Sur la théorie du mouvement brownien*", C. R. Acad. Sci. (Paris) **146**, pp. 530–533 (1908).

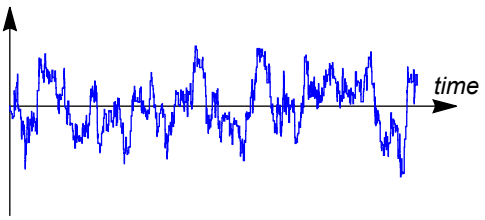


Figure 2: *A realization of the Ornstein-Uhlenbeck process $v(t)$ defined by (1.3) when $\xi(t)$ is a Gaussian white noise.*

This representation makes easy to deduce the statistical properties of $v(t)$ from those of $\xi(t)$. If the initial velocity is non random, we have

$$\langle v(t)\rangle = v(0)\,\mathrm{e}^{-t/\tau}\,. \tag{1.8}$$

After a time larger than $\tau = m/\gamma$, the memory of the initial velocity is lost and the velocity is independent of $v(0)$. We also get the correlator $\langle v(t)v(t')\rangle_c \stackrel{\text{def}}{=} \langle v(t)v(t')\rangle - \langle v(t)\rangle\,\langle v(t')\rangle$:

$$\langle v(t)v(t')\rangle_c = \frac{1}{m^2}\int_0^t \mathrm{d}t_1\,\mathrm{e}^{-(t-t_1)/\tau}\int_0^{t'}\mathrm{d}t_2\,\mathrm{e}^{-(t'-t_2)/\tau}\,\langle\xi(t_1)\,\xi(t_2)\rangle = \frac{C\,\mathrm{e}^{-(t+t')/\tau}}{m^2}\int_0^{\min(t,t')}\mathrm{d}t_1\,\mathrm{e}^{2t_1/\tau} \tag{1.9}$$

thus

$$\langle v(t)v(t')\rangle_c = \frac{C\,\tau}{2m^2}\left(\mathrm{e}^{-|t-t'|/\tau} - \mathrm{e}^{-(t+t')/\tau}\right)\,. \tag{1.10}$$

The correlations decay in time over the same time scale τ like the average time. The decorrelation of the velocity can be understood from the fact that the velocity decorrelates from the noise on the same time scale : we check easily that

$$\langle v(t)\xi(t')\rangle = \frac{C}{m}\,\theta_{\mathrm{H}}(t-t')\,\mathrm{e}^{-(t-t')/\tau}\,. \tag{1.11}$$

The stochastic process described by (1.3) where $\xi(t)$ is a Gaussian white noise is known as the "*Ornstein-Uhlenbeck process*".

✍ ***Exercice 1.1 Comparison between time average and statistical average :*** *One considers the random "function" given by the sum of impulses $\xi(t) = \sum_{n=1}^{N}\kappa_n\,\delta(t-t_n)$ defined over the interval $[0,T]$, where*

- *the t_n's are independent and identically distributed (i.i.d) random times uniformly distributed over $[0,T]$ (i.e. one t_n has distribution $p(t_n) = 1/T$). We denote by $\lambda = N/T$ (for $N\to\infty$ and $T\to\infty$) the rate of occurence of the random times.*
- *The κ_n's are i.i.d random variables with common distribution $w(\kappa)$ with finite $\langle\kappa_n^2\rangle$.*

a) Compute the time average of $\overline{\xi(t)}$, over the time interval $[0,T]$. Compare with the statistical average (over t_n's and κ_n's).

b) What is the condition on the random function $\xi(t)$ allowing to define a time averaged correlator $\widetilde{C}(t-t') = \overline{\xi(t)\xi(t')}^{c} = \overline{\xi(t)\xi(t')} - \overline{\xi(t)}\;\overline{\xi(t')}$? Compare to $C(t-t') = \langle\xi(t)\xi(t')\rangle_c = \langle\xi(t)\xi(t')\rangle - \langle\xi(t)\rangle\,\langle\xi(t')\rangle$.

1.2 A fluctuation-dissipation relation

After a sufficient long time, we expect that the particle is at thermal equilibrium with the fluid (which should be at thermal equilibrium), hence $\langle v(t)^2\rangle = k_{\mathrm{B}}T/m$ (equipartition theorem).

On the other hand, the outcome of the Langevin analysis is $\langle v(t)^2\rangle = C/(2m\gamma)$. Consistency of the previous analysis with equilibrium statistical physics imposes a constraint between the strength C of the Langevin noise (the fluctuations in the fluid), the friction coefficient γ and the temperature :

$$\underset{\text{fluctuations}}{\overset{}{C}} = 2 \overset{\text{dissipation}}{\overset{\uparrow}{\gamma}} k_{\rm B}T \tag{1.12}$$

this is a "*fluctuation-dissipation relation*" and a first formulation of the **fluctuation-dissipation theorem** (FDT). The mass has disappeared, which emphasizes that this is a property of the thermal bath (the fluid). We could write the correlator of the noise

$$\big\langle \xi(t)\xi(t')\big\rangle = 2\gamma\, k_{\rm B}T\, \delta(t-t')\,. \tag{1.13}$$

The phenomenological coefficients C, the strength of the Langevin force, and γ, the friction coefficient, are *not* two independent parameters (at least when thermal equilibrium holds). This reminds that friction and fluctuations have the same physical origin : the interaction of the particle with the molecules of the fluid. Below (§ p. 43), we will introduce a microscopic model of friction and try to clarify the origin of this relation.

✍ ***Exercice 1.2 Langevin equation for random initial velocity :*** *The correlator (1.10) corresponds to a fixed initial velocity. Consider now the case where the initial velocity is random, distributed according to* $P(v_0) \propto \exp\big\{-\frac{mv_0^2}{2k_BT}\big\}$.

a) Compute the new correlator, denoted $\langle v(t)v(t')\rangle^{\rm equil}$.

b) Can we compare the two correlators ?

✍ ***Exercice 1.3 Stationary measure of the Ornstein-Uhlenbeck process :*** *In the stationary regime, compare the correlator with the one obtained in Exercise* **??**. *Deduce what is the measure of the Ornstein-Uhlenbeck process.*

In Eq. (1.10), the second term is a transient term coming from the initial condition $v(0) = 0$. Hence for times $t\,,\ t' \gg \tau$ we can write

$$\big\langle v(t)v(t')\big\rangle = \frac{k_{\rm B}T}{m}\,{\rm e}^{-|t-t'|/\tau} \tag{1.14}$$

The correlations (1.11) between velocity and Langevin force can also be rewritten in terms of the temperature

$$\big\langle v(t)\xi(t')\big\rangle = \frac{2k_{\rm B}T}{\tau}\;\theta_{\rm H}(t-t')\,{\rm e}^{-(t-t')/\tau}\,. \tag{1.15}$$

✍ ***Exercice 1.4 Dissipation of the energy in the Langevin equation :*** *Consider the kinetic energy* $E_{\rm kin} = \frac{1}{2}mv^2$. *Give* $\frac{{\rm d}E_{\rm kin}}{{\rm d}t}$ *and deduce a differential equation for* $\langle E_{\rm kin}\rangle$. *Interpret the two terms and solve it.*

1.3 Diffusion

Now that we have obtained the statistical properties of the velocity, let us analyze the statistical properties of the position. The average position is simply

$$\langle x(t)\rangle = v(0)\tau\,\Big(1-{\rm e}^{-t/\tau}\Big) \tag{1.16}$$

On average, after a time $t \gg \tau$, the particule covers a distance $v(0)\tau$, which is not surprising as the memory of the initial velocity $v(0)$ is lost after time τ. What about the fluctuations ? In

the stationary regime the correlator of the speed is a "narrow function" of width τ, with weight

$$\int_{-\infty}^{+\infty} \mathrm{d}(t-t') \left\langle v(t)v(t') \right\rangle_c^{\text{equil}} = \frac{2k_{\mathrm{B}}T}{\gamma} \,. \tag{1.17}$$

As a result, neglecting the transient regime at short times, we can write

$$\left\langle x(t)^2 \right\rangle_c = \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \left\langle v(t_1)v(t_2) \right\rangle_c \simeq t \int_{-\infty}^{+\infty} \mathrm{d}(t_1-t_2) \left\langle v(t_1)v(t_2) \right\rangle_c^{\text{equil}} = \frac{2k_{\mathrm{B}}T}{\gamma}\, t \tag{1.18}$$

The linear behaviour characterizes **diffusion motion**. We introduce the *diffusive constant*

$$D \stackrel{\text{def}}{=} \lim_{t\to\infty} \frac{\left\langle x(t)^2 \right\rangle_c}{2t} \tag{1.19}$$

In other terms, we have obtained above a general relation between the velocity correlator and the diffusion constant

$$\boxed{D \stackrel{\text{def}}{=} \int_0^\infty \mathrm{d}t \, \left\langle v(t)v(0) \right\rangle} \tag{1.20}$$

Coming back to Langevin model, Eqs. (1.3,1.4), we get the expression

$$\boxed{D = \frac{k_{\mathrm{B}}T}{\gamma}} \tag{1.21}$$

which is known as the "*Einstein relation*". It was obtained in Einstein 1905's article on the Brownian motion. [4] It is also known as the "Einstein-Stokes law" or "Einstein-Stokes-Sutherland law". This is another formulation of the FDT, relating three different physical quantities, the diffusion constant characterizing the fluctuations of the motion, the friction coefficient characterizing the dissipation and the temperature.

✍ ***Exercice 1.5*** *: Choose initial conditions for a fixed initial velocity $x(0) = 0$ and $v(0) = v_0$. Compute $\langle x(t) \rangle$. Then, Study precisely $\left\langle x(t)^2 \right\rangle_c$. Analyze the crossover between the short time and large time $\left\langle x(t)^2 \right\rangle_c \propto t$ diffusive behaviour.*

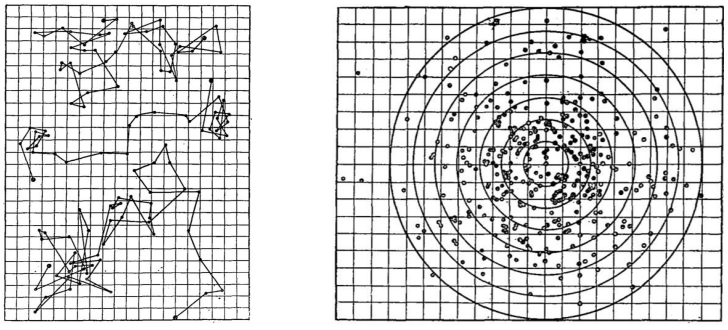


Figure 3: *Measurements of Jean Perrin (1908) ; from [35]. Left : few examples of trajectories. Right : final points after the several histories (for a fixed time).*

[4] A. Einstein, "*Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen*", Annalen der Physik **322**(8), 549–560 (1905).

✍ ***Exercice 1.6 Mean square displacement from the Langevin equation :*** *Our aim is to compute the mean square displacement* $\langle x(t)^2 \rangle$ *of a Brownian particle in a fluid We assume that* $x(0) = 0$ *and that the particle is initially at equilibrium with the fluid. We apply the method proposed by Langevin in his famous article (quoted in footnote 3).*

a) Prove that $\frac{\mathrm{d}^2}{\mathrm{d}t^2} x(t)^2 + \frac{1}{\tau} \frac{\mathrm{d}}{\mathrm{d}t} x(t)^2 = 2v(t)^2 + \frac{2}{m} x(t)\, \xi(t)$.

b) Give an argument to justify $\langle x(t)\, \xi(t) \rangle = 0$. *What is* $\langle v(t)^2 \rangle$ *?*

c) Argue that $\frac{\mathrm{d}}{\mathrm{d}t} \langle x(t)^2 \rangle \big|_{t=0} = 0$ *and deduce*

$$\langle x(t)^2 \rangle = \frac{2k_B T}{\gamma} \left[t - \tau \left(1 - \mathrm{e}^{-t/\tau} \right) \right] \tag{1.22}$$

Analyze carefully the limiting behaviours (interpret the $t \to 0$ *behaviour) and plot the function.*

1.4 Large scale properties and the overdamped regime

Over large time scales ($\gg \tau$), the correlator (1.14) seems a narrow function which can be replaced by a delta function

$$\langle v(t) v(t') \rangle_c^{\text{equil}} = \frac{C}{\gamma^2} \frac{\mathrm{e}^{-|t-t'|/\tau}}{2\tau} \overset{\text{large scale}}{\approx} \frac{C}{\gamma^2} \delta(t-t') = \frac{1}{\gamma^2} \langle \xi(t) \xi(t') \rangle \ . \tag{1.23}$$

Furthermore, assuming that $\xi(t)$ is Gaussian, [5] this corresponds to write

$$v(t) \overset{\text{large scale}}{\approx} \frac{1}{\gamma} \xi(t) \tag{1.24}$$

i.e. to neglect the acceleration term in Newton's equation :

$$0 \approx -\gamma v(t) + \xi(t) \qquad \text{(overdamped regime)} \ . \tag{1.25}$$

This approximation is called the "*overdamped regime*", which is achieved either by studying the process over large time scales, $\boxed{t \gg \tau}$, or by formally considering the limit of strong damping, $\gamma \to \infty$. As a result we obtain that the **velocity equals the force**.

Overdamped regime : "Aristote equation".— The pre-Galileo-Newtonian postulate, proposed by Aristote, asserted that velocity is proportional to force. [6] The above discussion has shown that this makes sense for the motion of a particle in a viscous fluid. If an additional (conservative) force $F(x)$ is introduced in the equation of motion for the overdamped regime (1.25), we have

$$\boxed{\frac{\mathrm{d}x(t)}{\mathrm{d}t} \approx \frac{1}{\gamma} \left[F(x(t)) + \xi(t) \right]} \qquad \text{(overdamped regime)} \ . \tag{1.26}$$

I call this equation the "Aristote equation", although this is a bit anachronistic (differential calculus was invented only at the end of XVIIth century by Leibniz and Newton).

[5] Gaussian processes have only two finite cumulants κ_1 and κ_2, all others being zero. Equality of averages and variances of two Gaussian processes implies that the have the same statistical properties.

[6] In the book "Aristote's Physics", it is claimed that the velocity of a falling body is proportional to its weight, i.e. the velocity is proportional to the force. In other terms the motion requires a force for Aristote (384-322 BC). It required almost two thousand years to understand that force induces acceleration, not motion : motion can exist without force. This was the achievement of Galileo Galilei (1564-1642 AC).

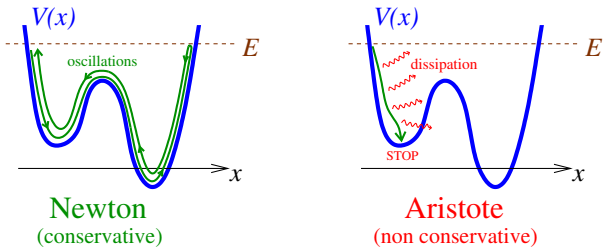


Figure 4: *The dynamics described by the Newton equation conserves the energy, whereas the energy is dissipated during the "Aristote dynamics".*

A last comment about the physical content of the "Aristote equation", which we rewrite

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = -\frac{1}{\gamma}\frac{\partial V(x)}{\partial x} + \sqrt{2D}\,\eta(t) \tag{1.27}$$

where $V(x)$ is the potential, such that $F(x) = -V'(x)$, and $\eta(t)$ a normalised Gaussian white noise, i.e. with $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = \delta(t-t')$. Contrary to the Newton equation, which describes a *conservative* dynamics, the Aristote equation describes a *non conservative* dynamics, along which energy is dissipated (cf. Exercise 1.4). In particular, in the $D \to 0$ limit, the trajectory converges towards the first stationary point (Fig. 4). If the first stationary point is a local minimum like on the figure, only a fluctuation (finite D) can untrap the particle.

We will come back later to a general analysis of this stochastic differential equation.

1.5 The free Brownian motion (the Wiener process)

In the overdamped regime, in the absence of the external force $F(x)$, the position is just the integral of a Gaussian white noise

$$x(t) = \underbrace{x(0)}_{=0} + \frac{1}{\gamma}\int_0^t \mathrm{d}u\,\xi(u) \tag{1.28}$$

Let us simplify the notations and introduce a normalised Gaussian white noise $\eta(t) = \xi(t)/\sqrt{C}$ so that

$$\langle \eta(t) \rangle = 0 \quad \text{and} \quad \langle \eta(t)\eta(t') \rangle = \delta(t-t')\,. \tag{1.29}$$

We now consider the normalised free Brownian motion, with no external force (the "Wiener process") by setting $x(t) = \frac{\sqrt{C}}{\gamma} W(t)$. Obviously

$$\frac{\mathrm{d}W(t)}{\mathrm{d}t} = \eta(t) \qquad \Rightarrow \qquad W(t) = \int_0^t \mathrm{d}u\,\eta(u) \tag{1.30}$$

thus

$$\langle W(t)W(t') \rangle = \int_0^t \mathrm{d}u \int_0^{t'} \mathrm{d}v\,\delta(u-v) = \int_0^{\min(t,t')} \mathrm{d}u \tag{1.31}$$

Finally

$$\boxed{\langle W(t)W(t') \rangle = \min\left(t,t'\right)} \tag{1.32}$$

Interpretation : consider the case $t < t'$, we have $\langle W(t)W(t') \rangle = \langle [W(t') - W(t)]W(t) \rangle + \langle W(t)^2 \rangle$. The second term is t (diffusion) ; the first term vanishes as the two increments $W(t') - W(t) = \int_t^{t'} \mathrm{d}u\,\eta(u)$ and $W(t) = \int_0^t \mathrm{d}u\,\eta(u)$ are independent.

✍ ***Exercice 1.7 :*** *Check that the increment depends only on the time difference*

$$\langle \left[W(t) - W(t')\right]^2 \rangle = |t - t'| \tag{1.33}$$

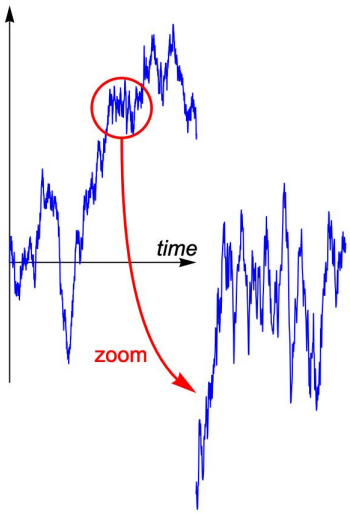


Figure 5: *A typical Brownian trajectory : $W(t)$ as a function of t. If one zooms, trajectory looks the same (scale invariance).*

Continuity.— In the limit $t \to t'$ we get $\lim_{t\to t'} \langle \big[W(t) - W(t')\big]^2 \rangle = 0$. This last equation suggests that the curve $W(t)$ is **continuous**. As a matter of fact the two statements are disconnected : the fact that this limit is zero does not imply continuity (cf. Exercise 2.5)!

In order to prove continuity, we should consider the probability

$$\text{Proba}\big\{|W(t) - W(t')| < \epsilon\big\} = \text{erf}\left(\frac{\epsilon}{\sqrt{2|t-t'|}}\right) . \tag{1.34}$$

This expression simply follows from the fact that the increment between times t and t' is Gaussian, with variance $|t - t'|$, hence the cumulative distribution related to the error function $\text{erf}(x)$ (see Appendix **??**). This expression shows that $\forall\, \epsilon > 0$, there exists a sufficiently small time difference, choose $|t - t'| \ll \epsilon^2$, so that we are sure that the distance is smaller than ϵ : $\text{Proba}\big\{|W(t) - W(t')| < \epsilon\big\} \simeq 1 - \mathcal{O}(\mathrm{e}^{-\epsilon^2/(2|t-t'|)})$. Because we can choose ϵ as small as we want, this corresponds to continuity of the process.

Continuity can also be understood in a simpler manner by constructing the Brownian motion from the discrete random walk, $W(t) = \sum_{\tau=1}^{t/\epsilon} \delta W_\tau$ where $\langle \delta W_\tau \rangle = 0$ and $\langle \delta W_\tau \delta W_{\tau'} \rangle = \epsilon\, \delta_{\tau,\tau'}$, and taking the continuum limit of small jumps $\delta W_\tau \sim \sqrt{\epsilon} \to 0$ occuring with high rate $1/\epsilon \to \infty$.

Non differentiability Another consequence of (1.33) is that

$$\left\langle \left(\frac{W(t) - W(t')}{t - t'}\right)^2 \right\rangle = \frac{1}{|t - t'|} \tag{1.35}$$

which goes to infinity when $t \to t'$: the derivative of typical curves is infinite, i.e. $W(t)$ is *non differentiable*. We can see on the plot that the curve is indeed extremely irregular (see Fig. 5).

Scaling This irregularity is related to *scale invariance* and fractal behaviour (with fractal dimension $1/2$). For a scaling factor $\alpha > 0$, it is clear that

$$\big\langle W(\alpha t) W(\alpha t') \big\rangle = \alpha \, \min\big(t, t'\big) = \alpha \, \big\langle W(t) W(t') \big\rangle \tag{1.36}$$

Because $W(t)$ is Gaussian, all statistical information is encoded in the two point function, hence this equality means that we can identify the statistical properties of $W(\alpha t)$ with those of

$\sqrt{\alpha}\,W(t)$. Mathematicians express this through and "*equality in law*" (or "*equality in distribution*")

$$\boxed{W(\alpha t) \overset{(\text{law})}{=} \sqrt{\alpha}\,W(t)} \tag{1.37}$$

(the "laws" of the two sides are equal). The same argument applies to the Gaussian white noise gives

$$\eta(\alpha t) \overset{(\text{law})}{=} \frac{1}{\sqrt{\alpha}}\,\eta(t)\,. \tag{1.38}$$

✍ ***Exercice 1.8 From the Wiener process to the Ornstein-Uhlenbeck process :*** *We consider the Wiener process described by the equation* $\frac{\mathrm{d}W(u)}{\mathrm{d}u} = \eta(u)$*, where* $\eta(u)$ *is a normalised Gaussian white noise.*

a) Consider $\varphi(u)$ *a monotonous function. Argue that*

$$\eta(\varphi(u)) \overset{(law)}{=} \frac{1}{\sqrt{|\varphi'(u)|}}\,\eta(u) \tag{1.39}$$

b) Deduce the stochastic differential equation for

$$x(t) = \frac{W(u)}{\sqrt{u}} \qquad \textit{with} \qquad u = u_0 \mathrm{e}^{2\gamma t} \tag{1.40}$$

☺ Important points

- Master the analysis of the linear Langevin equation (1.3) (integrate, average, etc)
- Fluctuation-dissipation relation (different forms) : Langevin force and damping force have the same origin, hence the relation.
- Wiener process : main properties.

2 Stochastic processes (2) : Markov processes and master equation

We have discussed above few simple stochastic processes (the Wiener process and the Ornstein-Uhlenbeck process). Let us now introduce some general ideas (vocabulary) allowing for a general analysis of stochastic processes.

Figure 6: *Marian von Smoluchowski (1872-1917) is considered as the father of the theory of stochastic processes.*

2.1 Generalities : joint probabilities, conditional probabilities

The aim of the section is to introduce some useful tools and concepts needed to describe random processes. In the previous section, we have obtained an integral representation of the trajectory in terms of the Langevin force, which has been used in order to analyze its statistical properties. In general, one considers a random process $X(t)$, i.e. a random function of the time, and one is interested in its statistical properties. Its probability weight should be given by a *functional* $P[X(t)]$, which is rather complicate to manipulate (for example an explicit calculation of an average might be difficult, e.g. $\langle X(t)\rangle = \int \mathcal{D}X(t)\, P[X(t)]\, X(t)$ requires to define how to perform the integral over the functions). For this reason we will introduce other tools more simple conceptually and practically : instead of considering a probability weight $\mathcal{D}X(t)\, P[X(t)]$ which allows to know the value of the process at *all* times, we introduce a joint distribution which provides statistical information at a discrete set of times.

Joint probability : In order to characterize the statistical properties of the random process, we can introduce the joint probability or the n-point function

$$\underbrace{P_n(x_n,t_n;\cdots;x_2,t_2;x_1,t_1)}_{\longleftarrow \text{time}} = \langle \delta(x_n - X(t_n)) \cdots \delta(x_1 - X(t_1))\rangle \tag{2.1}$$

corresponding to the probability (density) for the process to be equal to $x_1,\cdots,x_n$ at times $t_1,\cdots,t_n$. We can also write

$$P_n(x_n,t_n;\cdots;x_2,t_2;x_1,t_1)\,\mathrm{d}x_1\cdots\mathrm{d}x_n = \mathrm{Proba}\{X(t_1)\in[x_1,x_1{+}\mathrm{d}x_1]\ \&\ \cdots\ \&\ X(t_n)\in[x_n,x_n{+}\mathrm{d}x_n]\}$$

From the definition, it is clear that one integration connect the n-point to the $n-1$-point functions

$$\int \mathrm{d}x_k\, P_n(x_n,t_n;\cdots;x_{k+1},t_{k+1};\underline{x_k,t_k};x_{k-1},t_{k-1};\cdots;x_1,t_1) \tag{2.2}$$

$$= P_{n-1}(x_n,t_n;\cdots;x_{k+1},t_{k+1};x_{k-1},t_{k-1};\cdots;x_1,t_1) \tag{2.3}$$

It is clear from (2.1) that the joint distribution with n arguments is appropriate to express the n-point correlation function of the process :

$$\langle X(t_1)\rangle = \int \mathrm{d}x_1\, P_1(x_1,t_1)\, x_1 \tag{2.4}$$

$$\langle X(t_2)X(t_1)\rangle = \int \mathrm{d}x_1\mathrm{d}x_2\, P_2(x_2,t_2;x_1,t_1)\, x_2\, x_1 \tag{2.5}$$

etc.

Conditional probability : Another important concept is the one of conditional probability corresponding to the probability for the process to pass through $x_1,\cdots,x_n$ at successive times $t_1,\cdots,t_n$, *given* that it has previously passed through $y_1,\cdots,y_n$ at successive times $\tau_1,\cdots,\tau_n$:

$$P_{n|m}(x_n,t_n;\cdots;x_1,t_1\,|\,y_m,\tau_m;\cdots;y_1,\tau_1) = \frac{P_{n+m}(x_n,t_n;\cdots;x_1,t_1;y_m,\tau_m;\cdots;y_1,\tau_1)}{P_m(y_m,t_m;\cdots;y_1,\tau_1)} \tag{2.6}$$

In particular, the conditional probability is useful to write conditional averages. Example :

$$\langle X(t_2)X(t_1)\,|\,X(0)=x_0\rangle = \int \mathrm{d}x_1\mathrm{d}x_2\, x_2\, x_1\, P_{2|1}(x_2,t_2;x_1,t_1\,|\,x_0,0)\,, \tag{2.7}$$

which is the correlator over trajectories which all start from the same point $X(0)=x_0$.

2.2 Markov processes

A very important class of random processes are *Markov processes*. A Markov process is a random process whose evolution after time t_0 only depends on its value at time t_0. Mathematically, this property takes the form

$$P_{n|m}(x_n,t_n;\cdots;x_1,t_1\,|\,y_m,\tau_m;\underbrace{\cdots;y_1,\tau_1}_{\text{past history}}) = P_{n|1}(x_n,t_n;\cdots;x_1,t_1\,|\,y_m,\tau_m) \tag{2.8}$$

which expresses that history prior to τ_m does not matter : only the *last* position y_m at time τ_m determines the evolution at times $t_1,\cdots,t_n$.

Figure 7: *Andreï Andreïevich Markov (1856-1922).*

Let us examine the consequences of this assumption. Consider for example the three point function :

$$P_3(x_3,t_3;x_2,t_2;x_1,t_1) = P_{1|2}(x_3,t_3|x_2,t_2;x_1,t_1)\,P_2(x_2,t_2;x_1,t_1) \tag{2.9}$$

$$= P_{1|2}(x_3,t_3|x_2,t_2;x_1,t_1)\,P_{1|1}(x_2,t_2|x_1,t_1)\,P_1(x_1,t_1) \tag{2.10}$$

$$\overset{\text{Markov}}{=} P_{1|1}(x_3,t_3|x_2,t_2)\,P_{1|1}(x_2,t_2|x_1,t_1)\,P_1(x_1,t_1) \tag{2.11}$$

We can generalize this to any joint distribution. We simplify the notation as $P_{1|1}(x,t|y,t_0) \equiv P(x,t|y,t_0)$ and $P_1(x,t) \equiv P(x,t)$ and we conclude that

A Markov process is fully characterized by $P(x,t\|y,t_0)$ and $P(x,t)$ only.

Chapman-Kolmogorov equation : Start from the general property

$$\int \mathrm{d}x_2\, P_3(x_3,t_3;x_2,t_2;x_1,t_1) = P_2(x_3,t_3;x_1,t_1)\,. \tag{2.12}$$

For a Markov process, using (2.11), one gets the Chapman-Kolmogorov equation

$$\boxed{\int \mathrm{d}x_2\, P(x_3,t_3|x_2,t_2)\,P(x_2,t_2|x_1,t_1) = P(x_3,t_3|x_1,t_1)} \tag{2.13}$$

The probability to go from x_1 to x_3 is the sum over x_2 of the probabilities conditioned to passed through x_2.

Propagator : Integrating the two point-point function $P_2(x_f,t_f;x_i,t_i) = P(x_f,t_f|x_i,t_i)\,P(x_i,t_i)$ over the initial coordinate, we get

$$P(x_f,t_f) = \int \mathrm{d}x_i\, P(x_f,t_f|x_i,t_i)\,P(x_i,t_i) \tag{2.14}$$

Which shows that the conditional probability relates the distribution at initial time t_i to the distribution at final time t_f. For this reason, $P(x_f,t_f|x_i,t_i)$ is sometimes called the "*propagator*".

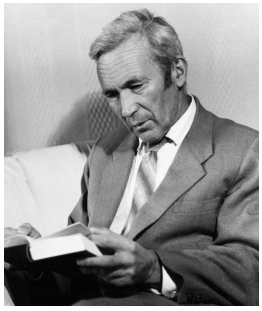


Figure 8: *Andreï Nikolaïevitch Kolmogorov (1903-1987), well-known by physicists for his major contributions to the theory of dynamical systems and probability.*

Homogeneous Markov processes : In the following, in order to simplify the discussion, we will restrict ourselves to Markov processes such that the transition probability is invariant under time translation

$$P(x_2,t_2|x_1,t_1) = P(x_2,t_2-t_1|x_1,0) \tag{2.15}$$

Such random processes are denoted "*homogeneous*". Since it only depends on the time difference, we will also write the propagator as $P_t(x|x_0)$.

a) A first example of Markov process

We can come back to the Langevin equation (1.3) for the velocity. (i) The equation for $v(t)$ is first order, hence the evolution at $t>0$ is fully determined by $v(0)=v_0$. (ii) The Langevin force is a white noise (ξ uncorrelated in time), thus no time correlations are hidden in the noise. From (i) & (ii) we conclude that the process is Markovian.

Let us now discuss the related fundamental probabilities $P(v,t)$ and $P(v,t|v_0,0)$, which can be easily obtained if we assume furthermore that the Langevin noise is **Gaussian**. [7] From the above calculations we have, cf. (1.8,1.10)

$$\langle v(t)\rangle = v_0\,\mathrm{e}^{-t/\tau} \tag{2.16}$$

$$\mathrm{Var}[v(t)] = \frac{k_{\mathrm{B}}T}{m}\left(1-\mathrm{e}^{-2t/\tau}\right) \tag{2.17}$$

The process $v(t)$ is a convolution of the Gaussian Langevin force $\xi(t)$, hence it is also Gaussian (a sum of Gaussian variables is also Gaussian). The knowledge of these two moments is sufficient to characterize the full distribution, which is here conditioned by the initial velocity : [8]

$$P_t(v|v_0) = \sqrt{\frac{m}{2\pi k_{\mathrm{B}}T\,\left(1-\mathrm{e}^{-2t/\tau}\right)}}\,\exp\left\{-\frac{m\,(v-v_0\,\mathrm{e}^{-t/\tau})^2}{2k_{\mathrm{B}}T\,\left(1-\mathrm{e}^{-2t/\tau}\right)}\right\}. \tag{2.18}$$

[7] The distribution of the noise is a Gaussian : $P[\xi] \propto \exp\left\{-\frac{1}{2C}\int \mathrm{d}t\,\xi(t)^2\right\}$. On can deduce from this that $\langle \xi(t)\xi(t')\rangle = C\,\delta(t-t')$ [hint : discretize the time to check this].

[8] This argument was used in the historical paper : G. E. Uhlenbeck and L. S. Ornstein, "*On the Theory of the Brownian Motion*", Phys. Rev. **36**(5), 823–841 (1930).

At large time, the conditional probability converges toward the equilibrium distribution

$$P_t(v|v_0) \underset{t\to\infty}{\longrightarrow} P(v) = \sqrt{\frac{m}{2\pi k_{\rm B}T}}\,{\rm e}^{-\frac{m}{2k_{\rm B}T}\,v^2} \tag{2.19}$$

(the Gibbs distribution). Here, the "one point distribution" $P(v)$ is independent of the time due to the existence of a stationary state (this is not always the case). This is also why the conditional probability rapidly converges (exponentially fast) toward the equilibrium distribution. The process described by equation (1.3), or the conditional probability (2.18), is known as the **Ornstein-Uhlenbeck process**. It is the subject of the Doob theorem (the only homogeneous Gaussian stationary random process is the Ornstein-Uhlenbeck process). [9]

✍ ***Exercice 2.1 :*** *Recover the correlator* $\langle v(t)v(t')\rangle_c$ *given by* (1.10) *from the conditional probability. Consider both cases of initially fixed velocity and random velocity.*

b) Markovian or non-Markovian ?

Random walk .— After each step, a random walker forgets past history (where he is coming from) : this is a Markov process.

Choosing clothes every morning.— Consider choosing clothes from a closet every morning as a stochastic process. The selection depends on the weather of the previous day : there is a memory effect hence the process is non Markovian.

$v(t)$ **is a Markov process.—** We have pointed out that the Langevin equation (1.3) describes a Markov process because
(i) the differential equation is first order, hence the solution for $t > 0$ depends only on some initial value $v(0)$;
(ii) the noise is δ-correlated, hence there is no memory hidden in the Langevin force.

$x(t)$ **is a non Markovian process.—** The position $x(t)$ of the particle is a non Markovian process. There are two points of view leading to this conclusion.

• it obeys the stochastic differential equation (SDE) $m\,\ddot{x}(t) = -\gamma\,\dot{x}(t) + \xi(t)$, which is *second* order. The noise is still δ-correlated, however, the solution of the differential equation is determined both by the initial position $x(0)$ *and* the initial velocity $\dot{x}(0)$, which depends on the history before $t = 0$ (velocity indicates where the particle comes from). We break point (i) while point (ii) holds. The process $x(t)$ is non Markovian.

• We could also argue that $x(t)$ obeys a first order SDE, $\dot{x}(t) = v(t)$, whose solution is determined only by $x(0)$, hence point (i) holds. The velocity now plays the role of the noise. This "noise" is now characterized by a finite correlation time (memory time), $\langle v(t)v(t')\rangle = \frac{k_{\rm B}T}{m}\,{\rm e}^{-|t-t'|/\tau}$ (one says that the SDE for $x(t)$ involves a "colored noise"). Within this point of view we break point (ii), which leads to the same conclusion, as it should, that $x(t)$ is non Markovian.

$(x(t), v(t))$ **is a 2D Markov process.—** $x(t)$ alone is a non Markovian process, however it can be considered as the first component of a two-dimensional Markov process $\vec{\psi}(t) = (x(t), v(t))$. Indeed, the system of differential equations for $(x(t), v(t))$ is *first* order and involves a δ-correlated noise. It presents the more general form of a *multidimensional Langevin equation*

$$\dot{\psi}_i = \Phi_i(\vec{\psi}) + B_{ij}\,\Xi_j(t) \tag{2.20}$$

[9] The Ornstein-Uhlenbeck process is more frequently introduced as a model for a particle attached to a spring in the overdamped regime : $\dot{x}(t) = -k\,x(t) + \xi(t)$ (I forget the friction coefficient γ).

where here $\vec{\Phi} = (v, F(x) - \gamma\, v)$ is the drift (we have added a conservative force). The noise $\vec{\Xi}(t) = (0, \xi(t))$ is uncorrelated in time. The matrix is $B_{xx} = B_{xv} = B_{vx} = 0$ and $B_{vv} = 1$. Hence it is a 2D Markovian process. We will see that the joint distribution $P_t(x, v)$ obeys the "Kramers equation" $\partial_t P_t = \big[-\partial_x v - \partial_v (F(x) - \gamma\, v) + \gamma k_{\rm B} T\, \partial_v^2 \big] P_t$.

Conclusion : The analysis of this example shows that the identification of a Markov process is sometimes a question of perspective, and also illustrates that Markov processes are elementary building blocks. Many non Markovian processes can be constructed from Markov processes.

2.3 Master equation

a) Master equation for continuous processes

Let us start with the case of continuous processes, which is more general. As we have seen, Eq. (2.14), the evolution of the distribution of a Markov process can be represented in terms of the conditional probability which plays the role of a "*propagator*"

$$P(x,t) = \int \mathrm{d}x_0\, P(x,t|x_0,t_0)\, P(x_0,t_0)\,. \tag{2.21}$$

However, this equation and (2.13) are not of great help to determine the two fundamental functions $P(x,t)$ and $P(x,t|x_0,t_0)$. The distribution is more conveniently obtained by solving an evolution equation for an infinitesimal time : such an evolution equation can be related to the above integral equation by considering the evolution during an infinitesimal time $\delta t \to 0$. In this case we expect

$$P(x, t+\delta t|x_0, t) \simeq \delta(x - x_0) + \delta t\, W_t(x|x_0) + \mathcal{O}(\delta t^2) \tag{2.22}$$

The linear correction follows from the Markov assumption : at short time, the transition probability is linear with time and involves a transition rate $W_t(x|x_0)\mathrm{d}x$ for performing the transition from x_0 to $[x, x + \mathrm{d}x]$.

If **we restrict ourselves to homogeneous processes** (time translation invariant) we have

$$W_t(x|x_0) \to W(x|x_0) \qquad \text{(homogeneous process)} \tag{2.23}$$

independent of time. For homogeneous processes, we find the differential equation (in time)

$$\boxed{\frac{\partial P(x,t)}{\partial t} = \int \mathrm{d}x'\, W(x|x')\, P(x',t)} \tag{2.24}$$

This is the general form of the Master equation for a continuous process. The fact that the differential equation in time is *first order* means that the future evolution of the probability density for times $t > 0$ depends only on the distribution $P(x, 0)$ and not on the past history (Markov property). This is the (*a posteriori*) justification for the expansion (2.22). Note that the conservation of probability requires that

$$\int \mathrm{d}x_f\, W(x_f|x_i) = 0 \quad \Rightarrow \quad \frac{\partial}{\partial t} \int \mathrm{d}x\, P(x,t) = 0 \;\; \forall\, t \tag{2.25}$$

so that probability $\int \mathrm{d}x\, P(x;t) = 1$ is conserved. This condition follows from the normalization condition of the conditional probability, in the expansion (2.22). Obviously, the conditional probability obeys the same equation

$$\frac{\partial P_t(x|x_0)}{\partial t} = \int \mathrm{d}x'\, W(x|x')\, P_t(x'|x_0) \quad \text{for initial condition } P_0(x|x_0) = \delta(x - x_0)\,. \tag{2.26}$$

In a specific problem, the transition "rates" $W(x|x_0)$ are given and the aim is to solve the master equation (2.24), or (2.26).

In the most general case, a Markov process can combine

- a diffusion : in this case the integral kernel is replaced by a second order differential operator
- jumps : leading to an integral term in the master equation, like in (2.24).

Below, we will give concrete examples.

b) Master equation for discrete processes

For simplicity, let us first consider a random process which takes discrete values $X(t) \in \{x_1, \cdots, x_{\mathcal{M}}\}$ and denote $P_n(t) = \text{Proba}\{X(t) = x_n\}$. The Markovian nature of the process implies that $P_n(t+\delta t)$ depends on the state of the process at time t, i.e. the probability $P_n(t)$, and the probability for some transition between t and $t+\delta t$. We denote by $W_{n,m} \geqslant 0$ the rate for a transition from m to n, with $n \neq m$, meaning that the probability to make a transition $m \to n$ on the interval $[t, t+\delta t]$ is $W_{n,m}\delta t$. Therefore

$$P_n(t+\delta t) \overset{\text{Markov}}{=} P_n(t)\Big(1 - \underbrace{\sum_{m(\neq n)} W_{m,n}\delta t}_{\text{proba to leave } n}\Big) + \sum_{m(\neq n)} \underbrace{W_{n,m}\delta t}_{\text{proba for } m\to n} P_m(t) \tag{2.27}$$

It is convenient to define the diagonal elements as $W_{n,n} \overset{\text{def}}{=} -\sum_{m\,(\neq n)} W_{m,n} < 0$. Letting $\delta t \to 0$, we obtain the *first order* differential equation

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}P_n(t) = \sum_m W_{n,m}P_m(t)} \tag{2.28}$$

Eq. (2.28) is the *master equation* for a discrete process. The coefficients $W_{n,m}$ form a $\mathcal{M}\times\mathcal{M}$ matrix W, which satisfies the condition

$$\sum_n W_{n,m} = 0 \tag{2.29}$$

ensuring the conservation of probability $\sum_n P_n(t) = 1\ \forall t$. Note that this condition is related to an asymmetry of the matrix ($W_{n,m} \neq W_{m,n}$ in general) : the sum of all elements of a column is zero, however summing elements along a line is non zero in general. By using $W_{n,n} = -\sum_{m\,(\neq n)} W_{m,n}$ we can rewrite the master equation as

$$\frac{\mathrm{d}}{\mathrm{d}t}P_n(t) = \sum_{m\,(\neq n)} [W_{n,m}P_m(t) - W_{m,n}P_n(t)] \tag{2.30}$$

(we can also replace $\sum_{m\,(\neq n)} \to \sum_n$). This form avoids to add the restriction (2.29).

Birth and death processes.— A subclass of these discrete processes are "birth and death processes". They correspond to the case where the transition matrix is tridiagonal, i.e. allows only transitions between nearest neighbour states. The master equation has the form

$$\frac{\mathrm{d}}{\mathrm{d}t}P_n(t) = d_{n+1}\,P_{n+1}(t) + b_{n-1}\,P_{n-1}(t) - (d_n + b_n)\,P_n(t) \tag{2.31}$$

where $d_n > 0$ and $b_n > 0$ are death and birth rates, respectively. A simple example is the Poisson process studied below in great detail. Another example will be discussed in Exercise 2.14.

We discuss now several examples of Markov processes (discrete or continuous).

c) The random telegraph process

We consider the *most simple Markov process* $X(t)$, taking only two possible values X_1 or X_2 (this is a "two level system" for stochastic processes). Hence we should introduce two probabilities $P_i(t) = \text{Proba}\{X(t) = X_i\}$ with $i \in \{1, 2\}$. In general, there are two different transition rates λ_1 (from X_1 to X_2) and λ_2 (from X_2 to X_1). A typical realization of the process is represented on Fig. 9. A physical realization is presented in Fig. 10.

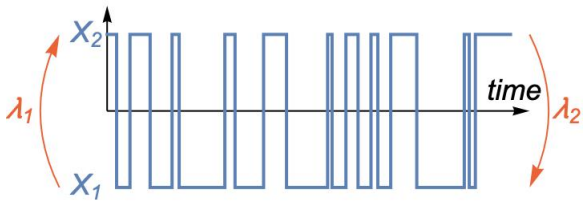


Figure 9: *Random telegraph process with* $X_1 = -1$ *and* $X_2 = +1$.

The two probability obey the set of differential equations

$$\frac{\mathrm{d}P_1(t)}{\mathrm{d}t} = -\lambda_1 P_1(t) + \lambda_2 P_2(t) \tag{2.32}$$

$$\frac{\mathrm{d}P_2(t)}{\mathrm{d}t} = +\lambda_1 P_1(t) - \lambda_2 P_2(t) \tag{2.33}$$

in each equation, one term populates the state and the other empties the state.

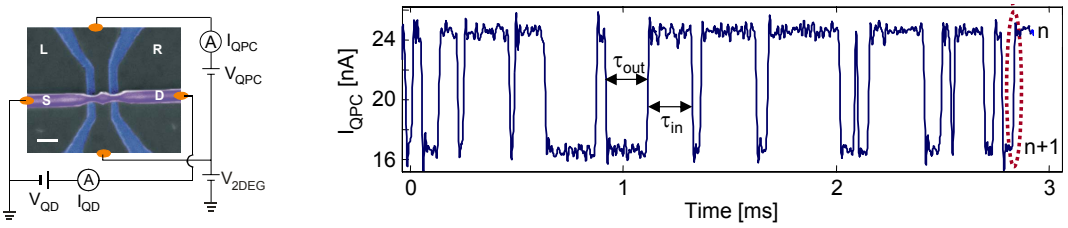


Figure 10: *A physical realization of the random telegraph process : the charge inside a quantum dot is measured as a function of the time with a neighbouring probe. The current* I_{QPC} *through the probe is proportional to the number of electrons inside the central island, which fluctuates by one unit (one electron). From Ref. [16].*

In the following exercice, we study the corresponding master equation, (2.28) for a 2×2 matrix W.

✍ ***Exercice 2.2 Random telegraph process :***
a) Derive the set of differential equations for $P_1(t)$ *and* $P_2(t)$. *Deduce a matricial form* $\frac{\mathrm{d}}{\mathrm{d}t}P(t) = W\,P(t)$, *where* $P = (P_1\ P_2)^{\mathrm{T}}$ *is the column vector (*$^{\mathrm{T}}$ *denotes tranposition).*

b) Find the stationary solution, denoted by P_i^*, *and give the general solution of the master equation.*

c) Determine the conditional probability $P_t(i|j)$. *Discuss detailed balance. Compute* $\sum_j P_t(n|j)\,P_j^*$ *and interpret.*

d) Express $\langle X(t)\rangle$ *and* $\langle X(t)X(t')\rangle$ *in the stationary regime. For simplicity, choose* $X_1 = 0$ *and* $X_2 = 1$. *Show that the correlator* $C(t-t') = \langle X(t)X(t')\rangle - \langle X(t)\rangle\,\langle X(t')\rangle$ *is*

$$C(t-t') = \frac{\lambda_1\lambda_2}{(\lambda_1+\lambda_2)^2}\,\mathrm{e}^{-(\lambda_1+\lambda_2)|t-t'|}\,. \tag{2.34}$$

e) Deduce the power spectrum $S(\omega)$ of the telegraphic noise (use the Wiener-Khintchine theorem discussed below, § 2.5, and the relation with the correlation function $C(t)$).

d) The Poisson process (statistics of uncorrelated events)

The Poisson process takes integer values $\mathscr{N}(t) \in \mathbb{N}$ and starts at initial time from $\mathscr{N}(0) = 0$. With probability rate λ, the process is incremented by one, i.e. during an interval of time of duration $\mathrm{d}t$, the process increases by one with probability $\lambda\,\mathrm{d}t$. We denote $P_n(t) = \mathrm{Proba}\{\mathscr{N}(t) = n\}$ its probability.

The Poisson process (PP) counts the occurences of *independent events*. For instance the number of drops of rain falling on the floor during a time interval t. Or the number of desintegrations in a radioactive material during a time t.

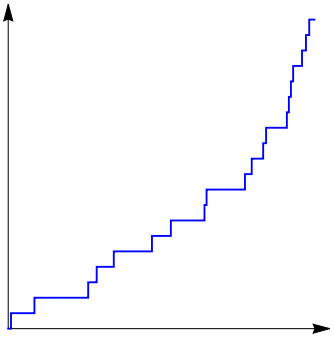


Figure 11: *A typical realization of the Poisson process : $\mathscr{N}(t)$ as a function of t.*

The master equation of the PP is

$$\begin{cases} \dfrac{\mathrm{d}P_n(t)}{\mathrm{d}t} = \lambda\, P_{n-1}(t) - \lambda\, P_n(t) \quad \text{for } n > 0 \\ \dfrac{\mathrm{d}P_0(t)}{\mathrm{d}t} = -\lambda\, P_0(t) \end{cases} \tag{2.35}$$

In other terms, the rate "matrix" has elements on the diagonal and just below the diagonal $W_{n,m} = \lambda\big(-\delta_{m,n} + \delta_{m,n-1}\big)$.

✍ ***Exercice 2.3 Master equation for the PP :***
a) Show that the master equation for the Poisson process is (2.35).

b) Introduce the generating function $G(z;t) \overset{\text{def}}{=} \sum_{n=0}^{\infty} z^n\, P_n(t)$. What is the value of $G(z;0)$? Get a differential equation for $G(z;t)$ and solve it.

c) Deduce that

$$P_n(t) = \frac{(\lambda t)^n}{n!}\, \mathrm{e}^{-\lambda t} \tag{2.36}$$

d) Determine the cumulants $\langle \mathscr{N}(t)^k \rangle_c$ of the Poisson process.

e) Give the distribution $q(\tau)$ of the time separating two successive events [indication : relate $q(\tau)$ and $P_0(t)$].

Note that (2.36) corresponds to the initial condition $\mathscr{N}(0) = 0$, hence the conditional probability of the Poisson process is $P_t(n|m) = P_{n-m}(t)$ for $n \geqslant m$ and $P_t(n|m) = 0$ for $n < m$.

This remark reflects the fact that the Poisson process is both *translation invariant* in time ($W_{n,m}$ does not depend on time) and "space"

$$W_{n,m} = \lambda\big(-\delta_{m-n,0} + \delta_{n-m,1}\big) = \text{function}(n-m)\,. \tag{2.37}$$

Using translation invariance, we deduce that the conditional probability of the Poisson process is

$$P_t(n|m) = \begin{cases} \frac{(\lambda t)^{n-m}}{(n-m)!}\, \mathrm{e}^{-\lambda t} & \text{for } n \geqslant m \\ 0 & \text{for } n < m \end{cases} \tag{2.38}$$

✍ ***Exercice 2.4 Conditional probability for the PP :*** *Consider the Poisson process with $\mathscr{N}(0) = 0$. Check that $\sum_m P_t(n|m)\, P_{t'}(m|n_0) = P_{t+t'}(n|n_0)$.*

✍ ***Exercice 2.5 Two-point correlator of the PP :***

a) For $\mathscr{N}(0) = 0$, express $\langle \mathscr{N}(t) \rangle$ in terms of the probability. Compute it.
b) Express $\langle \mathscr{N}(t)\mathscr{N}(t') \rangle$ as a double sum and compute it when $t' < t$. Deduce the correlator $\langle \mathscr{N}(t)\mathscr{N}(t') \rangle_c = \langle \mathscr{N}(t)\mathscr{N}(t') \rangle - \langle \mathscr{N}(t) \rangle \langle \mathscr{N}(t') \rangle$. Compare with the Wiener process.
c) Deduce $\left\langle \left[\mathscr{N}(t) - \mathscr{N}(t') \right]^2 \right\rangle_c$. Comment on the limit $t \to t'$.

✍ ***Exercice 2.6 Derivative of the PP :*** *We consider the noise $\xi(t) = \sum_n \delta(t - t_n)$, where the times are i.i.d. for a uniform density λ. I.e., when they are ordered, the events occur randomly and independently with rates λ. In other terms, the noise is the derivative of the Poisson process introduced above $\xi(t) = \mathscr{N}'(t)$.*
We introduce the generating function of the noise $G[h] \stackrel{\text{def}}{=} \left\langle \exp \int \mathrm{d}t\, h(t)\, \xi(t) \right\rangle$, where $\langle \bullet \rangle$ is the averaging over the random times t_n's.

a) Show that $G[h] = \exp\left\{ \lambda \int \mathrm{d}t (\mathrm{e}^{h(t)} - 1) \right\}$.
Hint: Consider that the N times are not ordered, distributed over $[0,T]^N$ with measure $\mathrm{d}t_1 \cdots \mathrm{d}t_N / T^N$.

b) Deduce the connex correlation functions (cumulants) : $\langle \xi(t) \rangle = \lambda$ and $\langle \xi(t_1) \cdots \xi(t_n) \rangle_c = \lambda\, \delta(t_1 - t_2) \cdots \delta(t_1 - t_n)$.
Hint: Consider functional derivatives of $\ln G[h]$.

In conclusion, $\xi(t) = \mathscr{N}'(t)$ is ***a non Gaussian white noise****.*

✍ ***Exercice 2.7 n-point correlations of the PP :*** *Using the result of Exercise 2.6, deduce the n-point correlations $\langle \mathscr{N}(t_1)\mathscr{N}(t_2) \cdots \mathscr{N}(t_n) \rangle_c$ for the Poisson process.*

e) The compound Poisson process

A natural generalization of the Poisson process is the *compound Poisson process* (CPP) [10] : we consider now that the process $X(t)$ makes random jumps

$$X(t_n^+) = X(t_n^-) + \eta_n \tag{2.39}$$

where the η_n's are i.i.d., distributed according to a distribution $w(\eta)$. As for the Poisson process, the jumps occur at random times t_n with rate λ. After a time t, the number of jumps $\mathscr{N}(t)$ is random (it is a PP), hence we can write the CPP in terms of the PP as

$$X(t) = \sum_{n=0}^{\mathscr{N}(t)} \eta_n \tag{2.40}$$

with $\eta_0 = X(0) = 0$.

Numerics : this form shows that it is very simple to simulate the CPP with a computer. One can generate two independent sequences of random numbers : the exponentially distributed random time intervals $\tau_n = t_n - t_{n-1} > 0$ (cf. Exercise 2.3) and the random amplitudes η_n's.

[10] in French: "processus de Poisson composé".

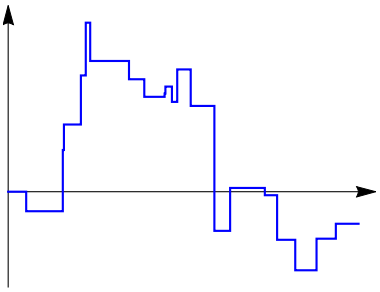


Figure 12: *Compound Poisson process $X(t)$ for Gaussian jumps.*

Master equation : The master equation of the CPP is

$$\frac{\partial P(x,t)}{\partial t} = \lambda \int \mathrm{d}\eta \, w(\eta) \, [P(x-\eta,t) - P(x,t)] \tag{2.41}$$

i.e. of the form (2.24) for

$$W(x|x_0) = \lambda \left[w(x-x_0) - \delta(x-x_0) \right] . \tag{2.42}$$

Note that here, the transition kernel is (time and space) translation invariant, as for the PP.

✍ ***Exercice 2.8 Master equation for the CPP :***
a) Show that the master equation for the CPP is (2.41).

b) Continuum limit.— Study the limit $\lambda \to \infty$ with $w \to 0$ such that $a = \lambda \langle \eta_n \rangle$ and $b = \lambda \langle \eta_n^2 \rangle$ are kept finite (argue that, in this limit, $\lambda \langle \eta_n^k \rangle \to 0$ for $k > 2$).

c) Introducing the Fourier transforms $\widehat{P}(k,t) = \int \mathrm{d}x \, \mathrm{e}^{-\mathrm{i}kx} \, P(x;t)$ and $\hat{w}(k) = \int \mathrm{d}\eta \, \mathrm{e}^{-\mathrm{i}k\eta} \, w(\eta)$, show that the solution is

$$P(x,t) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}k}{2\pi} \, \mathrm{e}^{\lambda t \, [\hat{w}(k)-1] + \mathrm{i}kx} . \tag{2.43}$$

Discuss the continuum limit.

*d) When $\langle \eta_n^2 \rangle = \infty$, the process belongs to the class of **Lévy flights**. For example, if $w(\eta) \sim c/\eta^2$ for $\eta \to \pm\infty$ we have $\hat{w}(k) \simeq 1 - c|k|$ for $k \to 0$. Deduce $P(x,t)$ over large scales. Discuss also the more general case where $\hat{w}(k) \simeq 1 - c|k|^\mu$ for $k \to 0$, with $\mu \in]0,2[$.*

✍ ***Exercice 2.9 Derivative of the CPP - a non Gaussian white noise :***
a) Using the representation $\xi(t) = X'(t) = \sum_n \eta_n \, \delta(t - t_n)$, where both the times t_n's and the coefficients η_n's are random, derive the connex correlation function of the noise $\langle \xi(t_1) \cdots \xi(t_n) \rangle_c$.
Hint: follow the same steps as in Exercise 2.6.

b) Show that the noise becomes a Gaussian white noise in a certain limit.

2.4 Markov chains

An important class of random processes are Markov chains, which are homogeneous random processes, discrete with respect to both the time and the state. This makes such processes rather convenient for numerical analysis.

a) Stochastic matrix

We consider a random process $X(t) \in \{1, \cdots, \mathcal{M}\}$ and denote $P_n(t) = \mathrm{Proba}\{X(t) = n\}$. The master equation (2.28) introduced above involves transitions at random times. For Markov

chain, the jumps occur at regular discrete times, thus the master equation takes the form

$$\boxed{P_n(t+1) = \sum_m M_{nm}\, P_m(t)} \tag{2.44}$$

where

$$M_{nm} = \text{Proba}\{m \to n\} \in [0,1] \tag{2.45}$$

is the $\mathcal{M} \times \mathcal{M}$ matrix of transition probabilities at each time step. M is called a "*stochastic matrix*". It satisfies

$$\boxed{\sum_n M_{nm} = 1} \tag{2.46}$$

Example of Markov chain : the biased RW.— A simple example is the case of the random walk on the line, where, at each time step, the walker jumps to the left with probability q or to the right with probability p. Then

$$M_{nm} = p\,\delta_{m,n-1} + q\,\delta_{m,n+1} \tag{2.47}$$

(with $p+q=1$). The problem is studied in detail in Exercise 2.12 below.

For the following, it is useful to rewrite the master equation (2.44) in a form closer to the differential equation (2.30) by using (2.46)

$$P_i(t+1) - P_i(t) = \sum_{j(\neq i)} \left[M_{ij}\, P_j(t) - M_{ji}\, P_i(t)\right] \tag{2.48}$$

✍ ***Exercice 2.10 Continuum limit of the Markov chain :*** *Consider a Markov chain with jumps occuring every δt. Argue that the master equation (2.28) is recovered by considering the continuum limit*

$$M_{ij} = \delta_{ij} + \delta t\, W_{ij} \qquad \textit{with } \delta t \to 0\,. \tag{2.49}$$

If M is a stochastic matrix, what is the constraint on the matrix W ?

b) The Perron-Fröbenius theorem and the stationary state

We can interpret the condition (2.46) as the existence of a left eigenvector $L^{(0)} = (1, \cdots, 1)^{\mathrm{T}}$ for eigenvalue $\lambda_0 = 1$:

$$L^{(0)\mathrm{T}} M = L^{(0)\mathrm{T}} \quad \text{or} \quad M^{\mathrm{T}} L^{(0)} = L^{(0)}\,, \tag{2.50}$$

where $(\cdot)^{\mathrm{T}}$ denotes transposition (the vectors are column vectors). The *Perron-Fröbenius theorem* states that (i) $\lambda_0 = 1$ is non-degenerate, (ii) it is the largest eigenvalue, (iii) the related right eigenvector

$$M\, R^{(0)} = R^{(0)}\,, \tag{2.51}$$

has positive components. For a finite number of states $\mathcal{M}$, this corresponds to the **stationary solution**, $R^{(0)} = (P_1^*, \cdots, P_{\mathcal{M}}^*)^{\mathrm{T}}$. Normalization condition reads $L^{(0)\mathrm{T}} R^{(0)} = \sum_i P_i^* = 1$ (the scalar product is the product of the line and the column vectors). We can rewrite equation (2.51) as

$$\sum_{j(\neq i)} \left[M_{ij}\, P_j^* - M_{ji}\, P_i^*\right] = 0\,. \tag{2.52}$$

c) Classification of Markov processes

We now discuss the different scenarii which might occur. We keep considering the case of Markov chains, although a similar discussion is more general.

(i) **Equilibrium.**— Often, the existence of a stationary solution is ensured by a condition *stronger* than (2.52), called the **detailed balance condition**

$$M_{ij}\,P_j^* - M_{ji}\,P_i^* = 0 \quad \forall\,(i,j) \qquad \text{(detailed balance)} \tag{2.53}$$

If detailed balance is fulfilled, one says that P_i^* is an *equilibrium state*. We can also conveniently relate the ratio of rates to the ratio of probabilities

$$\boxed{\frac{M_{ij}}{M_{ji}} = \frac{P_i^*}{P_j^*}} \qquad \text{(detailed balance} \equiv \text{equilibrium)} \tag{2.54}$$

The relation holds $\forall(i,j)$. For each pair of states, the ratio of occupations coincides with the ratio of transition probabilities. This is *a probabilistic definition of equilibrium.*

(ii) **NESS (non-equilibrium stationary state).**— If the detailed balance condition (2.53) is *not* fulfilled (at least for some couples (i,j)) but the condition

$$\sum_{j(\neq i)} \big[\underbrace{M_{ij}\,P_j^* - M_{ji}\,P_i^*}_{\neq 0}\big] = 0 \qquad \text{(stationarity)} \tag{2.55}$$

holds, one says that the stationary state is a *non-equilibrium steady state*. Such states are characterised by the existence of non zero *probability* fluxes.

(iii) **Transient process.**— When $\mathcal{M} \to \infty$ it is possible that the eigenvector $(\cdots, P_i^*, \cdots)^{\mathrm{T}}$ is not normalisable, so that there is no stationary state. One says that the process is *transient*.

Depending on the matrix M_{ij} which defines the Markov chain, one encounters one of the three situations.

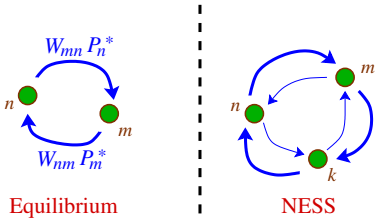


Figure 13: *Equilibrium state versus NESS : In equilibrium, probability currents should equilibrate for each pair of states. In the NESS, there exist loop(s) in which current(s) circulate (here, due to an imbalance $W_{mn}\,P_n^* > W_{nm}\,P_m^*$, there is a net circulation $n \to m \to k \to n$).*

With the master equation (2.28).— The form (2.30) is appropriate for the same discussion : Equilibrium requires detailed balance condition

$$W_{nm}\,P_m^* = W_{mn}\,P_n^* \quad \forall\,(n,m)\,. \tag{2.56}$$

W_{nm} being a rate, $J^*(m \to n) = W_{nm}\,P_m^*$ is the probability current between the two states, in the stationary state. In the stationary state, currents between states should compensate globally, if probability is conserved. Detailed balance means that probability currents between each pair of state equilibrate. There is no circulating probability current between more than two states (Fig. 13).

d) Spectral decomposition - Relaxation

✍ ***Exercice 2.11 Warm up : diagonalization of a non-symmetric*** 2×2 ***matrix:*** *We consider the real non-symmetric matrix*

$$M = \begin{pmatrix} 0 & \mathrm{e}^{-h} \\ \mathrm{e}^{h} & 0 \end{pmatrix} \tag{2.57}$$

Show that it is diagonalisable. Find the right and left eigenvectors and discuss the normalisation.

The stochastic matrix M, with positive matrix elements, is not symmetric in general, $M^{\mathrm{T}} \neq M$. We have seen above that its eigenvalue $\lambda_0 = 1$ is associated with a couple of left and right eigenvectors $L^{(0)}$ and $R^{(0)}$. If M is diagonalisable, its eigenvalues $\lambda_n < 1$ are associated with a biorthogonal set of left and right eigenvectors $L^{(n)}$ and $R^{(n)}$. We can choose the orthonormalisation condition as $L^{(n)\mathrm{T}} R^{(m)} = \delta_{n,m}$, which leads to the spectral representation

$$M = \sum_n \lambda_n R^{(n)} L^{(n)\mathrm{T}} \, . \tag{2.58}$$

This is useful in order to solve the master equation (2.44). Denoting by $P(0) = (P_1(0), \cdots, P_{\mathcal{M}}(0))^{\mathrm{T}}$ the initial conditions, we can write

$$P(t) = M^t \, P(0) \quad \text{i.e.} \quad P_n(t) = \sum_j \lambda_j^t \, R_n^{(j)} \underbrace{L^{(j)\mathrm{T}} P(0)}_{c_j \overset{\text{def}}{=}} \tag{2.59}$$

c_j is the coefficient of the initial vector on the basis of eigenvectors $P(0) = \sum_j c_j R^{(j)}$. Note that $c_0 = L^{(0)\mathrm{T}} P(0) = \sum_j P_j(0) = 1$ carries all the normalisation.

Conditional probability.— An example of initial condition is $P_n(0) = \delta_{nm}$ i.e. coefficients $c_j = L_m^{(j)}$. Then, the solution of the master equation (2.44) is the conditional probability

$$\boxed{P_t(n|m) = \left(M^t\right)_{nm}} \tag{2.60}$$

Relaxation towards stationary state.— Now let us discuss the large time behaviour. Using that $\lambda_0 = 1 > \lambda_1 > \lambda_2 > \cdots$, the large time behaviour takes the form

$$P_n(t) \underset{t\to\infty}{\simeq} \underbrace{P_n^*}_{\equiv R_n^{(0)}} + \underbrace{c_1 \, \lambda_1^t R_n^{(1)}}_{\underset{t\to\infty}{\longrightarrow} 0} \tag{2.61}$$

where we have used $c_0 = 1$ (normalisation). This shows that $1/\tau_{\mathrm{relax}} = -\ln \lambda_1$ is the relaxation rate towards the stationary state. Relaxation is usually exponentially fast, unless the gap in the spectrum vanishes and the spectrum is continuous.

Remark 1 : apart $\lambda_0 = 1$, the eigenvalues are not real in general , however complex eigenvalues should come in conjugate pairs since M is a real matrix (and the same for eigenvectors). Thus, in the general case, the rate of relaxation towards stationary state is

$$\boxed{\frac{1}{\tau_{\mathrm{relax}}} = -\ln |\lambda_1|} \tag{2.62}$$

Hence, in general the ranking of e.v. is $\lambda_0 > |\lambda_1| > |\lambda_2| > \cdots$, i.e. the *spectral radius* is one.

Remark 2 : When M is non symmetric, it is not always diagonalisable. However it can always be decomposed in terms of Jordan blocks.

✍ ***Exercice 2.12 Biased random walk in a ring :*** *Consider the random walk in a ring with L sites, such that with $M_{nm} = p\,\delta_{n,m+1} + q\,\delta_{n,m-1}$ for n, $m \in \{1, \cdots, L\}$. Periodic boundary conditions are $M_{1L} = p$ and $M_{L1} = q$.*

a) Argue that the stationary state is an equilibrium state when $p = q = 1/2$ and a NESS for $p \neq q$.

b) Give the spectrum of eigenvalues λ_k and eigenvectors (left/right) of the stochastic matrix M. Write $p = \frac{1+v}{2}$ and $q = \frac{1-v}{2}$ with $v \in [-1, +1]$. Check that the "spectral radius" is unity, i.e. $|\lambda_k| \leqslant 1\ \forall\, k$.

c) Decompose the conditional probability $P_t(n|m)$ over the eigenvalues and the eigenvectors.

d) Consider the limit $L \to \infty$ and discuss the bottom of the spectrum. Compute $P_t(n|m)$ in the two limiting cases $v = 0$ and $v = \pm 1$.

Remark 3 : All these spectral considerations also apply to the master equation (2.28) for continuous time.

✍ ***Exercice 2.13 Spectral analysis applied to Eq. (2.28) and Perron-Fröbenius th. :*** *a) Solve Eq. (2.28) by using spectral analysis (in the same spirit as it was done for the Markov chain). What is expected for the eigenvalues of W_{nm} ?*

b) What is the representation of the propagator equivalent to (2.60) ? Deduce that

$$\sum_m P_t(n|m)\, P^*_m = P^*_n\,. \tag{2.63}$$

e) Simple examples :

Molecular vapour at thermal equilibrium : consider a vapour of molecules at thermal equilibrium. Each molecule has energy levels ε_n, expected to be occupied according to canonical weights $P^*_n \propto \mathrm{e}^{-\beta\varepsilon_n}$. The molecule in an excited state falls in a state with lower energy by emission. Equilibrium and detailed balance imply that the absorption and emission rates between two levels fulfill the relation

$$\frac{\Gamma_{n\leftarrow m}}{\Gamma_{m\leftarrow n}} = \frac{P^*_n}{P^*_m} = \mathrm{e}^{-\beta(\varepsilon_n - \varepsilon_m)} \tag{2.64}$$

i.e. emission is more probable than absorption. This observation (Gibbs equilibrium is compatible with an imbalance between emission and absorption) is the key point of Einstein first theory of spontaneous emission (at the origin of the difference between emission and absorption). [11]

✍ ***Exercice 2.14 Illustration of the three scenarii for a birth and death process :*** *Let us consider the master equation describing the one dimensional diffusion on $\mathbb{Z}$ with transitions between nearest neighbour sites*

$$\partial_t P_n(t) = W_{n,n-1} P_{n-1}(t) + W_{n,n+1} P_{n+1}(t) - (W_{n-1,n} + W_{n+1,n})\, P_n(t) \tag{2.65}$$

i.e. $W_{n,m}$ is a tridiagonal (infinite) matrix with $W_{n,n} = -W_{n-1,n} - W_{n+1,n}$. Hence, this is an example of birth and death process.

[11] Albert Einstein, "*Zur Quantentheorie der Strahlung*", Physilakische Zeitschrift **18**, 121–128 (1917).
On trouvera l'article reproduit dans : A. Einstein, *Œuvres choisies. 1. Quanta*, Seuil (1989), textes choisis et présentés par F. Balibar, O. Darrigol & B. Jech.

a) Current : check that the master equation can be rewritten under the form

$$\partial_t P_n = -J_n + J_{n-1} \tag{2.66}$$

and express the probability current $J_n(t)$ related to the distribution $P_n(t)$ (J_n measures the current at time t between sites n and $n+1$).

We now choose the matrix such that

$$W_{n,m} = \mathrm{e}^{[V(m)-V(n)]/2} \tag{2.67}$$

where $V(x)$ is a known function.

b) Equilibrium ($J = 0$).— Show that

$$P_n^* = C\,\mathrm{e}^{-V(n)} \tag{2.68}$$

is a stationary solution corresponding to a vanishing probability current. Discuss the normalisability.

c) NESS ($J \neq 0$).— Find the stationary solution corresponding to $J_n = J\ \forall\, n$. Show that it is

$$P_n^* = J\,\mathrm{e}^{-V(n)} \sum_{m=n}^{\infty} \mathrm{e}^{[V(m+1)+V(m)]/2} \tag{2.69}$$

Discuss the normalisability (consider the continuum limit for simplicity).

d) Provide an example where there is no stationary state.

f) Detailed balance, reversibility and ergodicity

Let us consider a Markov chain with master equation (2.44), such that detailed balance is fulfilled. We denote by P_i^* the *equilibrium* solution. Define

$$\mathcal{D}_t \overset{\text{def}}{=} \sum_i \frac{(P_i(t) - P_i^*)^2}{P_i^*} = \sum_i \frac{P_i(t)^2}{P_i^*} - 1 \geqslant 0 \tag{2.70}$$

which measures the distance of the distribution at time t to the equilibrium distribution. One can study the evolution of the quantity by considering $\Delta\mathcal{D}_t = \mathcal{D}_{t+1} - \mathcal{D}_t$. Some algebra making use of detailed balance (2.54) leads to

$$\Delta\mathcal{D}_t = -\frac{1}{2} \sum_{i,j,k} M_{ji} M_{ki} P_i^* \left(\frac{P_j(t)}{P_j^*} - \frac{P_k(t)}{P_k^*} \right)^2 \leqslant 0 \tag{2.71}$$

Conclusion :

- $\mathcal{D}_t \geqslant 0$
- $\Delta\mathcal{D}_t \leqslant 0$
- We conclude that $\mathcal{D}_t \searrow$ and thus $P_i(t) \to P_i^*$.

This shows that detailed balance ensures that the system reaches equilibrium. This remark is borrowed from [24].

g) A practical (and important) application of Markov chains : the Monte Carlo method

Consider a physical observable $\mathcal{O}$. At thermal equilibrium, the probability of a microstate is $P_\ell \propto \mathrm{e}^{-\beta E_\ell}$. If the number of states $N_{\rm state}$ is too large, it might be difficult to compute numerically the sum

$$\langle \mathcal{O} \rangle_{\rm eq} = \sum_{\ell=1}^{N_{\rm state}} P_\ell \, \mathcal{O}_\ell \tag{2.72}$$

For example, if one considers N Ising spins, the sum runs over $N_{\rm state} = 2^N$ microstates, which becomes rapidly untracktable if N is large (a square of 10×10 spins $1/2$ has $N_{\rm state} \sim 10^{30}$ microstates).

Figure 14: *Nicholas Metropolis (1915-1999).*

The central idea of equilibrium statistical physics is to replace the study of the microscopic (deterministic) dynamics by a probabilistic description. The Monte Carlo method replaces the probabilistic description by a stochastic dynamics defined as follows : if the system is in state $|\, i \,\rangle$ at time t, a move to another state $|\, f \,\rangle$ chosen randomly is made with probability

$$\mathrm{Proba}\{i \to f\} \equiv M_{fi} = \min\left(1,\, \mathrm{e}^{-\beta(E_f - E_i)}\right) . \tag{2.73}$$

For example, in a spin system, one chooses a spin randomly and flip it, thus the difference of energy $E_f - E_i$ is due to a local change, and the energy difference is very easy to compute. This means that the matrix M_{nm} changes randomly at each time step. Assuming $E_f > E_i$, the stochastic matrix has the form

$$M = \begin{pmatrix} \ddots & & & \\ & 1 - \mathrm{e}^{-\beta(E_f - E_i)} & 1 & \\ & \mathrm{e}^{-\beta(E_f - E_i)} & 0 & \\ & & & \ddots \end{pmatrix} \begin{matrix} \\ \leftarrow \ |\, i \,\rangle \\ \leftarrow \ |\, f \,\rangle \\ \\ \end{matrix} \tag{2.74}$$

All other diagonal matrix elements are equal to one and all other non diagonal matrix elements equal to zero. This is the Metropolis algorithm (from the name of the inventor of the method, Nicholas Metropolis). Because $M_{fi}/M_{if} = \mathrm{e}^{-\beta(E_f - E_i)}$, such dynamics converges towards the Gibbs equilibrium. Finally the statistical average is replaced by the time average over the stochastic dynamics involving $N_{\rm step}$

$$\overline{\mathcal{O}(t)} = \frac{1}{N_{\rm step}} \sum_{t=1}^{N_{\rm step}} \mathcal{O}(t) \, . \tag{2.75}$$

The number of steps $N_{\rm step}$ can be chosen orders of magnitude smaller than $N_{\rm state}$, still large enough in order to ensure some ergodicity (see the book [19] for a detailed discussion).

Going from the microscopic dynamics to the Monte Carlo method, the scheme is the following :

Classical mechanics		Equilib. statistical physics		Monte Carlo method
deterministic evolution	$\longrightarrow$	probabilistic description	$\longrightarrow$	stochastic dynamics

2.5 Spectral analysis of stochastic processes – Wiener-Khintchine theorem

Convention for Fourier transform in time : We define the Fourier transform in time as

$$\widetilde{C}(\omega) = \int_{-\infty}^{+\infty} \mathrm{d}t\, C(t)\, \mathrm{e}^{\mathrm{i}\omega t} \quad \text{et} \quad C(t) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi}\, \widetilde{C}(\omega)\, \mathrm{e}^{-\mathrm{i}\omega t}\,. \tag{2.76}$$

Consider a homogeneous (time translation invariant) and **stationary** random process $x(t)$ defined on the interval $t \in [0, T]$, where T is the observation time. It is characterised by the correlation function $C_{xx}(\tau) \stackrel{\text{def}}{=} \langle x(t)\, x(t+\tau)\rangle$, assumed rapidly decreasing (assume $\langle x(t)\rangle = 0$ for simplicity). Because the process is stationary, we prefer to consider its discrete Fourier transform (cf. appendix page **??**) [12]

$$\tilde{x}_n = \int_0^T \frac{\mathrm{d}t}{T}\, x(t)\, \mathrm{e}^{+\mathrm{i}\omega_n t} \quad \text{et} \quad x(t) = \sum_n \tilde{x}_n \mathrm{e}^{-\mathrm{i}\omega_n t} \text{ où } \omega_n = \frac{2n\pi}{T} \text{ avec } n \in \mathbb{Z}\,. \tag{2.77}$$

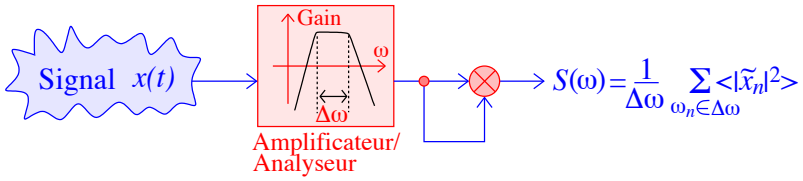


Figure 15: *Measure of the noise : the signal is amplified, duplicated and multiplied by itself. The result is averaged over a long time T.*

Noise spectrum.– Let $\Delta\omega$ be the bandwidth of the apparatus (with $\Delta\omega \gg 1/T$). We define the *noise spectrum* as the average of the square modulus of the Fourier components in the bandwidth, i.e. in the interval $[\omega, \omega + \Delta\omega]$:

$$\mathcal{S}(\omega) \stackrel{\text{def}}{=} \frac{1}{\Delta\omega} \sum_{\omega_n \in [\omega, \omega+\Delta\omega]} \langle |\tilde{x}_n|^2 \rangle \tag{2.78}$$

This is precisely the outcome of the device represented in figure 15 : sample → ampli/filter → multiplicator → measurement.

Wiener-Khintchine theorem.– From the above hypothesis, one can verify that :

$$\langle \tilde{x}_n \tilde{x}_m^* \rangle = \frac{1}{T} \delta_{n,m} \widetilde{C}_{xx}(\omega_n) \tag{2.79}$$

[12] Later, we will define the Fourier transform in space as $f_q = \int_V \mathrm{d}r\, f(r)\, \mathrm{e}^{-\mathrm{i}qr}$, where q is quantized if the volume is finite, and $f(r) = \frac{1}{V}\sum_q f_q\, \mathrm{e}^{+\mathrm{i}qr} \to \int \frac{\mathrm{d}q}{(2\pi)^d}\, f_q\, \mathrm{e}^{+\mathrm{i}qr}$.

Figure 16: *Norbert Wiener (1894-1964) & Aleksandr Yakovlevich Khinchin (1894-1959).*

where $\widetilde{C}_{xx}(\omega) = \int_{-\infty}^{+\infty} \mathrm{d}\tau\, C_{xx}(\tau)\, \mathrm{e}^{\mathrm{i}\omega\tau}$. Only components corresponding to opposite frequencies ω_n and ω_{-n} are correlated [13]. Thus one has : $\sum_{\omega_n \in [\omega, \omega+\Delta\omega]} \langle |\tilde{x}_n|^2 \rangle = \frac{\mathcal{N}_{\Delta\omega}}{T} \widetilde{C}_{xx}(\omega)$ where $\mathcal{N}_{\Delta\omega} = \Delta\omega T/2\pi$ is the number of frequencies ω_n in the bandwidth. Finally one gets

$$\boxed{\mathcal{S}(\omega) = \frac{\widetilde{C}_{xx}(\omega)}{2\pi}} \tag{2.80}$$

i.e. a relation between the noise spectrum (fluctuations at frequency ω) and the correlations. A random process characterized by short time correlations thus corresponds to a broad noise spectrum. The limit of correlation with zero range is called a "white noise" (flat spectrum).

Details of derivation of (2.79) : Write $\langle \tilde{x}_n \tilde{x}_m^* \rangle = \int_0^T \frac{\mathrm{d}t}{T} \int_0^T \frac{\mathrm{d}t'}{T} \mathrm{e}^{\mathrm{i}\omega_n t - \mathrm{i}\omega_m t'} C_{xx}(t-t') = \frac{1}{T} \int_0^T \frac{\mathrm{d}t'}{T} \mathrm{e}^{\mathrm{i}(\omega_n - \mathrm{i}\omega_m)t'} \int_{-t'}^{T-t'} \mathrm{d}(t-t') \mathrm{e}^{\mathrm{i}\omega_n (t-t')} C_{xx}(t-t')$. Short range correlation allows to write $\int_{-t'}^{T-t'} \mathrm{d}(t-t') \cdots \to \int_{-\infty}^{+\infty} \mathrm{d}(t-t') \cdots$.

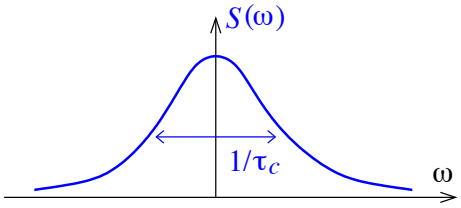


Figure 17: **Wiener-Khintchine theorem :** *width of noise spectrum is inversely proportional to the correlation time τ_c of the process (τ_c is the width of $C(\tau)$).*

✍ ***Exercice 2.15 :*** *As a simple application of the Wiener-Khintchine theorem, we analyze the correlation of the velocity for the process defined by the phenomenological Langevin equation*

$$\frac{\mathrm{d}v(t)}{\mathrm{d}t} = -\int \mathrm{d}t'\, \gamma(t-t')\, v(t') + \xi(t) \tag{2.81}$$

where $\xi(t)$ is the Langevin force (assumed to be a stationary random process with short time correlations). Here the friction is nonlocal in time, controlled by a causal function $\gamma(t)$, with finite width τ_m. Show that

$$C_{vv}(\tau) = \int_{-\infty}^{+\infty} \mathrm{d}\omega \underbrace{\frac{\widetilde{C}_{\xi\xi}(\omega)}{2\pi}}_{\mathcal{S}_{\mathrm{Force}}(\omega)} \frac{\mathrm{e}^{-\mathrm{i}\omega\tau}}{|\tilde{\gamma}(\omega) - \mathrm{i}\omega|^2} \tag{2.82}$$

Consider the limit $C_{\xi\xi}(\tau) = 2D\gamma^2\delta(\tau)$ et $\gamma(t) = \gamma\,\delta(t)$ and compute explicitly the correlator.

[13] One can as well consider a process defined on $\mathbb{R}$ by writing $T \to \infty$. The Fourier transform is then defined as $\tilde{x}(\omega) = \int \mathrm{d}t\, x(t) \mathrm{e}^{\mathrm{i}\omega t}$ and one can show that $\langle \tilde{x}(\omega) \tilde{x}(\omega') \rangle = 2\pi\delta(\omega+\omega') \widetilde{C}_{xx}(\omega)$. Correspondence between the two formulations is ensured by the substitutions $\tilde{x}(\omega) \leftrightarrow T\tilde{x}_n$ and $2\pi\delta(\omega-\omega') \leftrightarrow T\delta_{n,n'}$.

✍ ***Exercice 2.16 :*** *Consider now the case of a Langevin force correlated over the finite time τ_c (a microscopic time) : $C_{FF}(t) = 2D\gamma^2 \frac{1}{2\tau_c} e^{-|t|/\tau_c}$. We expect the function $\gamma(t)$ to be of finite width τ_m ; Assume $\gamma(t) = \gamma\,\theta(t)\frac{1}{\tau_m} e^{-t/\tau_m}$. The three time scales fulfill : $\tau_c \lesssim \tau_m \ll 1/\gamma$. Analyze the residus of $|\tilde{\gamma}(\omega) - i\omega|^{-2}$ justify that one can consider $\tau_m \to 0$ while keeping a finite τ_c, what simplifies the evaluation of the integral. Show then that $C_{vv}(\tau) = \frac{D\gamma}{1-(\gamma\tau_c)^2}[e^{-\gamma|t|} - \gamma\tau_c e^{-|t|/\tau_c}]$. Analyze the behaviour at short time as well.*

☺ Important points

- Markov process (definition).
- Be familiar with the various forms of the master equation (continuous/discrete ; Markov chain).
- A good exercise : recover the properties of the Poisson process (and the CPP).
- Definition of the stochastic matrix. Use of spectral information to solve the master equation.
- Detailed balance and the classification of Markov processes.
- Wiener-Khintchine theorem : relation between the correlation function of an homogeneous process and its noise spectrum.

3 Stochastic processes (3) : stochastic differential equations

In § 1, we have discussed a specific case of stochastic differential equation (SDE), the Langevin equation $m\frac{d}{dt}v(t) = -\gamma\, v(t) + \xi(t)$ involving a δ-correlated Langevin force. We took advantage of the linearity to obtain an integral representation of the solution, which makes easy the analysis of the statistical properties of the solution. The aim of this paragraph is to consider a more general situation and consider SDE of the form $\frac{d}{dt}x = F(x) + \sqrt{2D(x)}\,\eta(t)$, where $\eta(t)$ is a normalised Gaussian white noise.

SDE are particularly well suited for numerical simulations (it is easy to generate many realizations of such processes). Here, the aim is to introduce some tools allowing for a statistical analysis of the solution. Finally, let us stress that by considering that $\eta(t)$ is a Gaussian white noise, in this chapter we restrict ourselves to the study of **continuous Markov processes** (with no jump). [14]

3.1 SDE with drift and additive noise

Let us come back to the analysis of the stochastic process described by Eq. (1.26). We write

$$\frac{dx(t)}{dt} = F(x(t)) + \sqrt{2D}\,\eta(t) \tag{3.1}$$

where $\eta(t)$ is a normalised Gaussian white noise with

$$\langle \eta(t) \rangle = 0 \qquad \text{and} \qquad \langle \eta(t)\eta(t') \rangle = \delta(t-t')\,. \tag{3.2}$$

An analysis similar to the one of Section 1 is not possible (unless $F(x) \propto x$) due to the nonlinear character of the equation. Let us introduce the Wiener process

$$W(t) = \int_0^t dt'\,\eta(t') \tag{3.3}$$

[14] Remember the end of § 1 : the Wiener process $W(t) = \int_0^t du\,\eta(u)$ is continuous but not differentiable. The solution $x(t)$ of the SDE has the same regularity.

We could also write a differential equation for a Markov process with jumps by considering that a noise $\eta(t)$ such that $\int_0^t du\,\eta(u)$ is a Poisson process or a compound Poisson process, i.e. $\eta(t) = \sum_n \eta_n\,\delta(t-t_n)$. The analysis would be more complicated because the equation for $P_t(x)$ would then involve an *integral* operator instead of a *differential* operator, like in the Fokker-Planck equation (e.g. the equation (2.41) describing the simple case of the CPP involves an integral operator).

which allows to rewrite the SDE in a form popular in the Mathematical literature :

$$\mathrm{d}x(t) = F(x(t))\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}W(t)\,. \tag{3.4}$$

This emphasizes that $x(t)$ has the same regularity as the Wiener process $W(t)$: *continuous* but *non differentiable*. One of the question raised in this chapter is precisely to give a rigorous meaning to the differential equation for non differentiable functions !

Being interested in statistical properties of the solution, it is natural to consider its distribution, or at least to build an equation for it, the Fokker-Planck equation. Below we show that the corresponding FPE is

$$\frac{\partial P_t(x)}{\partial t} = -\frac{\partial}{\partial x}\left[F(x)\,P_t(x)\right] + D\,\frac{\partial^2}{\partial x^2}P_t(x) \tag{3.5}$$

where $P_t(x)$ is the distribution of $x(t)$. In the next section, we will furhter discuss how to solve this equation.

Proof : I define the increment $\delta W(t) = W(t+\delta t) - W(t)$. The most important observation is the **independence of the increments** (chapter 1) and the property

$$\boxed{\left\langle \delta W(t)^2 \right\rangle = \delta t \qquad \text{i.e.} \quad \delta W(t) \sim \mathcal{O}\big(\sqrt{\delta t}\big)} \tag{3.6}$$

see above, Eq. (1.33). The distribution of $\delta W(t)$ does not depend on time t, but only on the time difference δt. We now introduce the increment of the process

$$\delta x(t) \stackrel{\text{def}}{=} x(t+\delta t) - x(t) \simeq F(x(t))\,\delta t + \sqrt{2D}\,\delta W(t) \tag{3.7}$$

Consider a test function $\varphi(x)$. We study the evolution of $\langle \varphi(x(t)) \rangle$.

$$\begin{aligned}
&\langle \varphi(x(t+\delta t)) \rangle - \langle \varphi(x(t)) \rangle \\
&= \left\langle \varphi'(x)\,\left[F(x)\,\delta t + \sqrt{2D}\,\delta W\right] + \frac{1}{2}\varphi''(x)\,\left[F(x)\,\delta t + \sqrt{2D}\,\delta W\right]^2 + \cdots \right\rangle &(3.8)\\
&= \left\langle \varphi'(x(t))\,F(x(t)) \right\rangle \delta t + \sqrt{2D}\,\left\langle \varphi'(x(t))\,\delta W(t) \right\rangle + D\left\langle \varphi''(x(t)) \right\rangle \delta t + \cdots &(3.9)
\end{aligned}$$

where we have kept terms $\mathcal{O}(\delta t)$. Because $x(t)$ is only correlated with the increment $\delta W(t')$ for $t > t'$, we see that $x(t)$ and $\delta W(t)$ are uncorrelated, thus

$$\left\langle \varphi'(x(t))\,\delta W(t) \right\rangle = \left\langle \varphi'(x(t)) \right\rangle \langle \delta W(t) \rangle = 0\,. \tag{3.10}$$

Finally

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\langle \varphi(x(t)) \rangle = \left\langle \varphi'(x(t))\,F(x(t)) \right\rangle + D\left\langle \varphi''(x(t)) \right\rangle \tag{3.11}$$

The key point was that the expansion was performed up to second order in $\delta x(t)$ because the second order term in δW gives some first order contribution in δt, due to (3.6). We can now rewrite the equation in terms of the distribution

$$\begin{aligned}
\frac{\partial}{\partial t}\int \mathrm{d}x\,P_t(x)\,\varphi(x) &= \int \mathrm{d}x\,P_t(x)\,\left[\varphi'(x)\,F(x) + D\,\varphi''(x)\right] &(3.12)\\
&= \int \mathrm{d}x\,\varphi(x)\,\left(-\frac{\partial}{\partial x}\left[F(x)\,P_t(x)\right] + D\,\frac{\partial^2 P_t(x)}{\partial x^2}\right) &(3.13)
\end{aligned}$$

Because the equation is valid $\forall\,\varphi$, we can remove the integral, hence (3.5). QED.

3.2 SDE with multiplicative noise : Itô or Stratonovich ?

The SDE (3.1) is not the most general form of stochastic differential equation as it corresponds to the case where the diffusion constant is uniform in space. The aim of the paragraph is to discuss the case of SDE of the form

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = a(x(t)) + b(x(t))\,\eta(t) \qquad (\textit{not well defined!}) \tag{3.14}$$

where $b(x) = \sqrt{2D(x)}$ can be related to a x-dependent diffusion constant (note that the sign of $b(x)$ plays no role because $\eta(t) \overset{(\mathrm{law})}{=} -\eta(t)$). As we explain now, this form is however not well defined.

The noise is here multiplied by a function of the process : one says that the **noise is multiplicative**, whereas it is said additive in SDE (3.1). For a multiplicative white noise, with singular correlations $\langle \eta(t)\eta(t')\rangle = \delta(t-t')$, the differential equation (3.14) is ambiguous : something is missing in order to define precisely the solution of this differential equation. This is not surprising : if $\eta(t)$ is a Gaussian white noise, $x(t)$ has the same regularity as the Brownian motion, i.e. is continuous but not differentiable. The existence of a difficulty comes from the fact that we manipulate a differential equation involving objects which are not differentiable in the sense of functions !

If the difficulty comes from the singular nature of the white noise (δ-correlations), one could argue that we should rather study a different model for a more regular (non white) noise. However, that would be very painful ! The white noise is the simplest model which ensures that the process defined by the SDE is Markovian. The price to pay for this simplicity is that we have to add a prescription to interpret the SDE.

a) Discretization (numerical simulation)

A first approach to give a precise meaning to (3.14) could be to discretize time (this is natural for numerical implementation of the stochastic differential equation). We introduce $x_n = x(t = n\,\delta t)$ together with i.i.d. Gaussian variables δW_n such that $\langle \delta W_n\rangle = 0$ and $\langle \delta W_n \delta W_m\rangle = \delta t\,\delta_{n,m}$. The discretized SDE is

$$x_{n+1} = x_n + a(x_n)\,\delta t + b(x_n)\,\delta W_n\,. \tag{3.15}$$

Note that by construction x_n and δW_m are independent for $n \leqslant m$ (the process does not depend on the noise in the future or *at equal time*).

This discretization procedure is perfectly fine, however it turns out that in the limit $\delta t \to 0$, the resulting continuous function $x(t) = x_n$ does not obeys the usual rules of differential calculus (for regular functions), as we will see below. This is not necessarily a problem, however this deserves a clarification.

b) Origin of the ambiguity

To clarify this point, we come back to the continuous description and consider a slightly different type of noise, made of δ-peaks at random times

$$\eta(t) = \sum_n \delta(t - t_n) \tag{3.16}$$

(we could also add some random weigths, it would not change the discussion). If the times occur with a finite rate λ, the noise $\eta(t)$ is a white noise since $\langle \eta(t)\eta(t')\rangle_c = \lambda\,\delta(t-t')$, however it is of *non Gaussian* nature because higher cumulants are non zero (cf. Exercise 2.6, page 20).

In the close neighbourhood of time t_n, we can forget the drift and approximate the evolution as

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = \cdots + b(x(t))\,\delta(t-t_n) \qquad \text{for } t \sim t_n \tag{3.17}$$

This implies that $x(t)$ is discontinuous at t_n. When dealing with a continuous function $\psi(t)$ we can write $\psi(t)\,\delta(t-t_n) = \psi(t_n)\,\delta(t-t_n)$. The product is however not clearly defined when the function $\psi(t)$ is discontinuous at t_n... Should we replace $\psi(t)$ by $\psi(t_n^-)$, $\psi(t_n^+)$ or $\frac{1}{2}\big[\psi(t_n^-)+\psi(t_n^+)\big]$,... or something else ? Here, we are faced to this problem, which makes the time evolution ambiguous : Eq. (3.17) shows that $x(t)$ makes a jump whose amplitude is $b(x(t))$, i.e. depends on the process at a time where the process is discontinuous and still unkown ! How to choose this time ? We propose two possible interpretations of the evolution (3.17) :

(i) **Proposal 1 ($\leftrightarrow$ "Itô")** Interpret the equation as $\frac{\mathrm{d}}{\mathrm{d}t}x(t) = \cdots + b(x(t_n^-))\,\delta(t-t_n)$, then

$$x(t_n^+) = x(t_n^-) + b(x(t_n^-)) \tag{3.18}$$

This is a natural choice for numerics. This is analogous to (3.15).

(ii) **Proposal 2 ($\leftrightarrow$ "Stratonovich")** A physicist rather considers that the δ-peak is a mathematical model for a regular narrow function of finite width $\delta(t) \to \delta^\epsilon(t)$, for example $\delta^\epsilon(t) = \frac{1}{2\epsilon}\mathrm{e}^{-|t|/\epsilon}$. Then starting from (3.17) one writes $\mathrm{d}x(t)/b(x(t)) \simeq \delta^\epsilon(t-t_n)\,\mathrm{d}t$ and integrate around the δ^ϵ, eventually taking the limit $\epsilon \to 0^+$. One gets

$$\int_{x(t_n^-)}^{x(t_n^+)} \frac{\mathrm{d}x}{b(x)} = 1 \tag{3.19}$$

which obviously differs from (3.18).

✍ ***Exercice 3.1*** *: Consider a multiplicative noise with $b(x) = \sigma\, x$ where σ is a positive constant. Compare the two evolutions (3.18) and (3.19) in this case.*

The choice of the prescription, i.e. the precise meaning to give to the multiplicative noise term, determines the evolution and contribute to define the stochastic process with the SDE. We stress that given *two different* interpretations of the *same* equation (3.17) leads to two different evolutions, (3.18) or (3.19), i.e. define *two different processes*. A similar problem occurs with the SDE (3.14) where $\eta(t)$ is a Gaussian white noise. Several interpretations can be given to the multiplicative noise term.

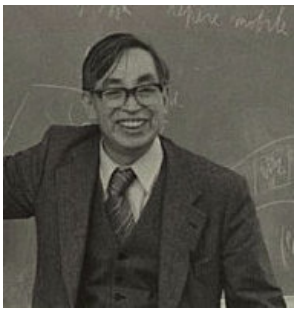



Figure 18: *Kiyoshi Itô (1915-2008) and Ruslan Leont'evich Stratonovich (1930-1997).*

The two evolutions (3.18) and (3.19) will be further studied in Exercise 3.9 below.

c) Itô convention and Itô calculus

The simpler choice which first comes in mind is to consider that the process and the increment at equal time are independent. This is a natural choice if one discretizes the evolution, as explained above, see Eq. (3.15). This is appropriate for numerical simulations. This is known as the *Itô convention*, corresponding to the "proposal 1" discussed above (and to discretization procedure, Eq. (3.15)). In order to specify in which sense the SDE is understood, we add a prescription

$$\mathrm{d}x(t) = a(x(t))\,\mathrm{d}t + b(x(t))\,\mathrm{d}W(t) \qquad \text{(Itô)}. \tag{3.20}$$

where the label "Itô" indicates that

$$\boxed{\text{Itô :} \quad x(t) \ \text{ and } \ \mathrm{d}W(t) \ \text{ are statistically independent at coinciding times}}$$

Itô calculus also makes use of

$$\boxed{\mathrm{d}W(t)^2 = \mathrm{d}t} \tag{3.21}$$

(we can omit the averaging when considering the infinitesimal noise increment ; see the appendix of this chapter on stochastic integrals in order to understand why $\langle\cdots\rangle$ can be omitted here, while it should be kept for $\langle \delta W(t)^2\rangle = \delta t$). Roughly speeking we have $\mathrm{d}W(t) \sim \mathcal{O}(\sqrt{\mathrm{d}t})$ and for this reason $\mathrm{d}W(t)^{2+n} = 0$ for $n > 0$.

Itô formula.— An important formula concerns the change of variable $x \to \varphi(x)$, where $\varphi(x)$ is a regular function, differentiable a least twice. If $x(t)$ obeys (3.20), we deduce

$$\boxed{\mathrm{d}\varphi(x(t)) = \left[\varphi'(x)\,a(x) + \frac{1}{2}\varphi''(x)\,b(x)^2\right]\mathrm{d}t + \varphi'(x)\,b(x)\,\mathrm{d}W(t) \qquad \text{(Itô)}} \tag{3.22}$$

(in the r.h.s. x stands for $x(t)$). This is known as the "*Itô formula*".

Proof : using Itô calculus, we must keep a second order term in equalities between infinitesimal increments :

$$\mathrm{d}\varphi(x) = \varphi'(x)\,\mathrm{d}x + \frac{1}{2}\varphi''(x)\,\mathrm{d}x^2\,. \tag{3.23}$$

This is due to (3.21) : a term $\mathcal{O}(\mathrm{d}t)$ is produced by the $\mathcal{O}(\mathrm{d}x^2)$ term : $\mathrm{d}x^2 = \big[a(x)\,\mathrm{d}t + b(x)\,\mathrm{d}W(t)\big]^2 = b(x)^2\,\mathrm{d}W(t)^2 + 2a(x)b(x)\mathrm{d}W(t)\mathrm{d}t + a(x)^2\mathrm{d}t^2 = b(x)^2\,\mathrm{d}t$. The first term dropped was $\mathcal{O}(\mathrm{d}W(t)\mathrm{d}t) = \mathcal{O}(\mathrm{d}t^{3/2})$ ($= 0$ in differential calculus).

✍ ***Exercice 3.2 :*** *Write the Itô formula for the multiplicative noise* $\mathrm{d}x(t) = \kappa\, x\,\mathrm{d}W(t)$. *The apply the formula to* $\varphi(x) = x^2$

Itô formula implies that **"Itô calculus" does not correspond with the "usual" differential calculus** when $W(t)$ is a regular (differentiable) function. Indeed, (3.22) shows that

$$\mathrm{d}\varphi(x(t)) \neq \varphi'(x(t))\,\mathrm{d}x(t) \qquad \text{(Itô)}. \tag{3.24}$$

Despite this drawback (for physicists), the Itô calculus is widely used by probabilists (and justified for certain physical situations). In particular, it is natural for financial mathematics, which is not a surprise as the time is discrete in finance : it corresponds to the discretization scheme mentioned above, Eq. (3.15), where δt is the elementary time step for trading on markets.

Remark : Within Itô convention, $x(t)$ and $W(t)$ are independent (at equal time). It follows that averaging (3.22) is straightforward (this is the interest of Itô's convention!) and gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\varphi(x(t)\rangle = \langle\varphi'(x(t))\,a(x(t))\rangle + \frac{1}{2}\langle\varphi''(x(t))\,b(x(t))^2\rangle\,. \tag{3.25}$$

Related FPE.– One can immediatly deduce the FPE related to the Itô equation (3.20). Write (3.25) as

$$\frac{\partial}{\partial t}\int \mathrm{d}x\, P_t(x)\,\varphi(x) = \int \mathrm{d}x\, P_t(x)\,\left[\varphi'(x)\,a(x) + \frac{1}{2}\varphi''(x)\,b(x)^2\right] \tag{3.26}$$

In the r.h.s, integrations by part allow to factorize $\varphi(x)$. Because the relation is true $\forall\,\varphi(x)$, we conclude that

$$\boxed{\frac{\partial P_t(x)}{\partial t} = -\frac{\partial}{\partial x}\left[a(x)\,P_t(x)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[b(x)^2\,P_t(x)\right]} \tag{3.27}$$

How to get the FPE from the SDE in a simple manner ? Above, the relation between the Itô SDE and the FPE was demonstrated by introducing a test function. A simpler way is to use $\langle \mathrm{d}W(t)^2\rangle_{\text{noise}} = \mathrm{d}t$ (physicist's notation) and to remark that the drift and the "diffusion" are given by

$$\langle a(x)\rangle = \frac{\langle \mathrm{d}x\rangle_{\text{noise}}}{\mathrm{d}t} \qquad \text{and} \qquad \langle b(x)^2\rangle = \frac{\langle \mathrm{d}x^2\rangle_{\text{noise}}}{\mathrm{d}t} \tag{3.28}$$

As an application we consider the multidimensional case

$$\mathrm{d}x_i(t) = a_i(\vec{x})\,\mathrm{d}t + b_{ij}(\vec{x})\,\mathrm{d}W_j(t) \qquad \text{(Itô)}. \tag{3.29}$$

with $\langle \mathrm{d}W_i(t)\mathrm{d}W_j(t)\rangle_{\text{noise}} = \delta_{ij}\mathrm{d}t$. Only the diffusion term is more complicated

$$\frac{\langle \mathrm{d}x_i \mathrm{d}x_j\rangle_{\text{noise}}}{\mathrm{d}t} = \langle b_{ik}b_{jk}\rangle \tag{3.30}$$

(with Einstein's convention for implicit summation over repeated indices). Then

$$\partial_t P_t(\vec{x}) = -\partial_i\left[a_i(\vec{x})P_t(\vec{x})\right] + \frac{1}{2}\partial_i\partial_j\left[b_{ik}(\vec{x})b_{jk}(\vec{x})P_t(\vec{x})\right]\,. \tag{3.31}$$

Application : Kramers and Smoluchowski equations.— Consider the equations

$$\begin{cases} \mathrm{d}x = v\,\mathrm{d}t \\ \mathrm{d}v = \left(-\frac{v}{\tau} + \frac{F(x)}{m}\right)\mathrm{d}t + \frac{1}{m}\sqrt{2k_{\mathrm{B}}T\gamma}\,\mathrm{d}W(t) \end{cases} \tag{3.32}$$

The drift terms are $a_x = \frac{\langle \mathrm{d}x\rangle_{\text{noise}}}{\mathrm{d}t} = v$ and $a_v = \frac{\langle \mathrm{d}v\rangle_{\text{noise}}}{\mathrm{d}t} = -\frac{v}{\tau} + \frac{F(x)}{m}$. The diffusive terms are $b_{xx}^2 = \langle \mathrm{d}x^2\rangle_{\text{noise}}/\mathrm{d}t = v^2\mathrm{d}t \to 0$, $b_{vv}^2 = \langle \mathrm{d}v^2\rangle_{\text{noise}}/\mathrm{d}t = 2k_{\mathrm{B}}T\gamma/m^2 = 2k_{\mathrm{B}}T/(m\tau)$ and $b_{xv}^2 = \langle \mathrm{d}x\mathrm{d}v\rangle_{\text{noise}}/\mathrm{d}t \sim \langle v\,\mathrm{d}W(t)\rangle_{\text{noise}} \to 0$. Finally, the FPE for the joint distribution is

$$\left(\partial_t + v\,\partial_x + \frac{F(x)}{m}\partial_v\right)P_t(x,v) = \frac{1}{\tau}\partial_v\left(v + \frac{k_{\mathrm{B}}T}{m}\partial_v\right)P_t(x,v) \tag{3.33}$$

This equation is called the *Kramers equation.*

✍ ***Exercice 3.3 Smoluchowski equation :*** *Using the overdamped limit introduced in § 1 get an equation for $P_t(x) = \int \mathrm{d}v\, P_t(x,v)$ in the limit of strong friction.*

d) Stratonovich convention

δ-function does not exist in real life : for physicists, it is only a mathematical model for an extremely narrow function. Similarly, white noise is only a mathematical model and physicists should find more natural to think at the Gaussian white noise in the SDE (3.14) as the limit of

a regular Gaussian noise with a finite but small correlation time. A concrete example of such a "real life" correlator is [15]

$$\langle \eta^\epsilon(t)\eta^\epsilon(t')\rangle = \frac{1}{2\epsilon}\mathrm{e}^{-|t-t'|/\epsilon} \tag{3.34}$$

with ϵ "small" (much smaller than all characteristic time scales of the problem). It is convenient to introduce the notation $W^\epsilon(t) = \int_0^t \mathrm{d}u\, \eta^\epsilon(u)$, which is regular (not only continuous, but *differentiable* now). In general we have

$$\langle \left[\partial_t W^\epsilon(t)\right]^2\rangle \sim 1/\epsilon \tag{3.35}$$

(for the correlator given above, we have $\langle \left[\partial_t W^\epsilon(t)\right]^2\rangle = 1/(2\epsilon)$). Let us write the regularised SDE

$$\mathrm{d}x^\epsilon(t) = \alpha(x^\epsilon)\,\mathrm{d}t + \beta(x^\epsilon)\,\mathrm{d}W^\epsilon(t) \tag{3.36}$$

The noise is regular, hence the solution $x^\epsilon(t)$ is also regular (this SDE is well defined). The standard rules of differential calculus for regular functions apply to $x^\epsilon(t)$: hence, the $\epsilon \to 0$ limit of this equation does not correspond to the Itô prescription.

Stratonovich SDE.— The limit $\epsilon \to 0^+$ of the regularised SDE (3.36) is our definition of the "*Stratonovich SDE*" :

$$\mathrm{d}x(t) = \alpha(x)\,\mathrm{d}t + \beta(x)\,\mathrm{d}W(t) \qquad \text{(Stratonovich)} \tag{3.37}$$

(Mathematicians proceed in a different manner). Because it is defined as a limit of a regular process, **ordinary rules of differential calculus hold within the Stratonovich convention** (this is its interest !) : what is true for $\epsilon > 0$ remains true at $\epsilon = 0$, which is not a singular point (this is the spirit of regularization in Physics). The drawback is that, as it differs from the Itô convention, the correlations at equal time are more difficult to characterize

Stratonovich : $x(t)$ and $\mathrm{d}W(t)$ are in general correlated at coinciding times

This is a bit subtle : $x(t)$ and $\mathrm{d}W(t')$ are uncorrelated for $t' > t$, as the process depends only on the noise in the *past* : $\langle \varphi(x(t))\,\mathrm{d}W(t')\rangle \propto \theta_{\mathrm{H}}(t-t')$ (causality). Within the Stratonovich convention, the process and the noise are correlated at *equal time* (these correlations are studied in Exercise 3.6 below). Note that this has to do with our definition of $\theta_{\mathrm{H}}(0)$.

Two questions :

- Q1: what is the FPE related to the Stratonovich SDE (3.37) ?
- Q2: what is the relation between the Stratonovich SDE (3.37) and the Itô SDE (3.20) (if they both aim to describe the same process) ?

Stratonovich SDE and FPE.— In the Exercise 3.4 below, we demonstrate that, using the usual rules of differential calculus (for regular functions), the Stratonovich SDE (3.37) is related to the FPE

$$\frac{\partial P_t(x)}{\partial t} = -\frac{\partial}{\partial x}\left[\alpha(x)\,P_t(x)\right] + \frac{1}{2}\frac{\partial}{\partial x}\left[\beta(x)\,\frac{\partial}{\partial x}\left[\beta(x)\,P_t(x)\right]\right] \tag{3.38}$$

[15] This choice is interesting because, from the theoretical point of view, we know how to generate such a non white noise from a white noise. We can simply solve the SDE $\frac{\mathrm{d}}{\mathrm{d}t}\eta^\epsilon(t) = -(1/\epsilon)\eta^\epsilon(t) + (1/\epsilon)\tilde{\eta}(t)$ where $\tilde{\eta}(t)$ is a white noise (this was done in chapter 1).

✍ ***Exercice 3.4 From the Stratonovich SDE to the FPE :*** *We consider the SDE* $\frac{\mathrm{d}x}{\mathrm{d}t} = \alpha(x) + \beta(x)\,\eta(t)$. *For additive noise* ($\beta(x) = \text{cste}$) *the mapping onto the FPE is simple and has been discussed above. Difficulties arise for* ***multiplicative noise****. To circumvent this, we perform a transformation of the SDE which leads to additive noise. Using ordinary rules of differential calculus means that we interpret the SDE with the Stratonovich interpretation.*

a) Consider $z(t) = \int^{x(t)} \mathrm{d}\tilde{x}/\beta(\tilde{x})$. *Write the SDE for* $z(t)$.

b) Give the FPE for $Q_t(z)$, *the distribution of* $z(t)$.

c) Deduce the FPE for $P_t(x)$, *the distribution of* $x(t)$.

Itô SDE *versus* Stratonovich SDE.— With this result in hand, it is easy to answer to the second question : we can rewrite the FPE Eq. (3.38) as

$$\frac{\partial P_t(x)}{\partial t} = -\frac{\partial}{\partial x}\left[\left(\alpha(x) + \frac{1}{2}\beta(x)\beta'(x)\right)\,P_t(x)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[\beta(x)^2\,P_t(x)\right] \tag{3.39}$$

which corresponds to (3.20) if

$$a(x) = \alpha(x) + \frac{1}{2}\beta(x)\,\beta'(x) \quad \text{and} \quad b(x) = \beta(x)\,. \tag{3.40}$$

Remark 1 : Note that Mathematicians follow a different strategy to define the Stratonovich SDE : in 1961, Stratonovich introduced a "symmetrized" form of stochastic integrals and differential forms (at the end of this chapter, the appendix on stochastic integrals give a flavour of this strategy).

Remark 2 : The study of the Langevin equation (chapter 1) suggests another approach to the problem. A way to introduce a regular noise with $\langle \eta^\epsilon(t)\eta^\epsilon(t')\rangle = \frac{1}{2\epsilon}\mathrm{e}^{-|t-t'|/\epsilon}$ is to add to (3.36) a differential equation for the noise. We recognize the correlations obtained in chapter 1. This provides a concrete way to analyze the limit $\epsilon \to 0$: we can study the couple of differential equations $\partial_t x^\epsilon(t) = a(x^\epsilon) + b(x^\epsilon)\,\eta^\epsilon(t)$, Eq. (3.36), and $\partial_t \eta^\epsilon(t) = -(1/\epsilon)\,\eta^\epsilon(t) + (1/\epsilon)\,\tilde{\eta}(t)$, where $\tilde{\eta}(t)$ is a Gaussian white noise. In this perspective, $\eta^\epsilon(t)$ is called a "**colored noise**" for the process $x^\epsilon(t)$. Clearly, the limit $\epsilon \to 0^+$ is the white noise limit, $\eta^\epsilon(t) \to \tilde{\eta}(t)$ (cf. the discussion of the overdamped regime in chapter 1). The analysis of the two coupled SDE in this limit can be achieved thanks to a "projection method" (see [12, 49] for discussions).

To close the paragraph, I emphasize :

- when $b(x)$ is not constant (case of multiplicative noise), the two SDE $\mathrm{d}x = a(x)\mathrm{d}t + b(x)\mathrm{d}W(t)$ (Itô) and $\mathrm{d}x = a(x)\mathrm{d}t + b(x)\mathrm{d}W(t)$ (Stratonovich) describe two *different* processes (related to different FPEs).
- Conversely $\mathrm{d}x = a(x)\mathrm{d}t + b(x)\mathrm{d}W(t)$ (Itô) and $\mathrm{d}x = \alpha(x)\mathrm{d}t + \beta(x)\mathrm{d}W(t)$ (Stratonovich) describe the *same* process provided (3.40) hold (then, they are related to the same FPE).

✍ ***Exercice 3.5 Stratonovich corresponds to standard differential calculus :*** *Let us check that the rules defined above for Stratonovich SDE are compatible with the usual rules of differential calculus for ordinary regular functions. Using the relation (3.40), transform the Itô formula (3.22) in the Stratonovich convention and check that*

$$\mathrm{d}\varphi(x(t)) = \varphi'(x(t))\,\mathrm{d}x(t) \qquad \textit{(Stratonovich)}. \tag{3.41}$$

I.e. within the Stratonovich's prescription, standard rules of differential calculus for regular functions do apply.

✍ ***Exercice 3.6 Correlation between the process and the noise (Stratonovich) :*** *Consider the Stratonovich equation (3.37).*

a) Denoting $\eta(t) = \mathrm{d}W(t)/\mathrm{d}t$, show that $\langle \beta(x(t))\,\eta(t)\rangle$ can be expressed as the average of a function of $x(t)$.

Hint : use the relation between Itô and Stratonovich SDE.

*b) Let us now consider a more general problem and analyze $\langle \Phi(x(t))\,\eta(t)\rangle$, where $\Phi(x)$ is an arbitrary function (in general $\Phi \neq \beta$) and where $x(t)$ solves (3.37). Noticing that the Gaussian white noise $\eta(t)$ is a Gaussian field and using the Furutsu-Novikov theorem (**??**), show that*

$$\boxed{\langle \Phi(x(t))\,\eta(t)\rangle = \frac{1}{2}\left\langle \Phi'(x(t))\beta(x(t))\right\rangle} \qquad \textit{(Stratonovich)} \tag{3.42}$$

e) Take home message

- If a SDE appears in a physical model, it should be most frequently interpreted in the Stratonovich sense (if the white noise is the limit of a regular noise with symmetric correlation function). Whithin the Stratonovich convention, ordinary rules of differential calculus hold.
- Remember how to relate the Stratonovich SDE (3.37) to the FPE (3.38) is the most important.
- Itô calculus is simple, however one must take care that rules of differential calculus should be changed in order to account for $\mathrm{d}W(t)^2 = \mathrm{d}t$: expansion must be performed up to second order $\mathrm{d}\varphi(x) = \varphi'(x)\,\mathrm{d}x + \frac{1}{2}\varphi''(x)\,\mathrm{d}x^2$, from which we recover the Itô formula.
- The relation between Itô SDE with FPE is given by Eq. (3.27) (straightforward to deduce from the Itô formula).
- Stratonovich SDE and Itô SDE (3.40) are related through a transformation of the drift term :

$$\text{Itô} \to \text{Stratonovich} : \quad \alpha(x) = a(x) - \frac{1}{2}b(x)\,b'(x) \quad \& \quad \beta(x) = b(x)$$
$$\text{Stratonovich} \to \text{Itô} : \quad a(x) = \alpha(x) + \frac{1}{2}\beta(x)\,\beta'(x) \quad \& \quad b(x) = \beta(x)$$

Bibliography : More can be found in the book of Gardiner [12]. For a presentation for mathematicians, see the book [30].

✍ ***Exercice 3.7 A student makes a computer simulation of a SDE :***
a) A student is doing his internship in finance. His advisor asks him to simulate numerically the SDE controlling the evolution of an asset, $\mathrm{d}S(t) = \left[r\,\mathrm{d}t + \sigma\,\mathrm{d}W(t)\right] S(t)$, where the actualization rate contains a fixed part, r, and a fluctuating part controlled by the volatility σ. What recurrence should the student implement on the computer to simulate this evolution ?

b) Another student is doing an internship in soft matter physics. His advisor asks him to simulate the equation for the position of a particle in a fluid, $\mathrm{d}x(t)/\mathrm{d}t = F(x(t)) + \sqrt{2D(x)}\,\eta(t)$, where $\eta(t)$ is a Gaussian white noise. Same question.

f) A simple illustration : evolution of an asset

In finance, the simplest model for the time evolution of an asset is to assume a growth rate with a fixed part and a random part, which corresponds to the simple SDE

$$\mathrm{d}x(t) = x(t)\,[r\,\mathrm{d}t + \sigma\,\mathrm{d}W(t)] \qquad \text{(Itô)}. \tag{3.43}$$

(the amplitude σ of the fluctuating part is the "volatility"). If $W(t)$ would be a regular (differentiable) function, one would simply divide the equation by x and use $\mathrm{d}\ln x = \mathrm{d}x/x$. This cannot be done here : within Itô calculus, the expression of $\mathrm{d}\ln x$ should account for the second order term $\mathrm{d}x^2$. We can proceed in two equivalent manners.

Method 1 (use Itô formula) : Application of Itô formula is easy from $\mathrm{d}\ln x = \frac{\mathrm{d}x}{x} - \frac{\mathrm{d}x^2}{2x^2}$. Here we have $\mathrm{d}x(t)^2 = \sigma^2\,x(t)^2\,\mathrm{d}W(t)^2 = \sigma^2\,x(t)^2\,\mathrm{d}t$. Thus

$$\mathrm{d}\ln x(t) = \left(r - \frac{\sigma^2}{2}\right)\mathrm{d}t + \sigma\,\mathrm{d}W(t) \qquad \text{(Itô)}. \tag{3.44}$$

Because the noise is additive, the SDE can be as well be interpreted in the Stratonovich sense. One can now simply integrate the equation

$$x(t) = x(0)\,\mathrm{e}^{\left(r-\frac{\sigma^2}{2}\right)t+\sigma\,W(t)} \tag{3.45}$$

This analysis shows that one must be careful with integration of Itô differential equation.

Note that a naive integration of (3.43) with the usual rules of integration (i.e. interpreting (3.43) within the Stratonovich sense), would have missed an exponential factor $\mathrm{e}^{-\frac{\sigma^2}{2}t}$).

Method 2 (use relation to the Stratonovich SDE) : Using the rule given above, we find that the Itô SDE is related to the SDE

$$\mathrm{d}x(t) = \left(r - \frac{\sigma^2}{2}\right)x(t)\,\mathrm{d}t + \sigma\,x(t)\,\mathrm{d}W(t) \qquad \text{(Stratonovich)}. \tag{3.46}$$

Now, we can safely divide the Stratonovich SDE by $x(t)$ and integrate. We obtain the same result, Eq. (3.45), as it should.

Let us stress an advantage of the Itô SDE : Using independence of $x(t)$ and $\mathrm{d}W(t)$ at the same time, we can average the Itô equation, leading to $\frac{\mathrm{d}}{\mathrm{d}t}\langle x(t)\rangle = r\,\langle x(t)\rangle$, hence $\langle x(t)\rangle = \langle x(0)\rangle\,\mathrm{e}^{rt}$. This is pretty straightforward.

Let us now average the solution (3.45) for fixed $x(0)$ in order to check that it is consistent with this result :

$$\langle x(t)\rangle = x(0)\,\mathrm{e}^{\left(r-\frac{\sigma^2}{2}\right)t}\left\langle \mathrm{e}^{\sigma W(t)}\right\rangle = x(0)\,\mathrm{e}^{(r-\sigma^2/2)t+\frac{1}{2}\sigma^2\langle W(t)^2\rangle} = x(0)\,\mathrm{e}^{rt} \tag{3.47}$$

where we have used the Gaussianity of $W(t)$. It was more direct to average the Itô SDE.

✍ ***Exercice 3.8 Vanishing of the mean velocity:*** *Consider the SDE for the drift $F(x)$ and the x-dependent diffusion constant $D(x)$:*

$$\mathrm{d}x(t) = F(x)\,\mathrm{d}t + \sqrt{2D(x)}\,\mathrm{d}W(t) \qquad \textit{(Stratonovich)}. \tag{3.48}$$

What is the drift ensuring that $\frac{\mathrm{d}}{\mathrm{d}t}\langle x(t)\rangle = 0$?

✍ ***Exercice 3.9 Itô and Stratonovich evolutions for non Gaussian white noise*** $\boldsymbol{\eta(t) = \sum_n \eta_n\, \delta(t - t_n)}$ ***:*** *In the beginning of § 3.2, we introduced a natural method to simulate an Itô SDE by discretizing time, cf. Eq. (3.15). Using the connection between Itô and Stratonovich SDE, we can also use (3.15) to simulate a Stratonovich SDE, by a careful choice of the drift (Exercise 3.7). In the present exercise, we discuss another approach, which allows to make a computer simulation of a Itô or Stratonovich SDE. The idea is based on the discussion of § 3.2 using non Gaussian white noise. We show here that, in a certain limit, the two evolutions (3.18) and (3.19) indeed correspond to Itô and Stratonovich conventions, respectively. These equations provide recurrences easy to implement on a computer.*

We consider the SDE

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = a(x(t)) + b(x(t))\,\eta(t) \qquad \text{where} \qquad \eta(t) = \sum_n \eta_n\, \delta(t - t_n) \tag{3.49}$$

is a non Gaussian white noise : t_n are random times occuring with rate λ and the i.i.d. amplitudes are chosen such that $\langle \eta_n \rangle = 0$ and $\lambda \langle \eta_n^2 \rangle = 1$. Then $\langle \eta(t)\eta(t') \rangle = \delta(t - t')$ (the noise is however non Gaussian : higher cumulants are non zero, as discussed in Exercise 2.9).

a) How do the two equations (3.18) ("Itô") and (3.19) ("Stratonovich") are modified by the introduction of the weights η_n ?

b) Consider first a simple example and set $a(x) = 0$ and $b(x) = \sigma\, x$ (like in Exercise 3.1). Write the two recurrences in this case.

c) What is the limit of the Gaussian white noise ? Show that the two rules correspond to Itô and Stratonovich SDE in this limit.
Hint : it is more easy to consider the evolution of $\ln x(t)$.

d) We now consider the general case (3.49). Study the two recurrences of question a) in the limit $\eta_n \to 0$ (up to second order). Deduce the corresponding SDE.

Historical note on Doblin-Itô calculus

Until 2000, Itô was considered as the foundator of what is usually denoted today the "Itô calculus". However in 2000, a sealed envelope ("pli cacheté" number 11-668), received in 1940 from a young mathematician named Vincent Doblin (born Wolfgang Döblin), was opened at Académie des Sciences de Paris, which showed that Doblin's contribution anticipated the work of Itô on stochastic calculus. Hence, we should rather name it "Doblin-Itô calculus".

Figure 19: *Vincent Doblin (1915-1940). A page of the pli cacheté (from [4]).*

Wolfgang Döblin was the son of a well-known german writer, Alfred Döblin. Because he was jewish and opponent to the nazism, Alfred Döblin escaped Germany to Zürich at the begining of 1933 with part of his family, followed by his son Wolgang. They arrived in Paris in the fall of 1933. Wolfgang obtained the french nationality in 1936, becoming "Vincent Doblin". In

1938 he passed his PhD, under the supervision of the famous mathematician Maurice Fréchet (Fig. **??**), however, at the end of 1938, he was incorporated in the French army. Refusing to serve as an officer, he was affected to the communications. During this period in the army, at the begining of the war, he was sent to the Ardennes and was able to produce important scientific results, which he chose to send to the Académie des Sciences under the form of a "pli cacheté", entitled "sur *l'équation de Kolmogoroff*, par Vincent Doblin". Just after the collapse of the French army, as his company was surrounded by germans in the Vosges region, Vincent Doblin tried unsuccessfully to cross the german lines and eventually preferred to commit suicide rather being captured. It was only possible to open the "pli cacheté" 60 years after his death. Although Vincent Doblin was already known in the mathematics community despite his youth, the importance of his contribution was not anticipated before 2000.

To learn more : look at the article [4] (available on the internet) written by the two probabilists Bernard Bru and Marc Yor, who analyzed the pli cacheté and recognized its scientific importance. Or the book by Marc Petit [36].

✍ ***Exercice 3.10 Electromagnetic noise :*** *We consider a model of electromagnetic noise : the two components of the electric field $E_x + \mathrm{i}\, E_y$ obey the two uncoupled SDE*

$$\begin{cases} \mathrm{d}E_x(t) = -\gamma\, E_x(t)\, \mathrm{d}t + \sqrt{D}\, \mathrm{d}W_x(t) \\ \mathrm{d}E_y(t) = -\gamma\, E_y(t)\, \mathrm{d}t + \sqrt{D}\, \mathrm{d}W_y(t) \end{cases} \tag{3.50}$$

where W_x and W_y are two independent Wiener processes, hence we can write

$$\mathrm{d}W_x^2 = \mathrm{d}W_y^2 = \mathrm{d}t \text{ and } \mathrm{d}W_x \mathrm{d}W_y = 0 \tag{3.51}$$

(remember that averages can be omitted for elementary differential increments).

1/ *We introduce the intensity and the phase : $E_x = A\cos\theta$ and $E_y = A\sin\theta$. Write the SDE for $A(t)$ and $\theta(t)$ within the Stratonovich convention.*

2/ *We write $E_x + \mathrm{i}\, E_y = A\, \mathrm{e}^{\mathrm{i}\theta} = \mathrm{e}^{\lambda + \mathrm{i}\theta}$.*

Using Itô calculus, express $\mathrm{d}\lambda + \mathrm{i}\, \mathrm{d}\theta$ as a function of λ, θ and the noises $\mathrm{d}W_x(t)$ and $\mathrm{d}W_y(t)$. Show that

$$\mathrm{d}W_A(t) = \cos\theta(t)\, \mathrm{d}W_x(t) + \sin\theta(t)\, \mathrm{d}W_y(t) \text{ and } \mathrm{d}W_\theta(t) = -\sin\theta(t)\, \mathrm{d}W_x(t) + \cos\theta(t)\, \mathrm{d}W_y(t) \tag{3.52}$$

are two independent noises. Deduce two Itô SDE for $\lambda(t)$ and $\theta(t)$ involving these new noises.

3/ *Using the Itô formula, deduce the Itô SDE for the amplitude $A = |E_x + \mathrm{i}\, E_y|$. Compare the related Stratonovich SDE for A to the one obtained in the question 1/. Discuss*

4/ *Write the SDE for the amplitude under the form*

$$\mathrm{d}A(t) = -V'(A(t))\, \mathrm{d}t + \sqrt{D}\, \mathrm{d}W_A(t) \tag{3.53}$$

and give the "potential" $V(A)$. Find its minimum and plot $V(A)$.

5/ *Write the FPE related to the SDE for $A(t)$. Deduce the equilibrium distribution. Discuss the distribution of the intensity $I = A^2$. Compute $\langle I \rangle$ and $\sqrt{\langle I^2 \rangle_c}$.*

APPENDIX : Stochastic integrals

If you feel unsatisfactory with the above presentation of Itô/Stratonovich convention, you can read this paragraph (borrowed from chapter 4 of [12]). Instead of considering the SDE, one considers integrals of the form $\int_0^t \mathrm{d}W(t')\, G(t')$ which requires the same discussion as for SDE.

Itô integral.— One defines the Itô integral as

$$\text{Itô}\int_0^t \mathrm{d}W(t')\,G(t') \stackrel{\text{def}}{=} \underset{N\to\infty}{\text{ms-lim}} \sum_{i=1}^{N} \delta W_i\, G(t_{i-1}) \tag{3.54}$$

where $\delta W_i = W(t_i) - W(t_{i-1})$. Here "ms-lim" stands for "mean-square limit" of a random variable, meaning that :

$$\underset{N\to\infty}{\text{ms-lim}}\, X_N = X_\infty \quad \text{if} \quad \lim_{N\to\infty} \langle [X_N - X_\infty]^2 \rangle = 0\,. \tag{3.55}$$

Let us study an example. Consider the integral Itô $\int_0^t \mathrm{d}W(t')\,W(t')$. One has to analyze the sum

$$\sum_{i=1}^{N} \delta W_i\, W_{i-1} = \frac{1}{2}\sum_{i=1}^{N} \left[(\delta W_i + W_{i-1})^2 - W_{i-1}^2 - \delta W_i^2\right] = \frac{1}{2}\sum_{i=1}^{N} W_i^2 - \frac{1}{2}\sum_{i=0}^{N-1} W_i^2 - \frac{1}{2}\sum_{i=1}^{N} \delta W_i^2$$
$$= \frac{1}{2}\left[W_N^2 - W_0^2\right] - \frac{1}{2}\sum_{i=1}^{N} \delta W_i^2 \tag{3.56}$$

It is easy to show that $\underset{N\to\infty}{\text{ms-lim}} \sum_{i=1}^{N} \delta W_i^2 = t$ (this is the reason why one writes $\mathrm{d}W(t)^2 = \mathrm{d}t$ without the average). Thus

$$\text{Itô}\int_0^t \mathrm{d}W(t')\,W(t') = \frac{1}{2}\left[W(t)^2 - W(0)^2 - t\right] \tag{3.57}$$

which differs (by $-t/2$) from the usual Riemann integral of a regular function.

Stratonovich integral.— Now introduce the definition of the Stratonovich integral

$$\int_0^t \mathrm{d}W(t')\,G(t') \stackrel{\text{def}}{=} \underset{N\to\infty}{\text{ms-lim}} \sum_{i=1}^{N} \delta W_i\, \frac{G(t_i) + G(t_{i-1})}{2} \tag{3.58}$$

(I use the standard notation for integration, anticipating that it will coincide with usual Riemann integrals).

Consider now the same integral as before $\int_0^t \mathrm{d}W(t')\,W(t')$ with the new convention. This time, one deals with

$$\sum_{i=1}^{N} \delta W_i\, \frac{W_i + W_{i-1}}{2} = \frac{1}{2}\sum_{i=1}^{N} W_i^2 - \frac{1}{2}\sum_{i=1}^{N} W_{i-1}^2 = \frac{1}{2}W_N^2 - \frac{1}{2}W_0^2 \tag{3.59}$$

so that we have recovered

$$\int_0^t \mathrm{d}W(t')\,W(t') = \frac{1}{2}\left[W(t)^2 - W(0)^2\right] \tag{3.60}$$

as for the integration of regular functions.

From stochastic integral to SDE : in the books [30, 12], stochastic integrals are first discussed along these lines, then SDE are introduced as derivatives of stochastic integrals.

APPENDIX : Microscopic foundations of the Langevin equation

The aim of this paragraph is to go beyond the phenomenological Langevin model and clarify the physical origin of the Langevin equation from a microscopic description. We introduce a model with a purely Hamiltonian *conservative* dynamics, within which will emerge the effective *dissipative* dynamics described by the Langevin equation. This will allow to identify the microscopic origin of the dissipation.

Model.— From Section 1, one would be tempted to model the collisions in the fluid, however the microscopic dynamics would be difficult to analyze. Instead, we consider a particle coupled to a macroscopic number of uncoupled harmonic oscillators modelling the "environment" (also called the "bath"). In this model, the oscillators represent the eigen-modes of the macroscopic system (like the phonon modes in a fluid). We now study the deterministic dynamics governed by the Hamiltonian

$$H = \frac{p^2}{2m} + V(x) + \sum_n \left[\frac{p_n^2}{2} + \frac{1}{2}\omega_n^2 \left(q_n - \frac{c_n\, x}{\omega_n^2} \right)^2 \right] \tag{3.61}$$

i.e.

$$H_{\rm sys}(x,p) = \frac{p^2}{2m} + V(x) \tag{3.62}$$

$$H_{\rm env}(\{q_n,p_n\}) = \sum_n \left[\frac{p_n^2}{2} + \frac{1}{2}\omega_n^2 q_n^2 \right] \tag{3.63}$$

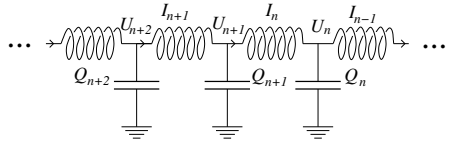
and the coupling is linear (this is very important for the following)

$$H_{\rm int} = -x \sum_n c_n\, q_n + \frac{1}{2}x^2 \sum_n \frac{c_n^2}{\omega_n^2} \tag{3.64}$$

Here c_n are coupling constants.

A physical realization is : an electron in an atom, coupled to the electromagnetic modes. Or : an electric device coupled to a L-C line.

✍ ***Exercice 3.11 Dissipation in a transmission line :*** *A perfect transmission line (a coaxial cable) is characterised by an inductance and a capacitance per length. A possible discrete model is a series of discrete capacitive and inductive elements (without resistance), i.e. only non-dissipative elements.*



We consider harmonic solutions $I_n(t) = \tilde{I}_n e^{-i\omega t}$. We recall that the impendance of the capacitance is $Z_C = 1/(-i\omega C)$ and that of the inductance $Z_L = -i\omega L$, where ω is the frequency.

1/ *We first study the eigenmodes of the infinite line. Using Kirchhoff laws, write the equations satisfied by the currents $\tilde{I}_n$.*

2/ Propagative modes.– *Show that the modes $I_n(t) = e^{iqn - i\omega(q)t}$ only exist in a finite bandwidth $\omega \in [0,\omega_0]$ where $\omega_0 \stackrel{\rm def}{=} 2/\sqrt{LC}$. Give the dispersion relation.*

3/ Evanescent modes.– *Study solutions of the form $I_n(t) = (-1)^n e^{qn - i\omega(q)t}$. Over what distance can propagate such modes ?*

4/ Impedance of semi-infinite line.– *We denote by Z_n the impedance of a finite line involving n couples of $L-C$ elements. Give the recurrence between Z_n and Z_{n+1}. Deduce the impedance of the semi-indinite line $Z_\infty \equiv Z(\omega)$. Plot* $\mathrm{Re}\, Z(\omega)$ *and* $\mathrm{Im}\, Z(\omega)$. *Discuss the fact that* $\mathrm{Re}\, Z(\omega) \neq 0$ *for a certain interval of frequencies (comment this at the light of question 1).*

Integration of the bath equations of motion.— We first derive the equations of motion

$$\begin{cases} m\,\ddot{x} = F(x) - x\sum_n \dfrac{c_n^2}{\omega_n^2} + \sum_n c_n q_n \\ \ddot{q}_n = -\omega_n^2 q_n + c_n\, x \end{cases} \tag{3.65}$$

where $F(x) = -V'(x)$. Let us integrate the equations of motion for the bath, which is possible thanks to the linearity. We can use that the retarded Green's function for the harmonic oscillator, i.e. the causal solution of $\ddot{G}^{\mathrm{R}}(t) + \omega_n^2 G^{\mathrm{R}}(t) = \delta(t)$ is $G^{\mathrm{R}}(t) = \theta_{\mathrm{H}}(t)\,\frac{\sin(\omega_n t)}{\omega_n}$. Thus we can solve the equation of motion for the oscillators

$$q_n(t) = q_n(0)\,\cos(\omega_n t) + \dot{q}_n(0)\,\frac{\sin(\omega_n t)}{\omega_n} + c_n \int_0^t \mathrm{d}t'\,\frac{\sin(\omega_n (t-t'))}{\omega_n}\,x(t') \tag{3.66}$$

We split the source term in Eq. (3.65) in two parts

$$\sum_n c_n\, q_n(t) = \overbrace{\sum_n c_n \left(q_n(0)\,\cos(\omega_n t) + \dot{q}_n(0)\,\frac{\sin(\omega_n t)}{\omega_n} \right)}^{\xi(t)} + \int_0^t \mathrm{d}t'\,\Gamma(t-t')\,x(t') \tag{3.67}$$

where

$$\Gamma(t) \overset{\text{def}}{=} \sum_n c_n^2 \frac{\sin(\omega_n t)}{\omega_n} \tag{3.68}$$

is a function depending of the microscopic parameters of the model. We denote $\xi(t)$ "the noise", which is controlled by the dynamical variables of the bath, i.e. a macroscopic number of degrees of freedom. For this reason, it is expected to exhibit a complex dynamics. Using $\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t} = \frac{1}{0^+ - \mathrm{i}\omega}$ we remark that

$$\int_0^\infty \mathrm{d}t\,\Gamma(t) = \sum_n \frac{c_n^2}{\omega_n^2} \tag{3.69}$$

which appears in the equation of motion above. With this definitions, we can rewrite the effective equation for the particle as

$$m\,\ddot{x}(t) = F(x(t)) - x(t)\int_0^\infty \mathrm{d}\tau\,\Gamma(\tau) + \int_0^t \mathrm{d}\tau\,\Gamma(\tau)\,x(t-\tau) + \xi(t) \tag{3.70}$$

Integration over the bath degrees of freedom is responsible for both the integral term and the "noise" term.

Noise and spectral function.— Because the bath involves a macroscopic number of degrees of freedom, it is natural to assume **thermal equilibrium for the bath**, say at $t = 0$, for the bath variables

$$P(\{q_n, p_n\}) \propto \mathrm{e}^{-\beta H_{\mathrm{env}}} \tag{3.71}$$

so that

$$\langle q_n(0)q_m(0)\rangle = \delta_{n,m}\,\frac{k_{\rm B}T}{\omega_n^2} \tag{3.72}$$

$$\langle \dot{q}_n(0)\dot{q}_m(0)\rangle = \delta_{n,m}\,k_{\rm B}T \tag{3.73}$$

Then the noise correlator is

$$C(t-t') = \big\langle \xi(t)\xi(t')\big\rangle = k_{\rm B}T\sum_n \frac{c_n^2\,\cos(\omega_n(t-t'))}{\omega_n^2} \tag{3.74}$$

At this stage it is useful to define the spectral function

$$J(\omega) \stackrel{\rm def}{=} \pi\sum_n \frac{c_n^2}{2\omega_n}\,\delta(\omega-\omega_n) \tag{3.75}$$

which depends on the distribution of frequencies and coupling constants. We can write the function

$$\Gamma(t) = \frac{2}{\pi}\int_0^\infty {\rm d}\omega\, J(\omega)\,\sin(\omega t) \tag{3.76}$$

and the correlator

$$C(t) = \frac{2k_{\rm B}T}{\pi}\int_0^\infty {\rm d}\omega\,\frac{J(\omega)}{\omega}\,\cos(\omega t) \tag{3.77}$$

in terms of the spectral function. Two remarks :

- In practice, we expect a dense spectrum of oscillators for frequencies $\omega \geqslant 0$ (it is natural to assume that the spectrum of eigenmodes start at $\omega = 0$ since there exist low frequency excitations ususally).
  What kind of behaviour can we expect for $J(\omega)$? Imagine that coupling constant is a smooth function of the frequency $c_n^2 = g(\omega_n)$. Then $J(\omega) = \frac{\pi}{2\omega}\sum_n g(\omega_n)\,\delta(\omega-\omega_n) \simeq \frac{\pi}{2\omega}g(\omega)\,\rho(\omega)$ for $\omega \to 0$, where $\rho(\omega)$ is the spectral density. For a linear spectrum (like photons, or phonons) we have $\rho(\omega) \sim \omega^{d-1}$ and thus we expect a power law $J(\omega) \sim g(\omega)\,\omega^{d-2}$ at low frequency. A simple assumption is $g(0)$ =cste.
- The spectrum of eigen-frequencies is usually cut off at a frequency ω_D related to the microscopic scale (for phonon modes in a crystal, ω_D is the Debye frequency, related to the lattice spacing).

The Ohmic case, $J(\omega) \propto \omega$ for small frequency : a concrete example.— assuming a broad spectrum of frequencies, of width ω_D of the form

$$J(\omega) = \gamma_0\,\omega\,\frac{\omega_D^2}{\omega^2+\omega_D^2} \tag{3.78}$$

gives

$$C(t) = k_{\rm B}T\,\gamma_0\,\omega_D\,{\rm e}^{-\omega_D|t|}\,. \tag{3.79}$$

Its integral is

$$\int_{-\infty}^{+\infty}{\rm d}t\,C(t) = 2\gamma_0\,k_{\rm B}T \tag{3.80}$$

which recall us something...

Effective equation of motion.— Let us come back to the analysis of the effective equation of motion (3.70). If the spectral function is broad (width $\sim \omega_D$), we expect the function $\Gamma(t)$ to be narrow in time (width $\sim 1/\omega_D$). For future convenience, we introduce

$$\gamma(t) = \int_t^\infty \mathrm{d}t'\, \Gamma(t') \tag{3.81}$$

which also decays rapidly over the scale $\sim 1/\omega_D$. We introduce a heaviside function in its definition to make it causal

$$\gamma(t) = \theta_{\mathrm{H}}(t) \sum_n \frac{c_n^2 \cos(\omega_n t)}{\omega_n^2} = \frac{2\,\theta_{\mathrm{H}}(t)}{\pi} \int_0^\infty \mathrm{d}\omega\, \frac{J(\omega)}{\omega} \cos(\omega t) \tag{3.82}$$

is a "narrow function" of width $1/\omega_D$.

An integration by parts gives

$$\int_0^t \mathrm{d}\tau\, \Gamma(\tau)\, x(t-\tau) = \gamma(0)\, x(t) - \gamma(t)\, x(0) - \int_0^t \mathrm{d}\tau\, \gamma(\tau)\, \dot{x}(t-\tau) \tag{3.83}$$

Considering times $t \gg 1/\omega_D$, we drop the term $\gamma(t)\, x(0)$. We end with the effective equation of motion

$$\boxed{m\,\ddot{x}(t) = F(x(t)) - \int_0^t \mathrm{d}\tau\, \gamma(\tau)\, \dot{x}(t-\tau) + \xi(t)} \tag{3.84}$$

This makes clear the physical interpretation of the integral term as a *friction* term, non local in time. The nonlocality is not a surprise after all, as, from a microscopic perspective, damping needs some time to establish.

FDT.— Finally we have the relation between the correlator of the noise and the friction

$$\boxed{C(\tau) = k_{\mathrm{B}} T\, \gamma(\tau) \quad \text{for } \tau > 0 \qquad \text{(FDT)}} \tag{3.85}$$

which relates the correlator of the noise to the damping (friction) function.

In the microscopic model, the damping term is an integral term. The relation between the damping and the strength of the noise results from the integration of the microscopic equation of motions, assuming equilibrium for the bath *only* (not for the particle, like in the phenomenological Langevin approach). We can compare the two approaches

- In the § 1 we have introduced two terms in the Langevin equation : the friction controlled by γ_0 and the noise controlled by the strength C. We have then assumed that the *particle* is at canonical equilibrium $P_{\mathrm{sys}}(x,p) \propto \exp[-\frac{\beta}{2} m v^2]$. Comparing with the statistical properties of the solution of the Langevin equation, we have deduced that the two parameters of the model cannot be independent but must be related by $C = 2\gamma_0 k_{\mathrm{B}} T$. To some extent, this relation was *assumed* for consistency.

- Here, we have only assumed that, being macroscopic, the *bath* is at thermal equilibrium $P_{\mathrm{bath}}(x,p) \propto \mathrm{e}^{-\beta H_{\mathrm{bath}}}$. As a result of the integration of the conservative dynamics, we have deduced the relation $C = 2\gamma_0 k_{\mathrm{B}} T$. A by-product is that if we study the statistic for the particle, one can show that it is described by canonical equilibrium (the particle reaches equilibrium because it interacts with the bath).

Quantum model : a very similar analysis can be performed within a quantum frame. Mainly, the correlator of the noise (i.e. of the initial bath variables) involves a different function and one is led to a "quantum Langevin equation" (cf. [13] or [45]).

Energetic considerations : We now study the energy of the system

$$\frac{\mathrm{d}}{\mathrm{d}t}H_{\rm sys} = \dot{x}\,[m\ddot{x} - F(x)] = -v(t)\int_0^t \mathrm{d}\tau\,\gamma(\tau)\,v(t-\tau) + v(t)\,\xi(t) \tag{3.86}$$

Clearly, the second term corresponds to the work of the Langevin force

$$\frac{\text{đ}W}{\mathrm{d}t} = v(t)\,\xi(t) \tag{3.87}$$

hence the first term should be interpreted as the heat received by the system

$$\frac{\text{đ}Q}{\mathrm{d}t} = -v(t)\int_0^t \mathrm{d}\tau\,\gamma(\tau)\,v(t-\tau)\,. \tag{3.88}$$

One can consider the model with $\gamma(\tau) = \gamma_0\,\omega_D\,\mathrm{e}^{-\omega_D\tau}$. Assuming $1/\omega_D \ll \tau = m/\gamma_0$, we expect that $v(t)$ is smooth on the scale $1/\omega_D$ so that we can treat $\xi(t)$ as a white noise. Hence $v(t) \simeq \frac{1}{m}\int_0^t \mathrm{d}t'\,\xi(t')\,\mathrm{e}^{-(t-t')/\tau}$. We can estimate the average work of the Langevin force

$$\frac{\langle \text{đ}W\rangle}{\mathrm{d}t} = \frac{1}{m}\int_0^t \mathrm{d}t'\,\left\langle \xi(t)\xi(t')\right\rangle\,\mathrm{e}^{-(t-t')/\tau} = \frac{C}{m}\,\theta_{\rm H}(0) = \frac{C}{2m} = \frac{k_{\rm B}T}{\tau} \tag{3.89}$$

where we have used that $\theta_{\rm H}(0) = 1/2$ (this is consistent with a symmetric regularised δ function). The averaged heat is

$$\frac{\langle \text{đ}Q\rangle}{\mathrm{d}t} = -\int_0^t \mathrm{d}t'\,\gamma(t-t')\,\left\langle v(t)v(t')\right\rangle \tag{3.90}$$

Because the correlator $\langle v(t)v(t')\rangle$ decays much slower than the damping function (we have assumed $\omega_D\tau \gg 1$) we can write $\gamma(t-t')\,\langle v(t)v(t')\rangle \simeq \gamma(t-t')\,\left\langle v(t)^2\right\rangle$, hence

$$\frac{\langle \text{đ}Q\rangle}{\mathrm{d}t} \simeq -\left\langle v(t)^2\right\rangle\int_0^\infty \mathrm{d}t''\,\gamma(t'') = -\frac{k_{\rm B}T}{m}\,\gamma_0 = -\frac{k_{\rm B}T}{\tau} \tag{3.91}$$

As it should the total energy is conserved on average

$$\langle \text{đ}W\rangle + \langle \text{đ}Q\rangle = 0 \tag{3.92}$$

The Langevin force furnishes some work to the particle and the bath receives the heat which is dissipated. The bath receives the entropy $\mathrm{d}S_{\rm bath} = -\text{đ}Q/T$, thus the dissipation corresponds to the production of entropy with rate

$$\boxed{\frac{\mathrm{d}\,\langle S_{\rm bath}\rangle}{\mathrm{d}t} = +\frac{k_{\rm B}}{\tau}} \tag{3.93}$$

Stochastic thermodynamics.— Here, I have applied some concepts of thermodynamics to a single particle. This type of question has attracted a lot of attention for ~ 25 years and is the subject of the field of "stochastic thermodynamics". If you are interested you can have a look to the reviews [23, 8, 27, 42, 41, 25] or to the lectures of Bernard Derrida at collège de France (2015-2016), `https://www.college-de-france.fr/site/bernard-derrida/`

☺ Important points

- Understand the difference between Itô and Stratonovich conventions (for multiplicative noise).
- For Itô calculus : remember $\mathrm{d}W(t)^2 = \mathrm{d}t$ and be careful with differential calculus ! Be able to recover the Itô formula.
- Be familiar with the relations between SDE (Itô or Stratonovich) and the FPE.

4 Stochastic processes (4) : the Fokker-Planck approach

When studying a stochastic process, the main goal is to determine its statistical properties, i.e. its distribution. The Fokker-Planck equation is an important equation which controls the evolution of the distribution of a Markov processes with no jump. In this chapter, we discuss several applications of the Fokker Planck equation and will demonstrate the power of the approach, compared to the stochastic differential equation approach : in particular we will see that we can address more subtle properties, like exit problem or first passage time.

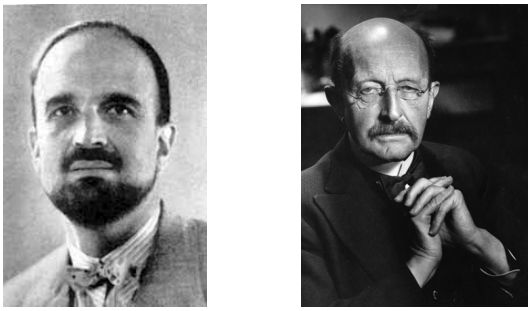


Figure 20: *Adriaan Fokker (1887-1972) and Max Planck (1858-1947)*

4.1 Interpretation of the Fokker-Planck equation

The Fokker-Planck equation (FPE) describes a specific class of stochastic processes for which the integro-differential master equation (2.24) can be reduced to a differential equation :

$$\frac{\partial P_t(x)}{\partial t} = -\frac{\partial}{\partial x}\left[F(x)\,P_t(x)\right] + \frac{\partial^2}{\partial x^2}\left[D(x)\,P_t(x)\right] \tag{4.1}$$

Below, we explain precisely in what limit and under what conditions we can go from (2.24) to (4.1). The equation is also known as the "*Kolmogorov equation*"or, for $D(x) \to D$, the "*Smoluchowski equation*". Let us first give the interpretation of the two terms in the Fokker-Planck equation (applications will be discussed below).

a) Drift : effect of the energy

Imagine that only the first term is present and that $F(x) \to F$ is uniform, we get

$$\frac{\partial P_t(x)}{\partial t} = -F\,\frac{\partial P_t(x)}{\partial x}\,. \tag{4.2}$$

The solution is $P_t(x) = \varphi(x - F\,t)$ thus F is the velocity (for uniform F, there is no deformation of the distribution). The first term in (4.1) is the **drift term**, where "the drift" $F(x)$ is interpreted as the force acting on the particle (remember that velocity=force). This is an effect of the energy as the force derives from a potential energy (at least in 1D).

b) Diffusion : effect of the entropy

Consider now the effect of the second term of (4.1) for a uniform $D(x) \to D$.

$$\frac{\partial P_t(x)}{\partial t} = D\frac{\partial^2 P_t(x)}{\partial x^2}\,. \tag{4.3}$$

As t grows, the distribution increases where the function is convex and diminishes where the function is concave (Fig. 21). This leads to a spreading of the distribution. The second term in

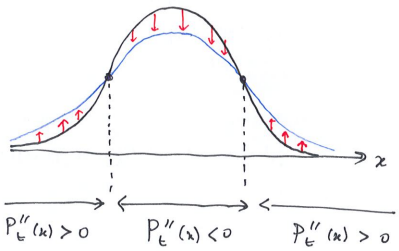


Figure 21: *the spreading of the distribution due to the diffusion term.*

(4.1) is the **diffusion term**, $D(x)$ playing the role of a x-dependent diffusion constant. This is an entropic effect (density tends to homogeneizes).

c) Current density

The Fokker-Planck equation can be rewritten under the form of a **conservation equation**

$$\frac{\partial P_t(x)}{\partial t} = -\frac{\partial J_t(x)}{\partial x} \tag{4.4}$$

where

$$\boxed{J_t(x) = \underbrace{F(x)\,P_t(x)}_{\text{drift current}} \overbrace{-\frac{\partial}{\partial x}\left[D(x)\,P_t(x)\right]}^{\text{diffusion current}}} \tag{4.5}$$

is the current density. The drift current is the usual velocity×density. The diffusion term accounts for the fact that when the density is not uniform, particles moves from high density regions to low density regions in order to homogenize the density (entropic effect).

In dimension d, the current density is a vectorial field and has dimension $[J] = L^{1-d}/T$ (in 1D this is a current).

4.2 From the master equation to the Fokker-Planck equation

In the previous chapter, we have related stochastic differential equations (SDE) to the FPE. This connection has relied on the fact that the noise in the SDE is a *Gaussian white noise*. The FPE thus describes a subclass of Markov processes. In this paragraph, we would like to understand the emergence of the FPE from a broader perspective, starting from the more fundamental master equation. We will show in which limit and under what conditions we can replace the master equation by the FPE.

a) Kramers-Moyal expansion

We consider the case where the state of the system is described by a coordinate which varies continuously in $\mathbb{R}$. Our starting point is the general master equation (2.24), i.e.

$$\frac{\partial P_t(x)}{\partial t} = \int \mathrm{d}x'\, W(x|x')\, P_t(x') \qquad \text{with} \int \mathrm{d}x\, W(x|x') = 0 \tag{4.6}$$

to ensure conservation of probability. This equation only relies on Markov assumption.

We have studied in detail the specific case of translation invariant jump processes (CPP, Exercise 2.8) : in this case the transition kernel $W(x|x')$ is a function of the difference $x - x'$ and takes the form $W(x|x') = \lambda\, w(x - x') - \lambda\, \delta(x - x')$, with a simple interpretation : λ is the jump rate and $w(\eta)$ the distribution of jump amplitude.

Let us now turn to a general jump process. Two remarks : (i) the kernel accounts for jump from x' to x, hence, in the master equation, the term $W(x|x')P_t(x')$ *increases* the probability at x, thus $W(x|x') \geqslant 0$ for $x \neq x'$. (ii) In order to fulfill the condition $\int \mathrm{d}x\, W(x|x') = 0$, the kernel must then contain a term $\propto -\delta(x-x')$. From these two remarks, we conclude that we can in general rewrite the transition kernel as

$$W(\underset{\text{final}}{\underset{\downarrow}{x}} \mid \underset{\text{initial}}{\underset{\downarrow}{x'}}) \equiv \tilde{w}(\underset{\text{initial}}{\underset{\downarrow}{x'}} ; \underset{\text{jump}}{\underset{\downarrow}{\eta = x - x'}}) - \delta(x-x') \int \mathrm{d}x''\, \tilde{w}(x'; x''-x') \,. \tag{4.7}$$

where $\tilde{w}(x';\eta) \geqslant 0$ is a positive function. Comparison with the CPP case shows that $\tilde{w}(x';\eta)$ can be interpreted as the distribution of the amplitude of the jumps made from the initial position x', multiplied by a jump rate. With this reparametrisation of the transition kernel, the master equation now reads

$$\frac{\partial P_t(x)}{\partial t} = \int \mathrm{d}\eta\, \tilde{w}(x-\eta;\eta)\, P_t(x-\eta) - P_t(x) \int \mathrm{d}\eta\, \tilde{w}(x;\eta) \,. \tag{4.8}$$

Although it will not much used below, we can introduce the rate to perform a jump from x :

$$\lambda(x) \overset{\text{def}}{=} \int \mathrm{d}\eta\, \tilde{w}(x;\eta) \tag{4.9}$$

and the distribution of the amplitude of jumps from x : $w(x;\eta) \overset{\text{def}}{=} \tilde{w}(x;\eta)/\lambda(x)$, which is now correctly normalised, $\int \mathrm{d}\eta\, w(x;\eta) = 1$.

The master equation being an integro-differential equation, its analysis is not straightforawrd in general (unless in simple cases where translation invariance holds, as it was shown in Exercise 2.8). We now want to show how (under what conditions) it can be replaced by a partial differential equation (PDE) much more easy to handle. The main assumptions are now

- $\tilde{w}(x';\eta)$ is a sharp function of η (small jumps dominate)
- $\tilde{w}(x';\eta)$ and $P(x';t)$ are smooth functions of x'.

These assumptions allow an expansion of the function of $x-\eta$ in powers of η

$$\int \mathrm{d}\eta\, \tilde{w}(x-\eta;\eta)\, P_t(x-\eta) = \int \mathrm{d}\eta \sum_{n=0}^{\infty} \frac{(-\eta)^n}{n!} \frac{\partial^n}{\partial x^n} \left[\tilde{w}(x;\eta)\, P_t(x)\right] \tag{4.10}$$

After introduction of this series in (4.8), the $n=0$ term is cancelled by the last term of Eq. (4.8). We can introduce

$$a_n(x) \overset{\text{def}}{=} \int \mathrm{d}\eta\, \eta^n\, \tilde{w}(x;\eta) \tag{4.11}$$

which is $\sim n$-th moment of the jumps from x, multiplied by a rate. Precisely, with the above notations : $a_n(x) = \lambda(x) \int \mathrm{d}\eta\, \eta^n\, w(x;\eta) = \lambda(x)\, \langle \eta^n \rangle_x$, where both the jump rate and the moment depend on x.

The condition that $\tilde{w}(\cdot;\eta)$ is a "narrow" function should be rather reformulated as $a_n(x) < \infty$ $\forall n$. Permuting integration over η and derivations with respect to x, we end with

$$\frac{\partial P_t(x)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial x^n} \left[a_n(x)\, P_t(x)\right] \tag{4.12}$$

which is known as the **Kramers-Moyal expansion**. Of course such an expansion only exists if the distribution of jumps is such that *all moments* $a_n(x)$ *are finite*. Under this form, the equation is not more easy to manipulate than the integral form from which we started. However, with

the above assumption that $\tilde{w}(x;\eta)$ is a narrow function of η, corresponding to small jumps at high rate, we expect the moments $a_n(x)$ to decay fast with n, which allows a truncation of the expansion. The truncated equation

$$\frac{\partial P_t(x)}{\partial t} = -\frac{\partial}{\partial x}\left[a_1(x)\,P_t(x)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[a_2(x)\,P_t(x)\right] \tag{4.13}$$

is the Fokker-Planck equation (4.1). [16] The FPE describes a *continuous* random process (i.e. the jumps disappear in the continuum limit, which is only possible if the original distribution of jumps is sufficiently narrow). [17]

Bibliography : This discussion is inspired by the book of van Kampen (chapter VIII) [49].

Pawula theorem : Can we truncate the Kramers-Moyal expansion (4.12) at any n ? The Pawula theorem states that it can only be stopped at $n = 1$ or $n = 2$. The positivity of the solution implies that if not stopped at $n = 1$ or $n = 2$, one should keep the infinite series (cf. § 4.3, [39]). This reminds us the Marcinkiewicz theorem about the generating function of cumulants.

FPE describes large scale properties of the master equation.— Having in mind the form $\tilde{w}(x;\eta) = \lambda(x)\,w(x;\eta)$ and assume that there exists a unique characteristic scale λ. Additionnally we assume that jumps are characterised by a unique scale ϵ (width of $w(\cdot;\eta)$). In the master equation, the time can be rescaled as $\tilde{t} = \lambda t$, so that it is equivalent considering large time or high rate. We expect the scaling of the coefficients $a_n(x) \sim \lambda\,\epsilon^n$. If we send $\lambda \to \infty$ and $\epsilon \to 0$ such that $a_2(x) \sim \lambda\epsilon^2 \sim 1$ is fixed (i.e. interesting physics occurs at the scale related to a_2), then higher coefficients go to zero $a_n(x) \sim \epsilon^{n-2} \to 0$, hence we end with the Fokker-Planck equation. In conclusion, provided that the Kramers Moyal expansion exists (or more precisely, at least the **two coefficients** $a_1(x)$ **and** $a_2(x)$ **are finite**), the large scale properties described the master equation (for jump process) coincide with those given by the Fokker-Planck equation (for continuous process).

b) Conclusion : jump process *versus* diffusion

In general, the master equation can be written under the form

$$\partial_t P_t(x) = \mathscr{L} P_t(x) \tag{4.14}$$

where $\mathscr{L}$ is a linear operator.

- For a *jump process*, the linear operator is an integral operator, of the form (4.6) or (4.8). For example, a simple **jump process** is the CPP studied above, for which $\big[\mathscr{L}\varphi\big](x) = \lambda \int \mathrm{d}\eta\, w(\eta)\big(\varphi(x-\eta) - \varphi(x)\big)$. In the general case, the distribution of the jump amplitude depends on the initial position, Eq. (4.8).
- If the linear operator is a differential operator, $\mathscr{L} = -\partial_x F(x) + \partial_x^2 D(x)$, one says that the process is "**a diffusion**". From the Pawula theorem, the differential operator can be at most second order. Physically, a diffusion is obtained as the limit of small jumps occuring with high rate. This is the type of stochastic processes discussed in the previous chapter on SDE and the present one on FPE.
- In general, a Markov process can combine a diffusion and jumps.

[16] A proper justification of the truncation requires a neat rescaling of the jumps and the rate, like it was done in the above Exercise 2.8. The argument follows the spirit of the central limit theorem.

[17] The condition "distribution of jumps sufficiently narrow" should have been made clear in Exercise 2.8. It is furhter discussed in Exercise **??**.

4.3 Spectral analysis of the Fokker Planck equation

In this section we discuss how the FPE can be solved by using spectral information, in principle at least. For simplicity, we mostly study processes with additive noise

$$\mathrm{d}x(t) = F(x(t))\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}W(t)\,, \tag{4.15}$$

i.e. Eq. (4.1) for $D(x) \to D$ (some properties will be extended to the general case in Exercise 4.4). Because we only consider here additive noise, Itô and Stratonovich interpretations of the SDE correspond to the same process. Furthermore, *we restrict the discussion to the one-dimensional case when the drift is such that there exists an equilibrium state*, i.e. when the potential

$$V(x) = -\int^x \mathrm{d}x'\, F(x') \tag{4.16}$$

is *confining*.

a) Generator of the diffusion

The related FPE was obtained above, Eq. (3.5). This form is not unfamiliar and recalls the Schrödinger equation in imaginary time $-\partial_t P = H_{\rm FP} P$. The reader is most probably familiar with spectral analysis in the quantum mechanical context. Here we have introduced $H_{\rm FP} = -D\,\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x}F(x)$, where the notation means that the operator $\frac{\partial}{\partial x}F(x) = F'(x) + F(x)\frac{\partial}{\partial x}$ must be understood as acting on a function $\phi(x)$ as $\frac{\partial}{\partial x}\big[F(x)\phi(x)\big] = F'(x)\phi(x) + F(x)\phi'(x)$. The operator $H_{\rm FP} = -D\,\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x}F(x)$ is therefore *not self-adjoint* in the presence of the drift, [18] $H_{\rm FP} \neq H_{\rm FP}^\dagger$. Instead of the notation $H_{\rm FP}$ used in [39], I will prefer the mathematicians' notation

$$\partial_t P_t(x) = \mathscr{G}^\dagger P_t(x) \quad \text{where} \quad \mathscr{G}^\dagger = D\,\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x}F(x) \tag{4.17}$$

is the "forward generator". By convention, probabilists call the adjoint of this operator

$$\mathscr{G} = D\,\frac{\partial^2}{\partial x^2} + F(x)\frac{\partial}{\partial x} \tag{4.18}$$

the "*generator of the diffusion*". I will also call it the "*backward generator*" as we will see that it governs the evolution of the density backward in time. We have used that $\big(\frac{\partial}{\partial x}\big)^\dagger = -\frac{\partial}{\partial x}$ (like in quantum mechanics).

It will be helpful for the following to rewrite the generator and its adjoint in the following form

$$\boxed{\mathscr{G}^\dagger = D\,\frac{\partial}{\partial x}\mathrm{e}^{-V(x)/D}\frac{\partial}{\partial x}\mathrm{e}^{V(x)/D}} \quad \text{and} \quad \mathscr{G} = D\,\mathrm{e}^{V(x)/D}\frac{\partial}{\partial x}\mathrm{e}^{-V(x)/D}\frac{\partial}{\partial x}\,, \tag{4.19}$$

where $F(x) = -V'(x)$. Several simple observations follow from this remark. For example, the generator and its adjoint car be related through the transformation $\mathscr{G}^\dagger = \mathrm{e}^{-V(x)/D}\mathscr{G}\mathrm{e}^{V(x)/D}$.

Equilibrium.— It makes clear that a stationary solution of the FPE, i.e. a solution of $\mathscr{G}^\dagger P = 0$, is

$$P_{\rm eq}(x) = C_0\,\mathrm{e}^{-V(x)/D} \qquad \Rightarrow \quad \mathscr{G}^\dagger P_{\rm eq}(x) = 0 \tag{4.20}$$

where C_0 is a normalisation constant. As a matter of factn we have identify the right vector for eigenvalue $\lambda_0 = 0$, i.e. $\mathscr{G}^\dagger \Phi_0^{\rm R}(x) = 0$. Similarly the left eigenvector such that $\mathscr{G}\Phi_0^{\rm L}(x) = 0$ is clearly a constant :

$$\boxed{\Phi_0^{\rm R}(x) = P_{\rm eq}(x) \quad \text{and} \quad \Phi_0^{\rm L}(x) = 1} \tag{4.21}$$

[18] Self-adjointness is not only broken by the drift term ; it can also be broken by the boundary conditions, if they induce a drift at the boundaries.

✍ ***Exercice 4.1 :*** *Argue that the solution (4.20) is an equilibrium solution (hint : analyze the related current). What is the condition on $V(x)$ for such an equilibrium state ?*

b) Solving the FPE

Let us apply the spectral method to solve the FPE $\partial_t P_t(x) = \mathscr{G}^\dagger P_t(x)$. We look for a solution of the "separable" form

$$P_t(x) = \Phi(x)\,\mathrm{e}^{-\lambda t} \quad \text{hence} \quad \mathscr{G}^\dagger \Phi(x) = -\lambda\,\Phi(x)\,. \tag{4.22}$$

Because the generator is not self adjoint, this last equation is an equation for a "right eigenvector" of $\mathscr{G}^\dagger$. Its spectrum involves a bi-orthognoal set of right and left eigenvectors

$$\mathscr{G}^\dagger \Phi_n^{\mathrm{R}}(x) = -\lambda_n\,\Phi_n^{\mathrm{R}}(x) \quad \text{and} \quad \mathscr{G}\Phi_n^{\mathrm{L}}(x) = -\lambda_n\,\Phi_n^{\mathrm{L}}(x) \tag{4.23}$$

with [19]

$$\int \mathrm{d}x\,\Phi_n^{\mathrm{L}}(x)\Phi_m^{\mathrm{R}}(x) = \delta_{nm} \tag{4.24}$$

(see the discrete version in Subsection d), page 24). When there exists a stationary state, the spectrum is real and the lowest eigenvalue $\lambda_0 = 0$ is isolated (there is a finite gap between λ_0 and the next eigenvalue). The next eigenvalue λ_1 corresponds to the *relaxation rate* toward stationary state (or $\mathrm{Re}(\lambda_1)$ if λ_1 is complex). When there exists an equilibrium, for a confining potential $V(x)$, the spectrum is real.

Let us use this spectral information to solve the FPE for a given initial condition $P_0(x)$. We first decompose this latter on the right eigenvectors

$$P_0(x) = \sum_n c_n\,\Phi_n^{\mathrm{R}}(x) \quad \text{where} \quad c_n = \int \mathrm{d}x\,\Phi_n^{\mathrm{L}}(x)P_0(x) \tag{4.25}$$

Then, the solution at time t reads

$$P_t(x) = \sum_n c_n\,\Phi_n^{\mathrm{R}}(x)\,\mathrm{e}^{-\lambda_n t}\,. \tag{4.26}$$

The conditional probability can be obtained along these lines : in this case, the initial condition is $P_0(x) = \delta(x - x_0)$, hence $c_n = \Phi_n^{\mathrm{L}}(x_0)$. Therefore the spectral decomposition of the conditional probability is

$$\boxed{P_t(x|x_0) = \sum_{n=0}^{\infty} \Phi_n^{\mathrm{R}}(x)\Phi_n^{\mathrm{L}}(x_0)\,\mathrm{e}^{-\lambda_n t}} \tag{4.27}$$

c) Supersymmetry

We already noticed that the generator has an interesting structure, which results in some important properties. In particular, $\mathscr{G}^\dagger$ has a negative spectrum : all its eigenvalues are negative

[19] Prove orthonormalisation : consider the difference

$$\int \mathrm{d}x\,\left[\Phi_m^{\mathrm{L}}(x)\mathscr{G}^\dagger\Phi_n^{\mathrm{R}}(x) - \Phi_n^{\mathrm{R}}(x)\mathscr{G}\Phi_m^{\mathrm{L}}(x)\right] = (\lambda_n - \lambda_m)\int \mathrm{d}x\,\Phi_n^{\mathrm{L}}(x)\Phi_m^{\mathrm{R}}(x)$$

The left hand side vanishes thanks to some integration by parts, since $\Phi_n^{\mathrm{L}}(x)\Phi_m^{\mathrm{R}}(x) \to 0$ for $|x| \to \infty$ (this is required by normalisation on $\mathbb{R}$). Hence $\int \mathrm{d}x\,\Phi_n^{\mathrm{L}}(x)\Phi_m^{\mathrm{R}}(x) \propto \delta_{nm}$.

or zero (i.e. $\lambda_n \geqslant 0$). We can prove this by stressing some interesting connection to a quantum mechanical operator H_+. We first perform the non unitary transformation

$$\begin{aligned} H_+ &= -\mathrm{e}^{V(x)/2D}\, \mathscr{G}^\dagger\, \mathrm{e}^{-V(x)/2D} = -\mathrm{e}^{-V(x)/2D}\, \mathscr{G}\, \mathrm{e}^{V(x)/2D} \\ &= -D\, \mathrm{e}^{V(x)/2D} \frac{\partial}{\partial x} \mathrm{e}^{-V(x)/D} \frac{\partial}{\partial x} \mathrm{e}^{V(x)/2D} \end{aligned} \tag{4.28}$$

which symmetrizes the structure of the operator. The transformation relates $-\mathscr{G}^\dagger$ to the self-adjoint operator H_+ (the two operators have the *same spectrum* of eigenvalues). [20] In other terms we consider the transformation of the FPE

$$\partial_t P_t(x) = \mathscr{G}^\dagger P_t(x) \qquad \overset{P_t(x)=\psi_0(x)\,\phi_t(x)}{\longrightarrow} \qquad -\partial_t \phi_t(x) = H_+ \phi_t(x) \tag{4.29}$$

where $\psi_0(x) = c_0\, \mathrm{e}^{-V(x)/2D} = \sqrt{P_{\mathrm{eq}}(x)}$. This Hamiltonian has a specific structure

$$\boxed{H_+ = \mathscr{Q}^\dagger \mathscr{Q}} \qquad \text{with } \mathscr{Q} \overset{\text{def}}{=} -\sqrt{D} \mathrm{e}^{-V(x)/2D} \frac{\partial}{\partial x} \mathrm{e}^{V(x)/2D} = \sqrt{D} \left(-\frac{\partial}{\partial x} + \frac{F(x)}{2D} \right) \tag{4.30}$$

known as "*supersymmetric*" (it is possible to introduce the supersymmetric partner $H_- = \mathscr{Q}\mathscr{Q}^\dagger$, the two operators having the same spectrum but the zero mode [21]). The structure $H_+ = \mathscr{Q}^\dagger \mathscr{Q}$ implies that the spectrum of the operator is strictly positive [22]

$$\mathrm{Spec}(H_+) = \mathrm{Spec}(-\mathscr{G}^\dagger) \subset \mathbb{R}_+ \,. \tag{4.31}$$

We have also

$$\boxed{H_+ = D \left(\frac{\partial}{\partial x} + \frac{F(x)}{2D} \right) \left(-\frac{\partial}{\partial x} + \frac{F(x)}{2D} \right) = -D \frac{\partial^2}{\partial x^2} + \frac{F(x)^2}{4D} + \frac{F'(x)}{2}} \tag{4.32}$$

The drift is such that there exists an equilibrium state, hence the effective potential $\mathcal{U}(x) = \frac{F(x)^2}{4D} + \frac{F'(x)}{2}$ is a confining potential and the Hamiltonian has a discrete spectrum :

$$H_+ \psi_n(x) = \lambda_n\, \psi_n(x) \qquad \text{with } \lambda_n \geqslant 0 \,. \tag{4.33}$$

In particular, the equilibrium solution $P_{\mathrm{eq}}(x)$ is related to the zero mode of H_+ :

$$H_+ \psi_0(x) = 0 \quad \text{with } \psi_0(x) = c_0\, \mathrm{e}^{-V(x)/2D} = \sqrt{P_{\mathrm{eq}}(x)}. \tag{4.34}$$

where c_0 is a normalisation.

✍ ***Exercice 4.2 Ornstein-Uhlenbeck process and the quantum harmonic oscillator:*** *Consider the case $F(x) = -k\,x$ (i.e. $V(x) = \frac{k}{2}\,x^2$). Check that H_+ is the quantum Hamiltonian for the harmonic oscillator. What are the two operators $\mathscr{Q}$ and $\mathscr{Q}^\dagger$?*
Deduce the spectrum of eigenvalues $\{\lambda_n\}_{n\in\mathbb{N}}$ of H_+ and $-\mathscr{G}^\dagger$.

[20] A subtle remark : boundary conditions for the FPE may differ from boundary conditions relevant for quantum mechanical problems. Although there is a mapping between the two differential operators H_+ and $\mathscr{G}^\dagger$, there are some situations where the boundary conditions of the FPE leads to break the self-adjointness of H_+, which explains how the spectrum may be complex (such a case appears in [11, 7]. For confining potential $V(x)$, this however does not happen : boundary conditions correspond to exponentially decaying wave functions of H_+ and right eigenvectors of $\mathscr{G}^\dagger$, with real spectrum.

[21] Only one of the two hamiltonians H_+ and H_- may have a zero mode. If none of them possesses a normalizable zero mode, the supersymmetry is said to be broken, cf. book [18].

[22] since $H_+|\,\psi\,\rangle = \lambda|\,\psi\,\rangle$ implies $\lambda = \langle\,\psi\,|\mathscr{Q}^\dagger\mathscr{Q}|\,\psi\,\rangle = ||\mathscr{Q}|\,\psi\,\rangle||^2 \geqslant 0$.

✍ ***Exercice 4.3 Linear confinment :*** *Find the spectrum of $\mathscr{G}^\dagger$ when the particle is submitted to the confining potential $V(x) = v\,|x|$.*
Hint : discuss H_+.

✍ ***Exercice 4.4 Generalized supersymmetry :*** *Consider the case of the diffusion for x-dependent diffusion constant*

$$\mathrm{d}x(t) = F(x)\,\mathrm{d}t + \sqrt{2D(x)}\,\mathrm{d}W(t) \qquad \textit{(Stratonovich)} \tag{4.35}$$

a) Give the generator $\mathscr{G}$ of this diffusion and show that it can be written under a form analogous to (4.19).

b) Deduce the expression of the equilibrium distribution $P_{\rm eq}(x)$. What is the condition which ensures that it exists ?

c) Now assuming the existence of a steady current J, give the related stationary distribution $P_{\rm st}(x)$.

d) How the operators H_+, $\mathscr{Q}$ and $\mathscr{Q}^\dagger$ are generalized ?

✍ ***Exercice 4.5 Solution for x-dependent diffusion constant and no drift :*** *We consider the SDE (4.35) for $F(x) = 0$. Write the FPE for $P_t(x)$. We introduce the change of variable*

$$y = \int^x \frac{\mathrm{d}\tilde{x}}{\sqrt{2D(\tilde{x})}} \tag{4.36}$$

Deduce the FPE for the distribution $Q_t(y)$. Solve it for the propagator and deduce $P_t(x|x_0)$.

d) Conditional probability (propagator)

An important object characterizing the diffusion is the propagator of the diffusion (the conditional probability), solution of

$$\partial_t P_t(x|x_0) = \mathscr{G}^\dagger P_t(x|x_0) \quad \text{ for initial condition } P_0(x|x_0) = \delta(x - x_0)\,. \tag{4.37}$$

We recall that we assumed a confining drift $F(x)$, such that there exists an equilibrium. Then the spectrum of $\mathscr{G}^\dagger$ (and of H_+) is discrete. Given the spectral information $\{\lambda_n, \psi_n(x)\}$ we can obtain a representation of the propagator.

Method n°1 : we can use the relation to supersymmetric quantum mechanics. The non unitary transformation $P_t(x) = \psi_0(x)\psi(x;t)$, where $\psi_0(x) \propto \mathrm{e}^{-V(x)/2D}$, maps the PDE for the conditional probability onto

$$-\partial_t \Psi_t(x|x_0) = H_+ \Psi_t(x|x_0) \quad \text{ for initial condition } \Psi_0(x|x_0) = \delta(x - x_0)\,. \tag{4.38}$$

The solution can be decomposed over the eigenstates of H_+ (this is the main motivation for spectral analysis!). Starting from the initial condition $\Psi_0(x|x_0) = \sum_{n=0}^\infty \psi_n(x)\psi_n(x_0)$ we get at time t,

$$\Psi_t(x|x_0) = \sum_{n=0}^\infty \psi_n(x)\psi_n(x_0)\,\mathrm{e}^{-\lambda_n t}\,. \tag{4.39}$$

We go back to the conditional probability. In order to satisfy the initial condition, we must write $P_t(x|x_0) = \psi_0(x)\Psi_t(x|x_0)/\psi_0(x_0)$, thus

$$\boxed{P_t(x|x_0) = \frac{\psi_0(x)}{\psi_0(x_0)} \sum_{n=0}^\infty \psi_n(x)\psi_n(x_0)\,\mathrm{e}^{-\lambda_n t}} \tag{4.40}$$

Method n°2 : It is more straightforward to manipulate operators : [23]

$$P_t(x|x_0) = \langle\, x\,|\mathrm{e}^{t\mathscr{G}^\dagger}|\, x_0\,\rangle = \langle\, x\,|\mathrm{e}^{-t\psi_0(\hat{x})H_+\psi_0(\hat{x})^{-1}}|\, x_0\,\rangle = \langle\, x\,|\psi_0(\hat{x})\mathrm{e}^{-tH_+}\psi_0(\hat{x})^{-1}|\, x_0\,\rangle$$
$$= \psi_0(x)\langle\, x\,|\mathrm{e}^{-tH_+}|\, x_0\,\rangle\frac{1}{\psi_0(x_0)} \tag{4.41}$$

where $\hat{x}$ is the "position operator" with $\hat{x}|\, x\,\rangle = x|\, x\,\rangle$. The propagator of H_+ can be decomposed over its eigenstates and we recover (4.40).

✍ ***Exercice 4.6 :*** *Check the normalisation* $\int \mathrm{d}x\, P_t(x|x_0) = 1$.
Argue that $\lim_{t\to\infty} P_t(x|x_0) = P_{\rm eq}(x)$.

This structure makes clear the relation $P_t(x|x_0)\psi_0(x_0)^2 = P_t(x_0|x)\psi_0(x)^2$ i.e.

$$\boxed{P_t(x|x_0)P_{\rm eq}(x_0) = P_t(x_0|x)P_{\rm eq}(x)} \tag{4.42}$$

which is reminiscent of the *detailed balance* condition, which was expected as we are dealing with a situation where an equilibrium exists ($V(x)$ is confining). Strictly speaking, detailed balance involves the transition rates, i.e. the $t \to 0$ limit : $P_t(x|x_0) \simeq \delta(x - x_0) + t\, W(x|x_0)$, then detailed balance is $W(x|x_0)P_{\rm eq}(x_0) = W(x_0|x)P_{\rm eq}(x)$.

Remark : This equation is the consequence of the identity between operators

$$P_{\rm eq}(\hat{x})^{-1}\,\mathscr{G}^\dagger\,P_{\rm eq}(\hat{x}) = \mathscr{G}\,. \tag{4.43}$$

✍ ***Exercice 4.7 The Ornstein-Uhlenbeck process and the quantum oscillator :*** *Using the expression of the propagator for the quantum mechanical harmonic oscillator*

$$\langle\, x\,|\mathrm{e}^{-tH_\omega}|\, x_0\,\rangle = \sqrt{\frac{m\omega}{2\pi\sinh\omega t}}\,\exp -\frac{m\omega}{2\sinh\omega t}\left[\cosh\omega t\,(x^2 + x_0^2) - 2xx_0\right] \tag{4.44}$$

for $H_\omega = -\frac{1}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2\, x^2$, *recover the propagator* (2.18) *of the Ornstein-Uhlenbeck process described by the SDE* $\mathrm{d}x = -k\,x\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}W(t)$.
Check the condition (4.42).

e) Right/left eigenvectors and supersymmetry

It is instructive to make the connection between the right/left eigenfunctions introduced above and the eigenfunctions of the supersymmetric Hamiltonian. Eq. (4.27) coincides with (4.40). This shows that the right and left eigenvectors can be simply related to the eigenfunctions of H_+ as follows

$$\Phi_n^{\rm R}(x) = \psi_0(x)\psi_n(x) \quad \text{and} \quad \Phi_n^{\rm L}(x) = \frac{\psi_n(x)}{\psi_0(x)} \tag{4.45}$$

In particular, for $\lambda_0 = 0$,

$$\Phi_0^{\rm R}(x) = \psi_0(x)^2 = P_{\rm eq}(x) \quad \text{and} \quad \Phi_0^{\rm L}(x) = 1\,. \tag{4.46}$$

[23] The two operators are related by a non-uniatry transformation of the form $\mathscr{G}^\dagger = -\mathcal{U}H_+\mathcal{U}^{-1}$. Exponentiating the equality we find $\exp\left[t\,\mathscr{G}^\dagger\right] = \exp\left[-t\,\mathcal{U}H_+\mathcal{U}^{-1}\right] = \mathcal{U}\exp\left[-t\,H_+\right]\mathcal{U}^{-1}$.

Example : We have discussed the relation between the Ornstein-Uhlenbeck process and the QM oscillator, Exercise 4.7. As a result, in this case

$$\Phi_n^{\rm R}(x) = c_n\, H_n\left(\sqrt{\frac{k}{2D}}\, x\right) \mathrm{e}^{-\frac{k}{2D}x^2} \quad \text{and} \quad \Phi_n^{\rm L}(x) = H_n\left(\sqrt{\frac{k}{2D}}\, x\right) \tag{4.47}$$

where $H_n(x)$ is a Hermite polynomial and $c_n = \frac{1}{2^n n!}\sqrt{\frac{k}{2D}}$ a normalisation [46]. Note that only the right eigenvectors vanish at infinity, while the left eigenvectors grow at infinity, $\Phi_n^{\rm L}(x) \sim x^n$.

f) Case of NESS

In this last paragraph of Section 4.3, let us forget the assumption that the potential is confining and make a remark on the case of diffusions with a NESS. In this case, the spectral analysis is more tricky and the spectrum of eigenvalues is not necessary real : a simple example is discussed in Exercise 4.8 (this exercise is the continuous version of Exercise 2.12).

✍ ***Exercice 4.8 Diffusion for a uniform drift on a ring:*** *The aim is to obtain the propagator $P_t(x|x_0)$ of the diffusion (3.5) for a uniform drift $F(x) = F_0$ on a ring, i.e. on the finite interval $[0, L]$ with periodic boundary conditions.*

a) Discuss the spectrum of the forward generator $\mathscr{G}^\dagger = D\partial_x^2 - F_0\partial_x$: eigenvalues, right and left eigenvectors.

b) Write $P_t(x|x_0)$ by using the spectral information. Analyze the $t \to \infty$ limit (identify a characteristic time τ_D).

*c) In order to analyze the limit $t \ll \tau_D$, get another representation of the conditional probability from the Poisson formula (**??**). Discuss the $L \to \infty$ limit.*

✍ ***Exercice 4.9 FPE on $\mathbb{R}$ for a non confining potential:*** *Consider the FPE $\partial_t P_t(x) = D\partial_x^2 P_t(x) + \partial_x\big[V'(x)P_t(x)\big]$ on $\mathbb{R}$ such that the drift $F(x) = -V'(x)$ drives the particle from $-\infty$ to $+\infty$. This requires that $V(x \to \pm\infty) \to \mp\infty$.*

1/ Give an example of $V(x)$ and discuss the typical trajectories.

2/ Argue that $\mathscr{G}^\dagger P = 0$ has two independent solutions.

3/ Show that the equilibrium solution is not normalisable and find the expression of the second solution (under the form of an integral).

4/ ***Condition for the NESS***
a) If the stationary solution exists, using the expression found above, show that it presents the asymptotic behaviour $P_{\rm st}(x) \simeq J/F(x)$ for $x \to +\infty$.
b) Deduce the condition for existence of the stationary state for the non confining potential.
c) Give an example of non confining drift with allows for a stationary state, and an example which does not.

5/ Compare with the results of Exercise 2.14 page 25.

4.4 Forward and backward FPE

We have solved above the forward FPE [24]

$$\boxed{\partial_t P_t(x|x_0) = \mathscr{G}_x^\dagger P_t(x|x_0)} \tag{4.48}$$

[24] This equation, formally $\partial_t P_t = \mathscr{G}^\dagger P_t = P_t \mathscr{G}$, is called the "*Kolmogorov equation*" by mathematicians.

where the forward generator is a differential operator acting on the *final* coordinate x. The above discussion makes clear that the generator of the diffusion is involved in the *backward FPE* [25]

$$\boxed{\partial_t P_t(x|x_0) = \mathscr{G}_{x_0} P_t(x|x_0)} \tag{4.49}$$

where the operator acts on the *initial* coordinate x_0. We will see some applications of this equation below.

✍ ***Exercice 4.10 BFPE from FFPE:*** *Deduce* (4.49) *from* (4.48) *by using* (4.42).

4.5 Boundary conditions for the FPE

So far we have not discussed the situation where the FPE is solved on a bounded domain. Let us discuss here the question of boundary conditions. For simplicity we consider the FPE $\partial_t P_t(x) = \big[D\partial_x^2 - \partial_x F(x)\big] P_t(x) = -\partial_x J_t(x)$ on $\mathbb{R}^+$ so that there is just one boundary at $x = 0$.

a) Reflecting boundary condition

The first natural boundary condition is the reflecting boundary condition, where the particle coming to $x > 0$ is simply reflected at $x = 0$. This is expressed by the condition of a vanishing current at the origin

$$J_t(0) = F(0)P_t(0) - DP_t'(0) = 0 \tag{4.50}$$

where $'$ means here derivation with respect to x. In the usual terminology, this corresponds to a "mixed boundary condition". [26]

Remark : reflecting boundary conditions for the conditional probability.— For the following we will have to impose the boundary conditions for the conditional probability $P_t(x|x_0)$. The reflecting boundary condition is

$$\big[D\partial_x - F(x)\big] P_t(x|x_0)\big|_{x=0} = 0 \tag{4.51}$$

We could aslo ask about the condition with respect to the initial coordinate : Using the relation (4.42), we have

$$\left(\partial_x - \frac{1}{D}F(x)\right) P_t(x|x_0) = \left(\partial_x + \frac{1}{D}V'(x)\right)\left[\frac{P_{\rm eq}(x)}{P_{\rm eq}(x_0)} P_t(x_0|x)\right] = \frac{P_{\rm eq}(x)}{P_{\rm eq}(x_0)}\partial_x P_t(x_0|x) \tag{4.52}$$

where I used that $P_{\rm eq}(x) \propto \exp[-V(x)/D]$. As a consequence, the presence of the reflecting boundary at $x = 0$ implies

$$\partial_{x_0} P_t(x|x_0)\big|_{x_0=0} = 0\,. \tag{4.53}$$

The reflecting boundary condition is not symmetric for the two coordinates.

---

[25] I have used $\langle \psi \,|\, A\chi \rangle = \langle A^\dagger \psi \,|\, \chi \rangle$; explicitly $\partial_t P_t(x|x_0) = \langle x \,|\mathscr{G}^\dagger \mathrm{e}^{t\mathscr{G}^\dagger}|\, x_0 \rangle = \mathscr{G}_x^\dagger \langle x \,|\mathrm{e}^{t\mathscr{G}^\dagger}|\, x_0 \rangle = \mathscr{G}_{x_0} \langle x \,|\mathrm{e}^{t\mathscr{G}^\dagger}|\, x_0 \rangle$.

[26] For a linear wave equation of second order for the wave $\psi(x)$, like the Schrödinger equation $-\psi''(x) + V(x)\psi(x) = E\psi(x)$, the standard terminology is : (i) Dirichlet boundary condition : $\psi(0) = 0$; (ii) Neumann boundary condition : $\psi'(0) = 0$; (iii) mixed boundary condition : $\psi(0)\cos\theta + \psi'(0)\sin\theta = 0$ (one recovers Dirichlet and Neumann b.c. for $\theta = 0$ and $\theta = \pi/2$, respectively).

b) General boundary condition

Let us now consider a general (mixed) boundary condition

$$\tilde{\lambda} P_t(0) = P_t'(0) \tag{4.54}$$

For $\tilde{\lambda} = F(0)/D$, this corresponds to the reflecting boundary condition. What is the meaning of this condition for arbitrary real $\tilde{\lambda} \neq F(0)/D$?

Consider

$$\partial_t \int_0^\infty \mathrm{d}x\, P_t(x) = -\int_0^\infty \mathrm{d}x\, \partial_x J_t(x) = J_t(0) \tag{4.55}$$

The current of probability through $x = 0$ makes the total probability decreases (for $J_t(0) < 0$). Making use of the boundary condition, we get

$$J_t(0) = \left[F(0) - D\tilde{\lambda}\right] P_t(0) \equiv -\lambda\, P_t(0) \tag{4.56}$$

where we have found convenient to introduce $\lambda = D\tilde{\lambda} - F(0)$. For $\lambda > 0$, the total probability decreases

$$\partial_t \int_0^\infty \mathrm{d}x\, P_t(x) = -\lambda\, P_t(0)\,. \tag{4.57}$$

Hence $\lambda > 0$ has roughly the meaning of the rate of escape, when the particle reaches the boundary at $x = 0$. Then, the particle is absorbed or reflected with finite probabilities when it reaches the boundary.

Figure 22: *A random walker (the mouse) with an absorbing boundary condition at $x = 0$.*

c) Absorbing boundary condition

Writing $P_t(0) = \tilde{\lambda}^{-1} P_t'(0)$ shows that the limit $\tilde{\lambda} \to \infty$, or $\lambda \to \infty$, corresponds to a Dirichlet boundary condition

$$P_t(0) = 0 \tag{4.58}$$

corresponding physically to the situation where the particle reaching the boundary is absorbed with probability one (Fig. 22).

4.6 First passage and exit problem (in 1D)

We now study the recurrence for general diffusions in one-dimension (the restriction to dimension one makes the calculations simple ; the method extends easily to dimensions $d > 1$).

a) Persistence of the free Brownian motion

Here, I come back to the problem studied in § **??** : we study (in Exercise 4.11) the question of the first return of the free Brownian motion. In the previous paragraph, we considered the same question for the discrete random walk ; here we reconsider the problem for a continuous Brownian motion. This is the "*persistence*" problem, as the first return probability at time t corresponds to the probability that the process "persists" to remain positive up to time t.

✍ ***Exercice 4.11 Persistence, first passage time and maximum of the BM :***
1/ Propagator on the half line.– *We consider the free diffusion on* $\mathbb{R}_+$ *with a Dirichlet boundary condition at the origin. Construct the solution of the diffusion equation*

$$\partial_t P_t(x) = D\partial_x^2 P_t(x) \qquad \text{for } x > 0 \text{ with } P_t(0) = 0 \tag{4.59}$$

(use the image method). Apply the method to get the propagator of the diffusion on $\mathbb{R}_+$*, denoted* $P_t^{(\mathrm{Dir})}(x|x_0)$*.*

2/ Survival probability.– *Dirichlet boundary condition describes absorption at* $x = 0$*. Compute the survival probability for a particle starting from* x_0 *:*

$$S_{x_0}(t) = \int_0^\infty \mathrm{d}x\, P_t^{(\mathrm{Dir})}(x|x_0) \tag{4.60}$$

What would have been the result for $P_t^{(\mathrm{Neu})}(x|x_0)$*, the solution for a Neunmann boundary condition,* $\partial_x P_t(x)\big|_{x=0} = 0$ *?*

3/ First passage time.– *We denote by* T_{x_0} *the first time at which the process starting from* $x_0 > 0$ *reaches* $x = 0$ *(it is a random quantity depending on the process), and* $\mathscr{P}_{x_0}(T)$ *its distribution. Deduce*

$$\mathscr{P}_{x_0}(T) = \frac{x_0}{\sqrt{4\pi D}\, T^{3/2}}\, \mathrm{e}^{-\frac{x_0^2}{4DT}}\ . \tag{4.61}$$

Plot neatly the distribution and compare with the result obtained for the RW on the lattice.

4/ Maximum of a BM.– *We now consider another property of the Brownian motion* $x(\tau)$ *with* $\tau \in [0,t]$ *starting from* $x_0 = 0$ *: we denote by* $M = \underset{\tau\in[0,t]}{\mathrm{Max}}\,(x(\tau)) \geqslant 0$ *its maximum and* $W_t(m)$ *the distribution of* M*. Show that* $W_t(m)$ *and* $S_{x_0}(t)$ *are related and deduce the expression of* $W_t(m)$*. What does* $W_t(0)$ *represent ? The exponent of the power law* $t^{-\theta}$ *is called the persistence exponent. Give* θ *for the Brownian motion.*

Hint : use Appendix **??** *with properties of the error function.*

Remark : we have recovered the results obtained within the discrete model of random walk (§ **??**) : the probability to return to the starting point is $P_t(0|0) \sim t^{-1/2}$ and the probability for the *first* return is $\mathscr{P}_{x_0}(t) \sim t^{-3/2}$ at large time.

Conclusion : Two important points :

- in order to study the first passage time at the origin, one should impose an absorbing boundary condition at $x = 0$.
- The definition of the survival probability suggests that one should first find the conditional probability, then integrate it to get the survival probability. In fact, the backward FPE provides a shortcut and allows to find an equation directly for the survival probability, as we will see.

b) First passage time for arbitrary drift

We consider the case of a diffusion with drift and uniform diffusion constant for simplicity

$$\mathrm{d}x(t) = F(x)\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}W(t) \tag{4.62}$$

The drift derives from a potential $F(x) = -V'(x)$ and $W(t)$ is the Wiener process. Consider that the diffusion starts from the initial condition $x(0) = x_0$.

The determination of the propagator $P_t(b|x_0)$ allows to answer the question : what is the probability that the process reaches the point $x = b$ in a (fixed) time t (i.e. the final position is the random variable). We now ask a dual question : **what is the time T_{x_0} needed to reach the point $x = b$ for the first time ?** $x(0) = x_0$ and $x(T_{x_0}) = b$ with $x(t) < b$ for $0 < t < T_{x_0}$. Hence we now fix the final position ($x = b$) and study the statistical properties of the random time T_{x_0}. We denote by $\mathscr{P}_{x_0}(T)$ its distribution.

The main idea is to introduce an **absorbing boundary** at $x = b$:

$$P_t(b|x_0) = P_t(x|b) = 0 \tag{4.63}$$

implying that the particle is absorbed when it reaches $x = b$. For simplicity for future calculations and analysis, we impose a *reflecting boundary condition* at another point $x = a$, i.e. we impose that the current vanishes

$$(F(x) - D\partial_x)\, P_t(x|x_0)\big|_{x=a} = \partial_{x_0} P_t(x|x_0)\big|_{x_0=a} = 0 \tag{4.64}$$

The boundary condition takes a different form with respect to the two arguments (this is expecetd as $P_t(x|x_0)$ is not a symmetric function of its two arguments in general, cf. § 4.5 page 58).

We introduce the survival probability

$$S_{x_0}(t) = \int_a^b \mathrm{d}x\, P_t(x|x_0)\,, \tag{4.65}$$

the probabilty that the particle has survived up to time t, i.e. has not reached the absorbing boundary at $x = b$. Due to the absorbing boundary, $S_{x_0}(t) \leqslant 1$. The survival probability is the probability for the particle to be absorbed after time t

$$S_{x_0}(t) = \mathrm{Proba}\{T_{x_0} \geqslant t\} = \int_t^\infty \mathrm{d}T\, \mathscr{P}_{x_0}(T)\,. \tag{4.66}$$

Then $\mathscr{P}_{x_0}(T) = -\partial_T S_{x_0}(T)$. Because we integrate over the final position x involved in the propagator, we see that it is interesting to make use of the *backward* FPE (4.49) :

$$\partial_t S_{x_0}(t) = \int_a^b \mathrm{d}x\, \mathscr{G}_{x_0} P_t(x|x_0) = \mathscr{G}_{x_0} S_{x_0}(t) \tag{4.67}$$

for the initial condition

$$S_{x_0}(0) = \begin{cases} 1 & \text{for } x_0 \in [a, b[\\ 0 & \text{for } x_0 \geqslant b \end{cases}\,. \tag{4.68}$$

Similarly the first passage time distribution obeys

$$\partial_t \mathscr{P}_{x_0}(t) = \mathscr{G}_{x_0} \mathscr{P}_{x_0}(t) \tag{4.69}$$

At this point it is useful to introduce the n-th moment of the time :

$$T_n(x_0) \overset{\text{def}}{=} \left\langle \left(T_{x_0}\right)^n \right\rangle = \int_0^\infty \mathrm{d}T\, T^n\, \mathscr{P}_{x_0}(T) \tag{4.70}$$

✍ ***Exercice 4.12 Moments of the first passage time :***
a) Show that the moments obey the recurrence

$$\mathscr{G}_{x_0}\, T_n(x_0) = -n\, T_{n-1}(x_0) \quad \text{and} \quad \mathscr{G}_{x_0}\, T_1(x_0) = -1\,. \tag{4.71}$$

b) Justify that the boundary conditions are $\partial_{x_0} T_n(x_0)\big|_{x_0=a} = 0$ and $T_n(b) = 0$.

c) Deduce (calculation requires to solve a first order linear differential equation: easy!)

$$\boxed{T_n(x_0) = \frac{n}{D}\int_{x_0}^{b} \mathrm{d}x\, \mathrm{e}^{V(x)/D} \int_a^x \mathrm{d}x'\, \mathrm{e}^{-V(x')/D}\, T_{n-1}(x')} \tag{4.72}$$

(with obviously $T_0(x_0) = 1$).

✍ ***Exercice 4.13 Trapping by a constant drift :*** *We consider the trapping by a constant drift $F(x) = -\mu$. The particle starts from $x_0 \in [0, b[$ with a reflection boundary at $x = 0$. The boundary at b is absorbing.*
a) Compute the mean first passage time $T_1(x_0)$.
b) Discuss the result : consider limiting cases (i) $\mu b/D \ll 1$, (ii) $\mu b/D \gg 1$ for $\mu > 0$, (iii) $|\mu| b/D \gg 1$ for $\mu < 0$.

✍ ***Exercice 4.14 First passage time for $D(x)$:*** *Generalize (4.72) for a x-dependent diffusion constant $D \to D(x)$.*

c) Arrhenius law

An important application of the above formalism is the analysis of the escape time for a particle trapped in a potential well. This problem is relevant in chemistry where chemical reactions are activated by overcoming some potential (activation) barriers in the configuration space of the molecules. For simplicity we consider a one-dimensional problem of a particle initially in a potential well (Fig. 23) : x_0 is close to the local minimum at x_1. We study the time needed to escape the well, i.e. jump in the region $x > x_2$.

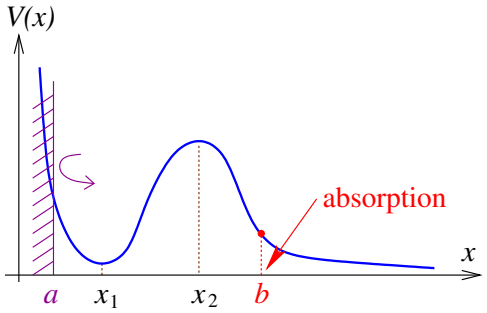


Figure 23: *A particle escapes from a metastable state.*

In a rather arbitrary manner, we introduce a reflecting boundary at $x = a$ at the left of the local minimum, and the absorbing boundary at $x = b$ at the right of the potential barrier (not too close from the top). As we have seen above the average time is given by

$$T_1(x_0) = \frac{1}{D}\int_{x_0}^{b} \mathrm{d}x\, \mathrm{e}^{V(x)/D} \int_a^x \mathrm{d}x'\, \mathrm{e}^{-V(x')/D}\,. \tag{4.73}$$

The integral can be analysed by using the steepest descent method. For $D \to 0$, the integral over x is dominated by the neighbourhood of $x = x_2$, hence we can replace the upper bound of the second integral $\int_a^x \to \int_a^{x_2}$, expand the potential in the exponential $\mathrm{e}^{V(x)/D} \simeq \exp\left\{\frac{1}{D}[V(x_2) - \frac{1}{\delta_2^2}(x-x_2)^2]\right\}$, where $\delta_2 = 1/\sqrt{-V''(x_2)}$, and perform the remaining Gaussian integral. Similarly, the integral over x' is dominated by the neighbourhood of $x' = x_1$; expanding similarly the integrand as $\mathrm{e}^{-V(x')/D} \simeq \exp\left\{\frac{1}{D}[-V(x_1) - \frac{1}{\delta_1^2}(x'-x_1)^2]\right\}$, where $\delta_1 = 1/\sqrt{V''(x_1)}$, we end with

$$\boxed{\langle T_{x_0}\rangle \equiv T_1(x_0) \simeq 2\pi\, \delta_1\, \delta_2\, \exp\frac{V(x_2) - V(x_1)}{D}} \tag{4.74}$$

The main result is that the average time is exponentially large in the height of the potential barrier $\Delta V = V(x_2) - V(x_1)$. It is pretty independent of x_0 (provided that it remains in the well) : for x_0 in the well, the particle is rapidly driven at the bottom of the well, where it is submitted to the fluctuations (the time scale is controlled by the curvature at x_1, like for the Ornstein-Uhlenbeck process) ; then it takes a long time to escape the well, thanks to large (and thus rare) thermal fluctuation.

Figure 24: *The swedish chemist Svante August Arrhenius (1859-1927), Nobel prize in chemistry in 1903.*

✍ ***Exercice 4.15 :*** *How far from the top of the barrier (at x_2) must be the absorbing boundary b so that the previous analysis is justified ? And how far the reflecting boundary at a should be from the bottom of the well (at x_1) ?*

✍ ***Exercice 4.16 Time needed to fall at the bottom of a harmonic well:*** *We discuss the situation where the initial point x_0 is far from the minimum of the well at $x = x_1$ and clarify a point of the previous discussion. We consider the Ornstein-Uhlenbeck process $\frac{\mathrm{d}}{\mathrm{d}t}x(t) = -\lambda\,(x - x_1) + \sqrt{2D}\,\eta(t)$. What is the typical time needed by a particle initially far from the minimum, $x(0) - x_1 = \Delta$ "large", to fall in the potential well ? Compare to the Arrhenius time.*

We can also analyze higher moments : applying the same arguments to (4.72) we get

$$T_n(x_0) \simeq n\, T_{n-1}(x_1)\, T_1(x_0) \tag{4.75}$$

for $D \to 0$. Using the independence in the initial position, we conclude that the moments are

$$T_n(x_0) \simeq n!\, [T_1(x_0)]^n \tag{4.76}$$

i.e. those of a Poisson distribution.

$$\boxed{\mathscr{P}_{x_0}(T) \simeq \frac{1}{\langle T_{x_0}\rangle} \exp -\frac{T}{\langle T_{x_0}\rangle}} \tag{4.77}$$

The exponential distribution was expected as in the $D \to 0$ limit, the particle is trapped a long time in the well, hence has time to decorrelate : the picture is that, starting from the initial position x_0, the particle falls after a short time in the vicinity of the minimum of the potential well $x(t) \sim x_1$. There, fluctuations are $\delta x \sim \sqrt{D}/\delta_1$. As long as the process remains in the well, it is approximatively described by the Langevin equation $\frac{\mathrm{d}}{\mathrm{d}t}x(t) \approx -\frac{1}{\delta_1^2}(x - x_1) + \sqrt{2D}\,\eta(t)$, where we have linearized $F(x) = -V'(x)$ near x_1. The correlation function is $\langle x(t)x(t')\rangle_c \simeq (D/\delta_1^2)\, \exp\big[-|t-t'|/\delta_1^2\big]$ (cf. chapter 1 on Langevin equation). Indeed, the decorrelation time is $\sim \delta_1^2$, which is exponentially smaller than the typical time to escape the well. This shows that the escape process can be approximatively considered Markovian, hence the exponential distribution (4.77).

Remark: this discussion is inspired by the book of Gardiner [12] and by the appendix of my paper [44], where an application for the statistics of energy levels in a quantum (Anderson) localisation [27] problem is discussed.

✍ ***Exercice 4.17 Lifetimes of metastable states :*** *We have obtained above the following formula for the average lifetime of a metastabel state corresponding to the well of Fig. 23 :* $\langle T_{x_0}\rangle \simeq \frac{2\pi}{\sqrt{-V''(x_1)V''(x_2)}}\,\exp\left\{\frac{V(x_2)-V(x_1)}{D}\right\}$, *valid in the* $D\to 0$ *limit.*
Derive some analogous formulae for the two potentials of Fig. 25.

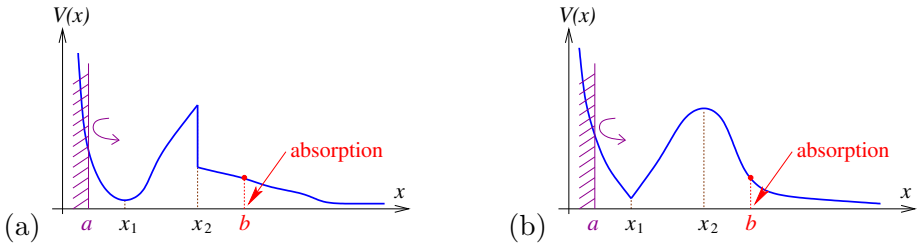


Figure 25: *Two other types of trapping potentials.*

✍ ***Exercice 4.18 Escape from the two boundaries :*** *We now consider the problem where a particle starts at* $x(0)=x_0\in]a,b[$ *and can escape the interval at one of the two boundaries. In this case one must solve the differential equation (4.71), i.e.*

$$\mathscr{G}_{x_0}T_n(x_0) = -n\,T_{n-1}(x_0) \qquad \text{i.e.} \quad \left(D\frac{\mathrm{d}}{\mathrm{d}x_0} - V'(x_0)\right)\frac{\mathrm{d}T_n(x_0)}{\mathrm{d}x_0} = -n\,T_{n-1}(x_0) \tag{4.78}$$

for two Dirichlet boundary conditions $T_n(a)=T_n(b)=0$. *For simplicity, we consider only the first moment.*

1/ *Denoting by* $\psi(x)=\exp[-V(x)/D]$ *(this is the equilibrium distribution, if normalisable), study the action of the generator* $\mathscr{G}_x$ *on*

$$\Phi(x) = \int_a^x \frac{\mathrm{d}y}{\psi(y)}\int_x^b \frac{\mathrm{d}x'}{\psi(x')}\int_a^{x'}\mathrm{d}z\,\psi(z) - \int_x^b \frac{\mathrm{d}y}{\psi(y)}\int_a^x \frac{\mathrm{d}x'}{\psi(x')}\int_a^{x'}\mathrm{d}z\,\psi(z) \tag{4.79}$$

2/ *Deduce* $T_1(x_0)$.

3/ *Study the limit* $D\to 0$ *for the potential of Fig. 26, when the initial condition is in the well. Introduce* $1/\delta_0^2 = V''(x_0)$ *and* $1/\delta_{1,2}^2 = -V''(x_{1,2})$. *Distinguish the general case* $V(x_1)\neq V(x_2)$ *and the case* $V(x_1)=V(x_2)$.

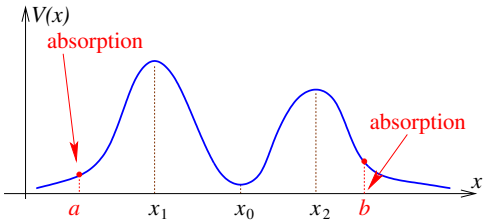


Figure 26: *Two absorbing boundaries.*

[27] Anderson localisation is the problem of localisation of a wave in a (static) random medium.

✍ ***Exercice 4.19 First passage time in dimension*** d ***:*** *We consider the problem of first passage time in dimension $d > 1$: a diffusive particle submitted to a centro-symmetric drift $\vec{F}(\vec{r}) = -V'(r)\,\vec{u}_r$ where $\vec{u}_r$ is the radial unit vector. The forward generator of the diffusion in $\mathbb{R}^d$ is $\mathscr{G}^\dagger = D\Delta - \vec{\nabla}\cdot\vec{F}$. The particle starts from $\vec{r}_0$ and we ask the question : when does it reachs a sphere of radius $b < r_0 = ||\vec{r}_0||$ for the first time ?*

a) Show that the moments of the first passage time obey the differential equation

$$\left[D\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{d-1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right) - V'(r)\frac{\mathrm{d}}{\mathrm{d}r}\right] T_n(r) = -n\,T_{n-1}(r) \tag{4.80}$$

Find an integral representation for $T_1(r_0)$.

b) When the dimension is increased, does the first passage time increases or decreases ?

☺ Important points

- Have in mind the meaning of the two terms in the FPE (drift and diffusion).
- Conservation equation $\partial_t P = -\partial_x J$ and expression of the current.
- You should have in mind the solution of the FPE in the free case, $\partial_t P = D\Delta\, P$ (in dimension d), or be able to recover it in two lines by Fourier tranform in space :
$P_t(\vec{r}|\vec{r}_0) = (4\pi D t)^{-d/2}\,\exp\big\{-(\vec{r}-\vec{r}_0)^2/(4Dt)\big\}$
- Existence of the BFPE
- Be familiar with the different types of boundary conditions (reflecting, absorbing)
- The problem of first passage time (relation between survival probability and the distribution of the first passage time) ; the use of the BFPE.
- Study of the first passage through point $x = b$ requires to consider an absorbing boundary at this place.
- The Arrhenius law.

5 Linear response theory

Previously, we have been mostly interested to present some tools allowing to analyze the properties of stochastic processes, i.e. to follow a more *phenomenological* approach (with the exception of § f)). In this last paragraph of this first part of the lectures, we are going to follow a more microscopic approach : we will however restrict ourselves to the study of **small disturbances on the top of equilibrium**, i.e. to the "linear regime". Our purpose is to describe the situation represented schematicall in Fig. 27.

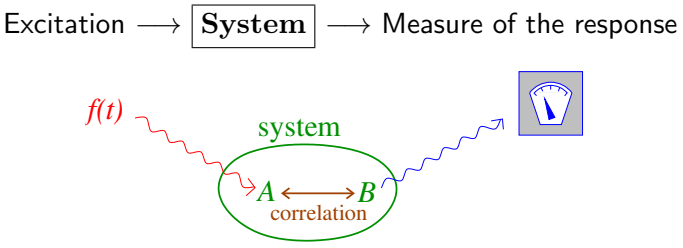


Figure 27: *Schematical representation of the situation under consideration : an excitation (external perturbation) acts on the system. A force $f(t)$ is coupled to an observable A of the system and another observable B is measured. The two observables are in general coupled by the time dynamics.*

A practical motivation could be to describe a bit more precisely the process of the measurement of an equilibrium property : the standard scheme to perform a measurement on a system at equilibrium consist in the introduction of a "small" perturbation (excitation) and the measurement of the response of the system (ex: an atomic vapor on which light is sent and which re-emit light by fluoresence).

First (§ 5.2), we start with a semi-phenomenological description based on thermdynamic properties (§ 5.1). In a second step (§ 5.3 to 5.5), we will develope the linear response theory.

5.1 Theory of thermodynamic fluctuations

This § was not discussed in the lectures due to lack of time.

Before entering into the (microscopic) approach of the linear response theory, it is useful to start with the more phenomenological approach of the thermodynamics of irreversible processes. We first start with the theory of thermodynamic fluctuations, which was developed by Einstein in 1910, among others [37]. In equilibrium thermodynamics, a fundamental function encoding all thermodynamic properties of a system is the entropy, which is an extensive function of a set of extensive variables (energy, number of particles, etc) characterizing the thermal state of the system :

$$S(\{X_i\}) \tag{5.1}$$

If the system is isolated, these extensive variables are fixed, however, if one considers extensive quantities characterizing a subpart of the system, there exist exchanges among different subparts : e.g. exchanges of energies, while the total energy of the isolated system is kept constant.

Conjugate thermodynamic forces : To each extensive variable X_i, we can associate an intensive conjugate force :

$$F_i = -\frac{\partial S}{\partial X_i} \tag{5.2}$$

Examples :

Obervable X_i	force F_i
Energy E	$-1/T$
Volume V	$-p/T$
Number N_a	μ_a/T

In particular, for a simple fluid made of a mixture of s species we have

$$\mathrm{d}S(E,V,\{N_a\}) = \frac{1}{T}\,\mathrm{d}E + \frac{p}{T}\,\mathrm{d}V - \sum_{a=1}^{s}\frac{\mu_a}{T}\,\mathrm{d}N_a \tag{5.3}$$

Note that extensivity $S(\{\lambda X_i\}) = \lambda\, S(\{X_i\})$ implies

$$S(\{X_i\}) = -\sum_j X_j\, F_j(\{X_i\}) \tag{5.4}$$

a) Preliminary – the thermal contact :

As a preliminary, let us recall the analysis of the thermal contact between two subparts of an isolated system [48]. Denote by $S(E)$ the entropy of the part of interest and $S_{\rm ext}(E_{\rm tot}-E)$ the entropy of the remaining of the system. $S_{\rm tot}(E) = S(E) + S_{\rm ext}(E_{\rm tot}-E)$ is the entropy of the isolated system for a fixed value E (here $S_{\rm tot}(E)$ is the reduced entropy). The fundamental postulate of statistical physics provide the distribution of the energy E as

$$w(E) \propto {\rm e}^{S_{\rm tot}(E)} \tag{5.5}$$

(for clarity I set $k_{\rm B}=1$). We introduce the "affinity"

$$\phi(E) \stackrel{\rm def}{=} -\frac{\partial S_{\rm tot}(E)}{\partial E} = -\frac{1}{T(E)} + \frac{1}{T_{\rm ext}(E_{\rm tot}-E)} \tag{5.6}$$

which is the difference of the two "forces", involving here the microcanonical temperatures T and $T_{\rm ext}$ are characterizing the two sub-systems. The equation giving the maximum of the distribution correspond to the vanishing of the affinity

$$\phi(E) = 0 \qquad \Rightarrow E = \overline{E} \tag{5.7}$$

and is also interpreted as the condition for thermal equilibrium $T = T_{\rm ext}$.

Consider a thermal fluctuation

$$\delta E = E - \overline{E} \tag{5.8}$$

then we can linearize the affinity $\phi(\overline{E}+\delta E) \simeq \kappa\, \delta E$ hence the probability of a fluctuation is

$$w \propto {\rm e}^{\delta S_{\rm tot}} \qquad \text{with } \delta S_{\rm tot} \simeq -\frac{1}{2}\kappa\, \delta E^2 \tag{5.9}$$

Here the coefficient κ has a clear interpretation

$$\kappa = \phi'(\overline{E}) = \frac{1}{T(\overline{E})^2}\left(\frac{1}{C_V(\overline{E})} + \frac{1}{C_V^{\rm ext}(E_{\rm tot}-\overline{E})}\right) \simeq \frac{1}{T(\overline{E})^2 C_V(\overline{E})} \tag{5.10}$$

where the second term can be necglected if the subsystem is much smaller than the external part. With this assumption, we can write the probability in terms of a function characterizing the subsytem alone

$$w \propto {\rm e}^{-\beta \mathcal{F}} \qquad \text{with } \mathcal{F} = E - TS(E) \tag{5.11}$$

where T is here the temperature of the external and $\mathcal{F}$ the free energy of the subpart of interest.

Since there is a bijection between the energy and the temperature, $\delta E \simeq C_V\, \delta T$, we can as well express the fluctuation of energy in terms of the temperature

$$w \propto {\rm e}^{\delta S_{\rm tot}} \qquad \text{with } \delta S_{\rm tot} \simeq -\frac{1}{2\kappa}\delta T^2 = -\frac{C_V}{2T^2}\delta T^2 \tag{5.12}$$

thus the temperature fluctuations are

$$\left\langle \delta T^2 \right\rangle = \frac{k_{\rm B}}{C_V}\, T^2 \tag{5.13}$$

where I have reintroduced the Boltzmann constant. I recall that C_V is here the heat capacity of the subpart in which the temperature fluctuations take place.

b) Affinities :

We now generalize these ideas to a set of extensive observables X_i. We consider a spontaneous thermal fluctuation

$$x_i = X_i - \overline{X_i} \tag{5.14}$$

and introduce the affinities corresponding to these observables

$$\phi_i \stackrel{\text{def}}{=} -\frac{\partial S_{\text{tot}}}{\partial X_i} = F_i - F_i^{\text{ext}} \tag{5.15}$$

Equilibrium state is characterised by the vanishing of all affinities $\phi_i = 0$.

In general we can write the entropy variation around its maximum (corresponding to the equilibrium state) as

$$\delta S_{\text{tot}} \simeq -\frac{1}{2}\sum_{i,j} \kappa_{ij} x_i x_j \tag{5.16}$$

where the coefficients κ_{ij} are encoded in the entropy function, the fundamental function characterizing the thermodynamic properties of the system, which is assumed known. Hence thermodynamic fluctuations are characterised by the Gaussian measure

$$w \propto \mathrm{e}^{\delta S_{\text{tot}}} = \mathrm{e}^{-\frac{1}{2}\sum_{i,j}\kappa_{ij}x_i x_j} \tag{5.17}$$

The affinities take the form

$$\phi_i = \sum_j \kappa_{ij} x_j \tag{5.18}$$

As a result of general properties of the Gaussian measure we have

$$\langle x_i x_j \rangle = (\kappa^{-1})_{ij} \tag{5.19}$$

(see appendix below). Using the linear relation between affinities and thermal fluctuations of observables, we get the correlator

$$\langle x_i \phi_j \rangle = \delta_{ij} \tag{5.20}$$

and

$$\langle \phi_i \phi_j \rangle = \kappa_{ij} \, . \tag{5.21}$$

Simple consequence : Eq. (5.20) shows that variables thermodynamically conjugated are uncorrelated. For example $\langle \delta T \delta V \rangle = 0$.

It is also interesting to split the variation of entropy in two parts

$$\delta S_{\text{tot}} = \delta S + \delta S_{\text{exch}} = \delta S + \sum_i F_i^{\text{ext}} \, \delta X_i \tag{5.22}$$

where the second term is the entropy exchanged between the system and the external. Note that in [37], the variation of entropy δS_{tot} is denoted δS_{int} as it is the entropy variation relative to the changes internal to the system (energy fluctuation of the system, etc).

Application : For example, if we consider the entropy as a function of the energy and the volume, $S(E,V)$, this gives the form

$$w \propto \exp -\frac{\delta E - T\delta S + p\delta V}{T} = \mathrm{e}^{-\beta\delta\mathcal{G}} \,, \tag{5.23}$$

where $\mathcal{G}$ is the free enthalpy. Expansion leads to

$$w \propto \exp\left\{-\frac{C_V \delta T^2}{2T^2} - \frac{\delta V^2}{2TV\kappa_T}\right\} \tag{5.24}$$

where $\kappa_T \overset{\text{def}}{=} -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T$ is the isothermal compressibility, which controls the volume fluctuations $\langle \delta V^2 \rangle = TV\kappa_T$.

Appendix : Gaussian integrals in $\mathbb{R}^N$ and Wick theorem

Consider the integral

$$\mathcal{N}^{-1} = \int_{\mathbb{R}^N} \mathrm{d}^N X \, \mathrm{e}^{-\frac{1}{2}X^{\mathrm{T}}AX} \tag{5.25}$$

where A is a real symmetric matrix. One can perform a rotation $X = \mathcal{O}Y$ which diagonalizes the matrix, $A = \mathcal{O}D\mathcal{O}^{\mathrm{T}}$ with $D = \mathrm{diag}(\lambda_1, \cdots, \lambda_N)$. Jacobian of the transformation equals unity $J = |\mathrm{D}X/\mathrm{D}Y| = |\det(\mathcal{O})| = 1$. This makes clear that the integral exists if the matrix is positive $A > 0$ (meaning $\lambda_i > 0 \; \forall \, i$). After diagonalization, the integral is separable, thus $\mathcal{N}^{-1} = \prod_i \sqrt{2\pi/\lambda_i} = (2\pi)^{N/2}/\sqrt{\det A}$.

Introduce the vector $B \in \mathbb{R}^N$ and the function

$$G(B) = \mathcal{N} \int_{\mathbb{R}^N} \mathrm{d}^N X \, \mathrm{e}^{-\frac{1}{2}X^{\mathrm{T}}AX + B^{\mathrm{T}}X} = \langle \mathrm{e}^{B^{\mathrm{T}}X} \rangle \tag{5.26}$$

which is interpreted as the generating function of the Gaussian variables X_i as derivations produce the correlation functions $\partial_{i_1} \cdots \partial_{i_m} G(B)|_{B=0} = \langle X_{i_1} \cdots X_{i_m} \rangle$. A simple manipulation is

$$X^{\mathrm{T}}AX - 2B^{\mathrm{T}}X = (X - A^{-1}B)^{\mathrm{T}} A (X - A^{-1}B) - B^{\mathrm{T}}A^{-1}B \tag{5.27}$$

leading to

$$G(B) = \mathrm{e}^{\frac{1}{2}B^{\mathrm{T}}A^{-1}B} \tag{5.28}$$

In particular we deduce the relation for the two point correlations $\langle X_i X_j \rangle = \frac{\partial^2 G(B)}{\partial B_i \partial B_j}\big|_{B=0}$:

$$\boxed{\langle X_i X_j \rangle = (A^{-1})_{ij}} \tag{5.29}$$

We conclude that the correlations of the Gaussian variable is already almost readable on the Gaussian measure itself $P(X) \propto \exp\{-\frac{1}{2}X^{\mathrm{T}}AX\}$. This is a very general and important result.

We can deduce the **Wick theorem**

$$\langle X_1 \cdots X_{2n} \rangle = \sum_{\text{contractions}} \langle X_{i_1} X_{j_1} \rangle \cdots \langle X_{i_n} X_{j_n} \rangle \tag{5.30}$$

where the sum runs over the $(2n-1)!!$ pair contractions. Example : for $2n = 4$, one needs to consider the $(4-1)!! = 3$ contractions

$$\langle X_1 X_2 X_3 X_4 \rangle = \langle X_1 X_2 \rangle \langle X_3 X_4 \rangle + \langle X_1 X_3 \rangle \langle X_2 X_4 \rangle + \langle X_1 X_4 \rangle \langle X_2 X_3 \rangle \tag{5.31}$$

The Wick theorem has many occurences and applications : in probability, in statistical physics, in statistical or quantum field theory.

5.2 Thermodynamics of irreversible processes

This § was not discussed in the lectures due to lack of time.

We now discuss the dynamics of observables when the system is driven slightly out-of-equilibrium (for example when inducing a current through a conductor by imposing a voltage drop). The main assumption is that the time scale which characterizes the dynamics is much longer than the time scale for relaxation towards equilibrium

$$\tau_{\rm dyn} \gg \tau_{\rm relax} \tag{5.32}$$

which ensures that the system follows equilibrium states described by equilibrium thermodynamic (in particular by the fundamental entropy function).

a) Fluxes

We introduce the flux related to the extensive variable X_i

$$J_i = \frac{{\rm d}X_i}{{\rm d}t} \, . \tag{5.33}$$

Denoting by $x_i(t) = X_i(t) - \overline{X_i}$ the deviation from equilibrium, we have also $J_i = \frac{{\rm d}x_i}{{\rm d}t}$. It is important to stress that although I use the same notation as the one used above for spontaneous thermal fluctuations, $x_i(t)$ designates here the change of the observable as a result of imposing a non zero affinity. The use of the same notation follows "**Onsager's regression hypothesis**" (1930), *assuming that the relaxation of non equilibrium disturbance is governed by the same laws as the regression of spontaneous microscopic fluctuations* [6].

If the system remains close to the equilibrium, it is natural to *assume* that the fluxes are linear in the deviations to equilibrium, i.e.

$$\frac{{\rm d}x_i}{{\rm d}t} = -\sum_j \lambda_{ij} x_j \, . \tag{5.34}$$

It is important to keep in mind that at this level, contrary to coefficients κ_{ij} introduced above, which are encoded in the entropy function and can be deduced in terms of (equilibrium) thermodynamic properties, as it was illustrated above, the new phenomenological coefficients λ_{ij} characterize the dynamic and require further information. Using the linear relation with the affinities, it is conventional to write

$$J_i = \frac{{\rm d}x_i}{{\rm d}t} = \sum_j \gamma_{ij} \phi_j \tag{5.35}$$

where γ_{ij} are the so-called "*kinetic coefficients*". The main object of the theory of irreversible processes is to find the relation between affinities and fluxes (this is similar to finding the relation between the voltage drop imposed by the external and the induced current, i.e. a formula for the conductance in terms of the microscopic parameter and the geometry of the conductor). At this stage, the description remains phenomenological. The sets of coefficients are clearly related by

$$\gamma_{ij} = -\sum_k \lambda_{ik} \, (\kappa^{-1})_{kj} \tag{5.36}$$

Figure 28: *Lars Onsager (1903-1976), Nobel prize in chemistry 1968.*

Example : the discussion is a bit formal. Let us give a concrete example : consider a conductor with charge Q (the "observable" X). The electrostatic energy is $H = QV$ so that the potential V is the "conjugated force ϕ"). The "flux J" is the electric current $I = \frac{\mathrm{d}Q}{\mathrm{d}t}$ and thus the kinetic coefficient is simply the conductance (inverse of resistance)

$$\gamma \longrightarrow G \tag{5.37}$$

as we usually writes $I = GV$).

b) Onsager symmetry relation

We now state the Onsager principle (1931) of the symmetry of kinetic coefficients

$$\boxed{\gamma_{ij} = \gamma_{ji}} \tag{5.38}$$

which relies on the time reversal symmetry, at equilibrium, as we now show.

Proof : We introduce the correlation function

$$C_{ij}(t) = \langle x_i(t) x_j(0) \rangle \tag{5.39}$$

Assuming *time reversal symmetry* we have

$$\langle x_i(t) x_j(0) \rangle = \langle x_i(0) x_j(-t) \rangle \overset{\text{TRS}}{=} \langle x_i(0) x_j(t) \rangle \qquad \Rightarrow \qquad C_{ij}(t) = C_{ji}(t)\,. \tag{5.40}$$

Now we differentiate the relation

$$\langle \frac{\mathrm{d}x_i(t)}{\mathrm{d}t} x_j(0) \rangle = \langle \frac{\mathrm{d}x_j(t)}{\mathrm{d}t} x_i(0) \rangle \tag{5.41}$$

and we use Onsager's regression hypothesis, which allows to make use of the kinetic coefficients

$$\sum_k \gamma_{ik} \langle \phi_k(t) x_j(0) \rangle = \sum_k \gamma_{jk} \langle \phi_k(t) x_i(0) \rangle \tag{5.42}$$

Because the relation holds $\forall\, t$ we can write

$$\sum_k \gamma_{ik} \underbrace{\langle \phi_k(0) x_j(0) \rangle}_{=\delta_{jk}} = \sum_k \gamma_{jk} \underbrace{\langle \phi_k(0) x_i(0) \rangle}_{=\delta_{ik}} \tag{5.43}$$

leading to (5.38).

Remarks :

- A standard illustration is the symmetry between transport of particles and transport of energy. Transport of particles can be induced by a modulation of the electrochemical potential $\bar{\mu} = \mu + V(\vec{r})$, where $V(\vec{r})$ is the potential (in the presence of an external potential, the "force" conjuguated to the local density is $\bar{\mu}$). Transport of energy can be induced by an imbalance of temperature (Fick's law). The local version gives the current of particles and the current of energy

$$\vec{J}_N = \gamma_{NN}\,\vec{\nabla}\left(\frac{\bar{\mu}}{T}\right) + \gamma_{NE}\,\vec{\nabla}\left(-\frac{1}{T}\right) \tag{5.44}$$

$$\vec{J}_E = \gamma_{EN}\,\vec{\nabla}\left(\frac{\bar{\mu}}{T}\right) + \gamma_{EE}\,\vec{\nabla}\left(-\frac{1}{T}\right) \tag{5.45}$$

  The coefficient γ_{NN} is proportional to the diffusion constant (or the conductivity for charged particles) and the coefficient γ_{EE} to the thermal conductivity. The Onsager symmetry relation is $\gamma_{NE} = \gamma_{EN}$. Its existence is related to the duality of two effects : the Seebeck and the Peltier effects [37, 24].
- The Onsager symmetry relations (5.38) was given here for observables invariant under time reversal symmetry. In general the observables can have a specific symmetry under TRS :

$$x_i(-t) = \epsilon_i\, x_i(t) \qquad \text{with } \epsilon_i = \pm 1\,. \tag{5.46}$$

  In the more general case, the Onsager symmetry relations take the form

$$\gamma_{ij}(\vec{B}, \vec{\Omega}) = \epsilon_i \epsilon_j\, \gamma_{ji}(-\vec{B}, -\vec{\Omega}) \tag{5.47}$$

  where $\vec{B}$ is the magnetic field and $\vec{\Omega}$ the angular velocity of rotation.
- **Equilibrium *versus* out-of-equilibrium.**— We will make clear below that, although they characterize how the system responds when put slightly out-of-equilibrium, the kinetic coefficients are properties of the *equilibrium* state. Thermal equilibrium is a crucial assumption for the Onsager symmetry relations to hold. In the out-of-equilibrium situation, Onsager symmetry can be broken.
- **Linear response *versus* non linear response.**— Another formulation of the previous remark : the fluxes are non zero because finite affinities are imposed from the external, hence the fluxes are functions of the affinities : $J_i(\{\phi_j\})$. We have written above the fluxes as $J_i(\{\phi_j\}) = \sum_j \gamma_{ij}\,\phi_j$. Assuming that the response is linear is equivalent to say that the kinetic coefficients are properties of the system for $\phi_i = 0\,\forall\, i$, $\gamma_{ij} = \mathcal{O}(\phi_k^0)$, i.e. that they are properties of the system *at equilibrium* (this is the essence of Onsager's regression hypothesis). Onsager symmetry relation holds for the linear response, however it has no reason to hold for the non-linear response, i.e. far from equilibrium.

  An example was discussed in [40, 43] (and further in [47]) : whereas it is well known that the linear conductance of a conductor with two contacts is a symmetric function of the magnetic field, the interaction between electrons was shown to induce an asymmetry of the nonlinear response under magnetic field reversal. This was observed experimentally in [51, 2].

c) Entropy production

The entropy production corresponds to dissipation

$$\frac{\mathrm{d}S_{\mathrm{tot}}}{\mathrm{d}t} = \sum_i \frac{\partial S_{\mathrm{tot}}}{\partial X_i}\,\frac{\mathrm{d}X_i}{\mathrm{d}t} = \sum_i \phi_i\, J_i \tag{5.48}$$

Hence the entropy production is a quadratic form

$$\frac{\mathrm{d}S_{\mathrm{tot}}}{\mathrm{d}t} = \sum_{ij} \gamma_{ij}\, \phi_i \phi_j \tag{5.49}$$

As a consequence of the 2nd "principle" of thermodynamic (demonstrated within the frame of statistical physics), $\mathrm{d}S_{\mathrm{tot}}/\mathrm{d}t \geqslant 0$, we have

$$\gamma_{ii} \geqslant 0 \tag{5.50}$$

and $\gamma_{ii}\gamma_{jj} \geqslant \frac{1}{4}(\gamma_{ij} + \gamma_{ji})^2$. More generally γ_{ij} is a positive matrix.

Bibliography:

- The chapter 12 of the Landau & Lifshitz [20] (the unpleasant notation $R_{\min}$ is used for the free energy or the free enthalpy).
- The chapter 2 of the book by Pottier [37] is well written (although the notations can be a bit confusing). The local version is developed. The chapter 2 of Livi and Politi's book [24] discusses this matter but is less detailed.
- The chapter 6 of Le Bellac et al's book [22].

5.3 Correlation functions and response functions

Let us now enter into the heart of linear response theory. Being a microscopic approach, it should be based on a description as microscopic as possible : we adopt the frame of classical mechanics and consider the distribution function in phase space.

- Phase space : we denote by $\vec{\Gamma}$ a point (the "microstate") in the D-dimensional phase space. For example, for a gas of N atoms, it is the vector $\vec{\Gamma} \equiv (\vec{r}_1, \cdots, \vec{r}_N, \vec{p}_1, \cdots, \vec{p}_N)$ with $D = 6N$ components.
- The dynamics of the system is controlled by the Hamiltonian $H(\vec{\Gamma})$.
- We adopt a probabilistic description and consider the distribution in phase space, denoted $\rho_t(\vec{\Gamma})$, which is the probability density in phase space at time t. It follows from the Hamiltonian equations of motion that it obeys the Liouville equation (see for example appendix of chapter 3 of [48])

  $$\frac{\partial}{\partial t}\rho_t = \{H\ ,\ \rho_t\} \tag{5.51}$$

  where

  $$\{A\ ,\ B\} \stackrel{\mathrm{def}}{=} \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i}\frac{\partial A}{\partial p_i} \right) \tag{5.52}$$

  is a Poisson bracket.
- Finally, considering an observable $A(\vec{\Gamma})$ (for example the kinetic energy $H_{\mathrm{kin}} = \frac{1}{2m}\sum_i \vec{p}_i{}^2$), the average at time t is given by

  $$\langle A \rangle_t = \int \mathrm{d}^D\vec{\Gamma}\, \rho_t(\vec{\Gamma})\, A(\vec{\Gamma})\,. \tag{5.53}$$

  Here, the evolution is carried by the density. Below, it will be conceptually more simple to write the average differently, with the evolution carried by the observable :

  $$\langle A \rangle_t = \int \mathrm{d}^D\vec{\Gamma}_0\, \rho_0(\vec{\Gamma}_0)\, A(\vec{\Gamma}(t)) \tag{5.54}$$

  where $\vec{\Gamma}(t)$ is the trajectory such that $\vec{\Gamma}(0) = \vec{\Gamma}_0$. The distinction between (5.53) and (5.54) is similar to the difference between Schrödinger and Heisenberg pictures in quantum mechanics. Below I will rather use the notation $\langle A \rangle_t \equiv \langle A(t) \rangle$ (a more consistent notation should be $\langle A(\vec{\Gamma}(t)) \rangle$ but it is too heavy).

a) Equilibrium and static response

Consider a modification of the Hamilonian

$$H_0(\vec{\Gamma}) \longrightarrow H_f(\vec{\Gamma}) = H_0(\vec{\Gamma}) - f\, A(\vec{\Gamma}) \tag{5.55}$$

where A is a certain "observable" and f the conjugate force (here in the sense of classical mechanics). I.e. the observable can be obtained by differentiation with respect to this parameter $A(\vec{\Gamma}) = -\frac{\partial}{\partial f} H_0(\vec{\Gamma})$. Assume canonical equilibrium

$$\rho^f(\vec{\Gamma}) = \frac{1}{Z_f}\, \mathrm{e}^{-\beta H_f(\vec{\Gamma})} \qquad \text{with } Z_f = \int \mathrm{d}^D\vec{\Gamma}\, \mathrm{e}^{-\beta H_f(\vec{\Gamma})}\,. \tag{5.56}$$

Consider the average of another observable

$$\langle B\rangle_f = \int \mathrm{d}^D\vec{\Gamma}\, \rho^f(\vec{\Gamma})\, B(\vec{\Gamma}) \tag{5.57}$$

Question : given $\langle B\rangle_0 = \int \mathrm{d}^D\vec{\Gamma}\, \rho^0(\vec{\Gamma})\, B(\vec{\Gamma})$, can we study the variation of the average due to the introduction of the force f ? As a preliminary, let us expand the partition Z_f in powers of f :

$$Z_f \simeq \int \mathrm{d}^D\vec{\Gamma}\, \mathrm{e}^{-\beta H_0(\vec{\Gamma})} \Big(1 + \beta f A(\vec{\Gamma}) + \cdots\Big) = Z_0\, (1 + \beta f\, \langle A\rangle_0 + \cdots)\,. \tag{5.58}$$

Similarly, we can expand the average

$$\langle B\rangle_f \simeq \int \mathrm{d}^D\vec{\Gamma}\, B(\vec{\Gamma})\, \frac{\mathrm{e}^{-\beta H_0}}{Z_0} \frac{1 + \beta f A(\vec{\Gamma}) + \cdots}{1 + \beta f\, \langle A\rangle_0 + \cdots} \tag{5.59}$$

Finally we can write

$$\langle B\rangle_f = \langle B\rangle_0 + f\, \chi^{\mathrm{stat}}_{BA} + \mathcal{O}(f^2) \tag{5.60}$$

where

$$\chi^{\mathrm{stat}}_{BA} = \beta\, (\langle BA\rangle_0 - \langle B\rangle_0\, \langle A\rangle_0) \tag{5.61}$$

is the "static response function". At lowest order in f, the properties of observables in the presence of the force are controlled by a *correlator* characterizing the equilibrium state ρ^0.

Example: consider a magnetic system with magnetic energy $H_{\mathrm{magn}} = -\mathcal{B}\, M$ where M is the magnetization. The **magnetic susceptibility** is the response of the magnetization to the magnetic field $\langle M\rangle_0 \simeq \chi\, \mathcal{B}$ for $\mathcal{B} \to 0$. Application of the formula shows that the susceptibility is related to the fluctuations of magnetization :

$$\chi = \frac{\langle \delta M^2\rangle_0}{k_{\mathrm{B}} T} \tag{5.62}$$

(cf. chap. 10 of [48]).

b) Relaxation

Let us now consider the problem of *relaxation*, i.e. a specific protocol to study the out-of-equilibrium situation where the system is submitted to a time dependent perturbation. We consider the dynamics induced by

$$H(\vec{\Gamma}, t) = H_0(\vec{\Gamma}) - f_R\, \theta_{\mathrm{H}}(-t)\, A(\vec{\Gamma})\,, \tag{5.63}$$

i.e. a situation where a static perturbation $\delta H_{\rm pert} = -f_R\, A$ is switched off at time $t = 0$. Up to time $t = 0$, we can write $\langle B\rangle_{f_R} \simeq \langle B\rangle_0 + f_R\, \chi^{\rm stat}_{BA}$. For time $t \geqslant 0$, the dynamics is controlled by the Hamiltonian H_0, we write

$$\langle B(t)\rangle_f = \int {\rm d}^D\vec{\Gamma}_0\, \rho^{f_R}(\vec{\Gamma}_0)\, B(\vec{\Gamma}(t)) \tag{5.64}$$

where $\vec{\Gamma}(0) = \vec{\Gamma}_0$, with $\boldsymbol{\vec{\Gamma}(t)}$ **solving the equation of motions for** $\boldsymbol{H_0}$**.** Here, it is indeed convenient that the time dependence is carried by the observable B, which allows us to expand the distribution ρ^{f_R} at time $t = 0$ in the same way as above :

$$\langle B(t)\rangle_f \simeq \int {\rm d}^D\vec{\Gamma}_0\, \frac{{\rm e}^{-\beta H_0(\vec{\Gamma}_0)}}{Z_0}\, \frac{1 + \beta f_R A(\vec{\Gamma}_0) + \cdots}{1 + \beta f_R \langle A\rangle_0 + \cdots}\, B(\vec{\Gamma}(t)) \tag{5.65}$$

We get

$$\langle B(t)\rangle_f \simeq \langle B\rangle_0 + f_R\, R_{BA}(t) \qquad \text{for } t > 0\,, \qquad \text{where } R_{BA}(t) = \beta\left(\langle B(t)\, A(0)\rangle_0 - \langle B\rangle_0\, \langle A\rangle_0\right) \tag{5.66}$$

is the relaxation function.[28] We have used that the averages are time independent at equilibrium, $\langle B(t)\rangle_0 = \langle B\rangle_0$. The relaxation is characterised by a correlation function of the model in the absence of the force. I stress that both the time evolution of observable B and the average refer to the "free" Hamiltonian H_0.

c) Dynamical response

Consider now a general perturbation

$$H(\vec{\Gamma}, t) = H_0(\vec{\Gamma}) - f(t)\, A(\vec{\Gamma}) \tag{5.67}$$

where f is an arbitrary function. In general, at lowest order in the force, the average must be a convolution of the force

$$\langle B(t)\rangle_f = \langle B\rangle_0 + \int {\rm d}t'\, \chi_{BA}(t - t')\, f(t') + \mathcal{O}(f^2) \tag{5.68}$$

where $\chi_{BA}(t)$ is by definition the "response function". The question is now to determine this function. First of all, causality imposes

$$\chi_{BA}(t) \propto \theta_{\rm H}(t) \tag{5.69}$$

Next, we relate this function to the relaxation function. The case of relaxation corresponds to $f(t) = f_R\, \theta_{\rm H}(-t)$, thus

$$R_{BA}(t) = \int {\rm d}t'\, \overbrace{\chi_{BA}(t - t')}^{\propto \theta_{\rm H}(t-t')}\, \theta_{\rm H}(-t') = \int_{-\infty}^{\min(t,0)} {\rm d}t'\, \chi_{BA}(t - t') \tag{5.70}$$

$$= \int_t^{\infty} {\rm d}t''\, \chi_{BA}(t'') \qquad \text{for } t > 0 \tag{5.71}$$

thus $\chi_{BA}(t) = -\frac{\rm d}{{\rm d}t} R_{BA}(t)$ for $t > 0$. Finally

$$\boxed{\chi_{BA}(t) = -\beta\, \theta_{\rm H}(t) \frac{\rm d}{{\rm d}t} \langle B(t)\, A(0)\rangle_0} \tag{5.72}$$

Once again, rephrasing Onsager : the response of the system put out-of-equilibrium by the introduction of the force $f(t)$, is controlled by a correlation function characterizing the equilibrium state. However, it is not an "hypothesis", this is perturbation theory!

[28] Once more, the notation for the correlation function refers to $\langle B(t)\, A(0)\rangle_0 = \int {\rm d}^D\vec{\Gamma}_0\, \rho^0(\vec{\Gamma}_0)\, B(\vec{\Gamma}(t))\, A(\vec{\Gamma}_0)$ where $\vec{\Gamma}(t)$ is the trajectory starting from $\vec{\Gamma}_0$ and $\rho^0(\vec{\Gamma}) \propto {\rm e}^{-\beta H_0(\vec{\Gamma})}$.

Important (but academic) example : the harmonic oscillator.— Consider

$$H_0(q,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\, q^2 \tag{5.73}$$

and introduce the perturbation $\delta H(t) = -f(t)\, q$. We apply the formula to compute $\chi_{qq}(t)$. Given $q(0) = q_0$ and $p(0) = p_0$ we have

$$q(t) = q_0\, \cos\omega t + \frac{p_0}{m\omega}\, \sin\omega t \tag{5.74}$$

Thus the correlation function is

$$C_{qq}(t) = \langle q(t)q(0)\rangle = \left\langle q_0^2\right\rangle\, \cos\omega t + \frac{\langle q_0 p_0\rangle}{m\omega}\, \sin\omega t \tag{5.75}$$

Given that the equilibrium distribution is $\rho \propto \mathrm{e}^{-\beta H_0}$ we have $\left\langle q_0^2\right\rangle = k_{\rm B}T/(m\omega^2)$ and $\langle q_0 p_0\rangle = 0$ hence

$$C_{qq}(t) = \frac{k_{\rm B}T}{m\omega^2}\, \cos\omega t \tag{5.76}$$

from which we deduce

$$R_{qq}(t) = \frac{1}{m\omega^2}\, \cos\omega t \quad \text{and} \quad \chi_{qq}(t) = \frac{\theta_{\rm H}(t)}{m\omega}\, \sin\omega t \tag{5.77}$$

Remark: it is relatively easy to understand why the response function is independent of the temperature (and in fact independent of the distribution function). This can be explained by the fact that the system is linear.

✍ ***Exercice 5.1 Anharmonic oscillator :*** *The response function $\chi(t)$for a harmonic (linear) oscillator, $\ddot{x}(t) - \omega_0^2 x(t) = f(t)$ is the Green's function of the equation, i.e. solves the differential equation $\ddot{\chi}(t) - \omega_0^2\chi(t) = \delta(t)$.*
We consider now the classical anharmonic oscillator forced by an external force $f(t)$: $\ddot{x}(t) - F(x(t)) = f(t)$, where $F(x)$ derives from a confining potential (e.g. $V(x) = \frac{1}{2}\omega^2x^2 + \frac{1}{4}\lambda x^4$). Deduce the differential equation satisfied by the response function. Discuss the differences with the harmonic case.

Example 2: conductivity.— consider now a particle submitted to an electric field $\mathcal{E}(t)$

$$H(t) = H_0 - q\, x\, \mathcal{E}(t) \tag{5.78}$$

The current density is

$$\langle j(t)\rangle_{\mathcal{E}} = nq\, \langle v(t)\rangle_{\mathcal{E}} = nq^2 \int \mathrm{d}t'\, \chi(t-t')\, \mathcal{E}(t') + \mathcal{O}(\mathcal{E}^2) \tag{5.79}$$

where n is the carrier density and $\chi(t-t')$ characterizes the response of the velocity to the electric field (coupled here to the position). From the general formula derived above we have

$$\chi(t-t') = -\,\theta_{\rm H}(t-t')\beta\frac{\mathrm{d}}{\mathrm{d}t}\left\langle v(t)x(t')\right\rangle = \theta_{\rm H}(t-t')\beta\left\langle v(t)v(t')\right\rangle \tag{5.80}$$

(I have used time translation invariance $\langle v(t)x(t')\rangle = \langle v(0)x(t'-t)\rangle$). In Fourier

$$\left\langle \tilde{j}_\omega\right\rangle = nq^2\widetilde{\chi}(\omega)\, \widetilde{\mathcal{E}}_\omega \equiv \tilde{\sigma}(\omega)\, \widetilde{\mathcal{E}}_\omega \tag{5.81}$$

So that the condutivity is the Fourier transform of the velocity-velocity correlator

$$\tilde{\sigma}(\omega) = nq^2\widetilde{\chi}(\omega) \tag{5.82}$$

The study of the phenomenological Langevin equation has led to

$$\langle v(t)v(0)\rangle = \frac{D}{\tau}\,\mathrm{e}^{-|t|/\tau} \tag{5.83}$$

where $D = k_{\mathrm{B}}T/\gamma = k_{\mathrm{B}}T\,\tau/m$ is the diffusion constant (cf. § 1). Then

$$\tilde{\sigma}(\omega) = \frac{nq^2\tau}{m}\frac{1}{1-\mathrm{i}\omega\tau} \tag{5.84}$$

we have recovered the Drude formula $\sigma_0 = \frac{nq^2\tau}{m}$.

5.4 Once more the fluctuation-dissipation theorem

We write the perturbation added to the free Hamiltonian under the form $H_{\mathrm{pert}}(t) = -f(t)\,A(t)$. Hence, $A(t)$ plays the same role as a "coordonate", coupled to an external "force" $f(t)$ (cf. the example of the Harmonic oscillator). The dissipative power is given by the product of the force and the velocity

$$\mathcal{P}_{\mathrm{diss}}(t) = f(t)\left\langle\frac{\mathrm{d}A(t)}{\mathrm{d}t}\right\rangle_f . \tag{5.85}$$

Consider an harmonic excitation $f(t) = f_\omega\cos\omega t = \mathrm{Re}[f_\omega \mathrm{e}^{-\mathrm{i}\omega t}]$. The linear response of observable A reads

$$\langle A(t)\rangle_f \simeq \mathrm{Re}\left[\widetilde{\chi}_{AA}(\omega)\,f_\omega \mathrm{e}^{-\mathrm{i}\omega t}\right] = f_\omega\left(\widetilde{\chi}'_{AA}(\omega)\,\cos\omega t + \widetilde{\chi}''_{AA}(\omega)\,\sin\omega t\right) \tag{5.86}$$

where $\widetilde{\chi}_{AA} = \widetilde{\chi}'_{AA} + \mathrm{i}\widetilde{\chi}''_{AA}$.

Dissipated power is given by : $\mathcal{P}_{\mathrm{diss}}(t) = f_\omega^2\,\omega\,\cos\omega t\,(-\widetilde{\chi}'_{AA}\sin\omega t + \widetilde{\chi}''_{AA}\cos\omega t)$. Averaging over time, one gets :

$$\overline{\mathcal{P}}_{\mathrm{diss}} = \frac{1}{2}\omega {f_\omega}^2\,\widetilde{\chi}''_{AA}(\omega)\,. \tag{5.87}$$

The imaginary part $\mathrm{Im}\,\widetilde{\chi}_{AA}(\omega)$ of the response function controls the dissipation.

✍ ***Exercice 5.2 :*** *On considère un oscillateur harmonique classique amorti décrit par l'équation $\ddot{x} + \frac{2}{\tau}\dot{x} + \omega_0^2 x = \frac{1}{m}f(t)$. Déduire la fonction de réponse fréquentielle $\widetilde{\chi}_{xx}(\omega)$. Analyser ses pôles ; on distinguera les régimes fortement ($1/\tau > \omega_0$) et faiblement ($1/\tau < \omega_0$) amortis. Dans ce second cas, montrer que $\widetilde{\chi}_{xx}(\omega)$ possède la même structure que dans le cas non amorti à condition de remplacer 0^+ par $1/\tau$.*

✍ ***Exercice 5.3 :*** *The response function of the damped harmonic oscillator takes the form (exercice 5.2) : $\widetilde{\chi}_{xx}(\omega) = \frac{1}{m}\frac{1}{\tilde{\omega}_0^2 - (\omega + \frac{\mathrm{i}}{\tau})^2}$ where $\tilde{\omega}_0 = \omega_0^2 - \frac{1}{\tau^2}$. Plot real and imaginary parts. Plot the dissipative power $\overline{\mathcal{P}}_{\mathrm{diss}} \propto \omega\,\mathrm{Im}\,\widetilde{\chi}_{xx}(\omega)$.*

Admittance : The dissipative power $\mathcal{P}_{\mathrm{diss}}(t) = f(t)\langle\dot{A}(t)\rangle$ involves the response of the "velocity" $\dot{A}$ to the perturbation $H_{\mathrm{pert}}(t) = -f(t)\,A(t)$. The corresponding reponse function is known as the *complex admittance* : $Y(\omega) \overset{\mathrm{def}}{=} \widetilde{\chi}_{\dot{A}A}(\omega) = -\mathrm{i}\omega\,\widetilde{\chi}_{AA}(\omega)$. It is also related to the *impedance* $Z(\omega) = 1/Y(\omega)$.

$$\boxed{\overline{\mathcal{P}}_{\mathrm{diss}} = \frac{1}{2}\omega {f_\omega}^2\,\mathrm{Im}\,\widetilde{\chi}_{AA}(\omega) = \frac{1}{2}{f_\omega}^2\,\mathrm{Re}\,Y(\omega)} \tag{5.88}$$

Examples :

- *Conductance.–* If $A \to Q$ is the electric charge, the conjugated "force" is the electric potential : $\delta E = V\delta Q$. The admittance characterizes the response of the current : $I(\omega) = \dot{Q}(\omega) = Y(\omega)V(\omega)$ (this is the conductance, usually denoted G). The dissipative power is proportional to $\mathrm{Re}\, Y(\omega) = \mathrm{Re}\, Z(\omega)/|Z(\omega)|^2$.
- *Conductivity.–* The conductance G of a wire of length L of cross section S is related to the conductivity as $G = S\sigma/L$. The Drude model gives : $\sigma(\omega) = \frac{ne^2\tau}{m}\frac{1}{1-\mathrm{i}\omega\tau}$ where τ is the collision time for electrons. As it is well known the *real* part of the conductivity characterizes the dissipation. Note that the imaginary part of the conductivity is proportional to the real part of the dielectric function (hence to the refraction phenomenon).

5.5 Causality and Kramers-Kronig relations

Causality of response functions is at the heart of a deep relation between the reactive ($\mathrm{Re}\,\widetilde{\chi}_{AA}(\omega)$) and dissipative ($\mathrm{Im}\,\widetilde{\chi}_{AA}(\omega)$) parts of the response function. As a consequence, in an experiment, it is sufficient to measure one of the two to get the full response function. For example, if one considers the complex refraction index in optics, $\nu(\omega) = n(\omega) + \mathrm{i}\kappa(\omega)$, the real part characterizes the refraction, i.e. the change of direction of a radius at the interface, whereas the imaginary part characterizes the absorption of the light by the medium.

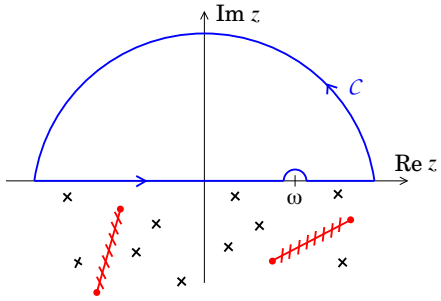


Figure 29: *Contour of integration considered to get Eq. (5.90). Crosses represent the poles of the function $\widetilde{\chi}(z)$, and the lines the branch cut.*

The response function is causal :

$$\boxed{\chi(t) = 0 \quad \text{for } t < 0} \tag{5.89}$$

Let us assume for simplicity that its Fourier transform is square integrable [29] : $\int_{-\infty}^{+\infty} \mathrm{d}\omega\, |\widetilde{\chi}(\omega)|^2 < \infty$. Because $\chi(t) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi}\widetilde{\chi}(\omega)\, \mathrm{e}^{-\mathrm{i}\omega t}$, all poles and branch cut of $\widetilde{\chi}(\omega)$ must belong to the lower half complex place. [29] Write the integral $\oint_{\mathcal{C}} \mathrm{d}z\, \frac{\widetilde{\chi}(z)}{z-\omega}$ over the contour represented in figure 29, and consider the limit where radius of external and internal semi-circles go to ∞ and 0, respectively. We get :

$$\widetilde{\chi}(\omega) = \frac{1}{\mathrm{i}\pi}\fint_{-\infty}^{+\infty} \mathrm{d}\omega'\, \frac{\widetilde{\chi}(\omega')}{\omega' - \omega} \tag{5.90}$$

[29] Démonstration : montrons que $\widetilde{\chi}(z) = \int_0^\infty \mathrm{d}t\, \chi(t)\, \mathrm{e}^{+\mathrm{i}zt}$ est analytique dans le plan complexe supérieur. Pour cela nous souhaitons vérifier que $\partial\widetilde{\chi}(z)/\partial z^* = 0$. La permutation entre dérivation et intégrale n'est permise que si l'intégrand et sa dérivée partielle sont bornés par une fonction sommable indépendante de z (théorème de convergence dominée). Or $|\chi(t)\mathrm{e}^{+\mathrm{i}zt}| = |\chi(t)|\mathrm{e}^{-t\,\mathrm{Im}(z)} \leqslant |\chi(t)|$ pour $\mathrm{Im}(z) \geqslant 0$. La permutation de $\partial/\partial z^*$ et $\int \mathrm{d}t$ n'est donc autorisée que si $\mathrm{Im}(z) \geqslant 0$; dans ce cas $\partial\widetilde{\chi}(z)/\partial z^* = \int_0^\infty \mathrm{d}t\, \chi(t)\, \partial\mathrm{e}^{+\mathrm{i}zt}/\partial z^* = 0$ puisque la fonction exponentielle est analytique. QED.

This shows that real and imaginary parts are related through Hilbert transforms :

$$\mathrm{Re}\,\widetilde{\chi}(\omega) = \frac{1}{\pi}\fint_{-\infty}^{+\infty} \mathrm{d}\omega' \,\frac{\mathrm{Im}\,\widetilde{\chi}(\omega')}{\omega'-\omega} \tag{5.91}$$

$$\mathrm{Im}\,\widetilde{\chi}(\omega) = -\frac{1}{\pi}\fint_{-\infty}^{+\infty} \mathrm{d}\omega' \,\frac{\mathrm{Re}\,\widetilde{\chi}(\omega')}{\omega'-\omega} \tag{5.92}$$

These dispersion relations are known as **Kramers-Kronig relations** (or Plemelj formulae) :

Figure 30: *Hendrik Anthony Kramers (1894-1952) & Ralph de Laer Kronig (1904-1995).*

Remarks :

- *Substractions.–* The function $\widetilde{\chi}(\omega)$ might not be square integrable. In this case, given $\mathrm{Im}\,\widetilde{\chi}(\omega)$, causality is not sufficient to fully determine $\mathrm{Re}\,\widetilde{\chi}(\omega)$. However, dispersions relations can be obtained by performing "substractions" [29]. For example, consider $\widetilde{\chi}(\omega)$ bounded at infinity $|\widetilde{\chi}(\infty)| < \infty$, a single substraction is sufficient. One applies the procedure described above to the function $\frac{\widetilde{\chi}(\omega)-\widetilde{\chi}(\omega_0)}{\omega-\omega_0}$ (which is square integrable). One gets :

$$\widetilde{\chi}(\omega) = \widetilde{\chi}(\omega_0) + \frac{\omega-\omega_0}{\mathrm{i}\pi}\fint_{-\infty}^{+\infty} \mathrm{d}\omega' \,\frac{\widetilde{\chi}(\omega')-\widetilde{\chi}(\omega_0)}{\omega'-\omega_0}\,\frac{1}{\omega'-\omega} \tag{5.93}$$

  where ω_0 is chosen at will (for example $\omega_0 = \infty$ can simplify the relation).
- In optics causality should be stated as follows : "the effect of a perturbation propagates slower that the light velocity c", i.e. the causal response is non zero inside the light cone.
- The two previous remarks should be applied to the celebrated case of the refraction index of a medium $\nu(\omega) = n(\omega)+\mathrm{i}\kappa(\omega)$. Because the medium becomes transparent at high frequency, the index has the property $\nu(\omega\to\infty) = 1$. Introduce the notation $\kappa(\omega) = c\beta(\omega)/2\omega$. Kramers-Kronig relation reads $n(\omega)-1 = \frac{c}{\pi}\fint_0^{+\infty}\mathrm{d}\omega'\,\frac{\beta(\omega')}{\omega'^2-\omega^2}$ (R. de L. Kronig, 1926 & H. A. Kramers, 1927). This relation between the refraction index and the extinction coefficient is the first known dispersion relation [29]. For this reason, the Plemelj relations are called Kramers-Kronig relations by physicists.

✍ ***Exercice 5.4 :*** *One gives* $\mathrm{Im}\,\widetilde{\chi}(\omega) = \frac{-1}{1+\omega^2}$, *show that* $\widetilde{\chi}(\omega) = \frac{1}{\omega+\mathrm{i}}$ *by using the Kramers-Kronig relations.*
Similarly, given $\mathrm{Im}\,\widetilde{\chi}(\omega) = \frac{1}{1/\tau^2+(\omega-\omega_0)^2}$, *find* $\widetilde{\chi}(\omega)$.

✍ ***Exercice 5.5 Analytic structure of the response function :***
1/ *Harmonic oscillator.– We consider the harmonic oscillator described by the equation of motion* $\ddot{x}+\omega_0^2 x = \frac{1}{m}f(t)$. *Show that the response function* $\chi(t)$ *characterising the response of* $x(t)$ *to the force* $f(t)$ *coupled to* x *is the Green's function of the differential equation. Check that the causal Green's function is* $\chi(t) = \theta_{\mathrm{H}}(t)\frac{\sin\omega_0 t}{m\omega_0}$. *Compute its Fourier transform* $\widetilde{\chi}(\omega)$ *(for this purpose it is necessary to introduce a regulator* $\mathrm{e}^{-\epsilon t}$ *with* $\epsilon\to 0^+$ *in the integral). Plot neatly* $\widetilde{\chi}(\omega)$.

2/ *Damped harmonic oscillator.–* *We consider now a damped harmonic oscillator submitted to the external force :*

$$\ddot{x} + \frac{2}{\tau}\dot{x} + \omega_0^2 x = \frac{1}{m} f(t) \tag{5.94}$$

Compute the Fourier transform of the response function $\widetilde{\chi}(\omega)$*. Analyse the poles of this function : study how the poles move in the complex plane as the damping rate* $1/\tau$ *varies from* $+\infty$ *to* 0^+*. Plot neatly* $\mathrm{Re}\,\widetilde{\chi}(\omega)$ *and* $\mathrm{Im}\,\widetilde{\chi}(\omega)$ *in the weak damping limit (to be defined). Come back to the first question and interpret physically the regulator* $\epsilon \to 0^+$*.*

☺ Important points

• The "response-correlation relation" (main idea of linear response theory) : for small external perturbations, the response of the system is controlled by an *equilibrium* correlation function.
• Be familiar with the expression of the response function.
• Fluctuation-dissipation ; $\mathrm{Im}\,\widetilde{\chi}_{AA}(\omega)$ is the dissipative part.
• Consequence of causality on the analytic structure of the response function (Kramers-Kronig).

PART 2 : Introduction to phase transitions and critical phenomena

This second part of the lecture notes is devoted to the study of phase transitions, which is probably the most difficult part of a course on *equilibrium* statistical physics. The reason is that phase transitions arise from the competition between thermal fluctuations (entropy) and local interactions (energy), which can lead to different phases of matter. [30] The study of problems with interactions is always a difficult task. Phase transitions usually manifest through a order/disorder transition, between a low-T ordered phase (when energy dominates) and a high-T disordered phase (when entropy dominates). The remarkable point is that a *microscopic range interaction* can mediate cooperative effects responsible for ordering at a *macroscopic scale*.

The study of phase transitions is interesting and important for different reasons. The first is that it concerns the understanding of the different organisations of matter. The second is that certain types of phase transitions, of "second order", exhibit critical phenomena (scale invariance and scaling laws) with a universal character : some properties are completely insensitive to the microscopic details and moreover can be the same for different physical problems : such properties are called "*universal*".

6 Mean field

6.1 Introduction : the liquid-gas transition

Let us start with a concrete (and important) example of phase transition, which will allow to introduce several important ideas. The study of the liquid phase within the frame of statistical physics, i.e. based on a microscopic model, is the most difficul to study :

(i) in the gaseous phase, the atoms (or the molecules) can be considered as *independent particles*. This is due to the fact that collisions between atoms are sufficiently rare so that the interaction energy of the atoms in the gas can be considered negligible compared to the kinetic energy : $E_{\rm kin} \gg E_{\rm int}$.

(ii) In a solid, this is exactly the opposite, atoms are attached to sites of the crystalline lattice and vibrate around their equilibrium positions. Interaction energy dominates (in the sense that the atoms cannot overcome the potential barriers) : $E_{\rm kin} \ll E_{\rm int}$. It is however still possible to identify *independent degrees of freedom* (collective vibration modes, phonon modes), which makes the analysis simple.

(iii) The liquid state is the most difficult to study : in this case kinetic energy and interaction energy are of the same order $E_{\rm kin} \sim E_{\rm int}$.

a) Description of the phenomenon

A standard protocol is to perform a decompression of the fluid at fixed temperature : Fig 31. Increasing the volume, the pressure of the liquid rapidly decreases (compressibility of the liquid is usually extremely small). For some value V_L, part of the liquid evaporates and two phases coexist. The pressure is then constant, which correspond to the "*liquefaction plateau*" (flat part of the isotherm). When all the liquid has been converted into vapour, the volume reaches the value V_G. If the volume is further increased, the pressure again diminishes slowly (compressibility of the gas is very high). This is represented schematically in Fig. 32 for different temperatures.

[30] Phase transition can also occur at zero temperature, and can be driven by a parameter. An example is the Anderson transition in disordered metals, between a metallic phase (with finite conductivity) and Anderson insulating phase, when the disorder strength (or the electron density) is varied.

The two volumes $V_L(T)$ and $V_G(T)$ and the pressure of the plateau $p_s(T)$ are functions of the temperature. The figure 33 shows real data for carbon dioxyde.

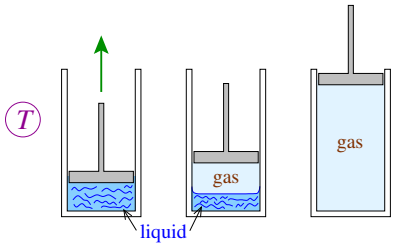


Figure 31: *Decompression (at constant temperature) of a fluid initially in the liquid phase.*

The volume V (or the density $n = N/V$) is the observable allowing to distinguish the two phases, it plays the role of the "*order parameter*". Because it makes a jump when the fluid goes from the liquid to the gaseous phase, one says that the liquid-gas transition is a **discontinuous phase transition**. A different representation is shown on the right parts of the figures 6.15 and 33 : in the plane (p, T), the coexistence between liquid and gas takes place on the line $p = p_s(T)$. This emphasizes that the Gibbs free energy [31] $G(T, p, N)$ presents a singular behaviour on this line : the volume being the derivative of the Gibbs free energy, $V = \frac{\partial G}{\partial p}$, we have $\frac{\partial G}{\partial p}\big|_L \neq \frac{\partial G}{\partial p}\big|_G$. Hence, the transition is also said to be a **first order phase transition**, according to the Erhenfest classification (a phase transition is said to be of order n if the nth-derivatives of the thermodynamic potentials present discontinuities or singular behaviours).

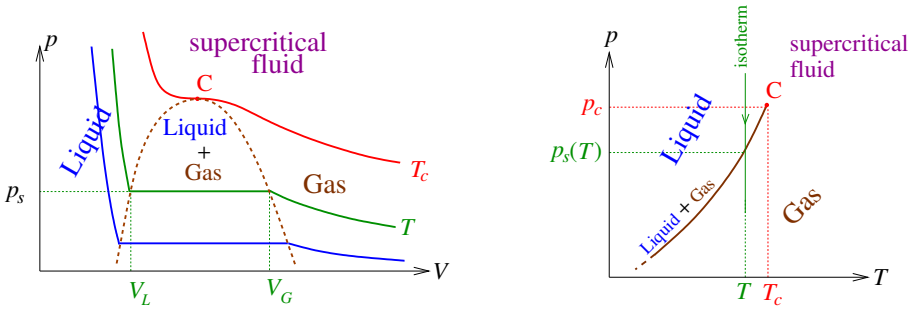


Figure 32: *Sketch of isotherms in the Clapeyron diagram. The isotherm at temperature T_c is the critical isotherm and C the critical point. Above the critical isotherm, the state is know as a supercritical fluid.* Right : *In the (p, T) representation, liquid and gas coexist on a line.*

If temperature is increased, the width of the liquefaction plateau diminishes and eventually vanishes at a temperature T_c called the "*critical temperature*" (Fig. 32 and Fig. 33 for experimental data) : $V_G(T) - V_L(T) \to 0$ as $T \to T_c^-$. The point C where the liquefaction plateau shrinks is called the "*critical point*". Hence $\frac{\partial G}{\partial p}$ is continuous for $T = T_c$ (and discontinuous for $T < T_c$). The critical isotherm being flat at the critical point, $\frac{\partial p}{\partial V}\big|_C = 0$, the isothermal compressibility $\chi_T = -\frac{1}{V}\frac{\partial^2 G}{\partial p^2}\big|_C = \infty$ is infinite at the critical point. It is now the second derivative of G which exhibits an "accident", hence according to the Ehrenfest classification, one says that the transition at C is a **second order phase transition**. Because the order parameter is continuous at T_c, the phenomenon is also called a **continuous phase transition**.

[31] Reminder of **theory of thermodynamic potentials** : $F(T, V, N)$ is the Helmholtz free energy (or simply the "free energy") and $G(T, p, N)$ is the Gibbs free energy (or the "free enthalpy"). They are related through Legendre transforms $G(T, p, N) = \min_V \{F(T, V, N) + pV\}$.

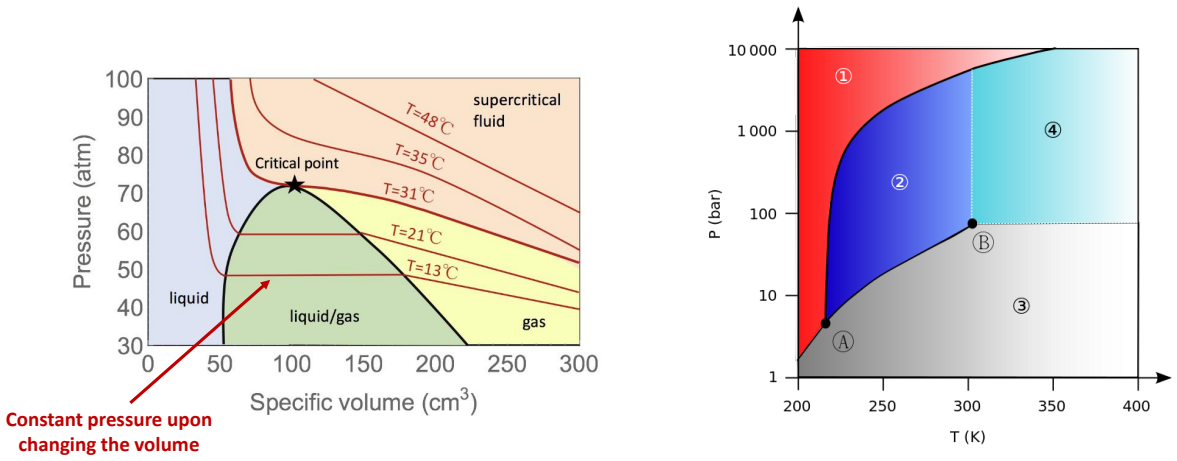


Figure 33: *Phase diagram of carbon-dioxyde (right figure from* `wikipedia`*: the red zone corresponds to the solid phase. The point* B *is the critical point and the point* A *the "triple point").*

Above T_c, there is no more distinction between liquid and gas and one says that the fluid is *supercritical*. This occurs at $T_c = 374\,^{\circ}\mathrm{C}$ in water (with $p_c = 220\,\mathrm{atm}$) or at $T_c = 31.1\,^{\circ}\mathrm{C}$ in CO_2 (with $p_c = 73\,\mathrm{atm}$, cf. Fig. 33). Critical temperatures and pressures for other fluids can be found at `https://en.wikipedia.org/wiki/Critical_point_(thermodynamics)`.

b) The van der Waals model

We now introduce a microscopic model which describes the transition (this paragraph is a brief presentation of the first part of chap. 10 of [48]) We consider N atoms, or molecules, assumed to interact only through *pair interactions* :

$$H = \sum_i \frac{\vec{p}_i{}^2}{2m} + \frac{1}{2}\sum_{i,j\ (\neq)} u_{\mathrm{LJ}}(||\vec{r}_i - \vec{r}_j||) = H_{\mathrm{kin}} + U\,. \tag{6.1}$$

The potential Lennard-Jones $u_{\mathrm{LJ}}(r) = u_0\big[(\frac{r_0}{r})^{12} - 2(\frac{r_0}{r})^6\big]$ correctly describes interaction between two atoms, with strong repulsion at short distance and weak attraction at large distance. It involves two microscopic parameters : the range r_0 of the potential (position of the minimum), and its depth $u_{\mathrm{LJ}}(r_0) = -u_0$. For example, interaction between Argon atoms is well described by the Lennard-Jones potential for $u_0 \simeq 2.5\,\mathrm{meV}$ ($\leftrightarrow 30\,\mathrm{K}$) and $r_0 \simeq 3.35\,\text{Å}$.

In order to simplify the analysis, we replace the Lennard-Jones potential by a potential $u_{\mathrm{LJ}}(r) \longrightarrow u(r)$ with $u(r) = \infty$ for $r < r_0$ (hard sphere repulsion) and $u(r) = u_{\mathrm{LJ}}(r)$ for $r > r_0$. This defines an *excluded volume* $v = \frac{4\pi}{3} r_0^3$ around each atom.

Our aim is now to compute the partition function of the gas

$$Z_N = \frac{1}{N! h^{3N}} \int \mathrm{d}^3\vec{p}_1 \cdots \int \mathrm{d}^3\vec{p}_N \int_V \mathrm{d}^3\vec{r}_1 \cdots \int_V \mathrm{d}^3\vec{r}_N\, \mathrm{e}^{-\beta H} = \frac{1}{N!\lambda_T^{3N}}\, Q_N \tag{6.2}$$

where $\lambda_T = \sqrt{2\pi\hbar^2/(mk_{\mathrm{B}}T)}$ is the thermal length and

$$Q_N = \int_V \mathrm{d}^3\vec{r}_1 \cdots \int_V \mathrm{d}^3\vec{r}_N\, \mathrm{e}^{-\beta U} \tag{6.3}$$

is the "*configurational integral*".

Hard sphere repulsion.– In order to estimate Q_N, we first consider the hard sphere repulsion and forget the attractive part of the potential (this is similar to do $u(r) \longrightarrow u_{\rm HS}(r) = \infty$ for $r < r_0$ and $u_{\rm HS}(r) = 0$ for $r > r_0$). Q_N is given by an integral over the available space : $Q_1 = V$. Fixing $\vec{r}_1$, the avalaible space for $\vec{r}_2$ is $V - v$, where v is the excluded volume, then $Q_2 = V\,(V - v)$ (see Fig. 34). For three atoms, $Q_3 \simeq V\,(V - v)\,(V - 2v)$ is an approximation as it results from the exclusion of atoms taken by pairs, and ignore the three body effect. Neverthelees, we can proceed and get [32]

$$Q_N \simeq \prod_{n=0}^{N-1} (V - n\,v)\,. \tag{6.4}$$

Assuming $V \gg Nv$, we have

$$Q_N \simeq (V - Nb)^N \qquad \text{for } V > Nb \tag{6.5}$$

with

$$\boxed{b \stackrel{\rm def}{=} \frac{v}{2} = \frac{2\pi}{3} r_0^3} \tag{6.6}$$

which is the first parameter of the van der Waals equation. The first conclusion is that we can account for the hard sphere repulsion by replacing the volume by $V \longrightarrow V - Nb$.

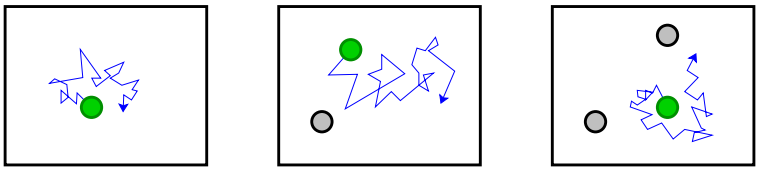


Figure 34: *Configuration integral : the first particle can move in a volum V, thus $Q_1 = V$, the second in a volume $V - v$, thus $Q_2 = V(V - v)$, the third in a volume $V - 2v$, hence $Q_3 \simeq V(V - v)(V - 2v)$, etc.*

✍ ***Exercice 6.1 :*** *The mean field approximation predicts that the fluid of hard spheres has a maximum density $n_c^{\rm mf} = 1/b = 3/(2\pi r_0^3)$ in $d = 3$.*
a) In $d = 2$, a similar argument gives $n_c^{\rm mf} = 1/b = 2/(\pi r_0^2)$. Compare with the (exact) density for the dense packed phase.
b) Same question in $d = 3$.

Weak attraction.– Because the integral over positions is uniform, we can interpret the configurational integral (6.3) as

$$Q_N \simeq (V - Nb)^N \langle {\rm e}^{-\beta U} \rangle_{\substack{\text{available} \\ \text{volume}}}\,, \tag{6.7}$$

what we approximate by

$$Q_N \simeq (V - Nb)^N \exp\Big[- \beta \langle U \rangle_{\substack{\text{available} \\ \text{volume}}} \Big]\,. \tag{6.8}$$

Let us now estimate $\langle U \rangle$: one atom, say atom 1, "sees" the averaged potential $\simeq n \int_{\rho > r_0} {\rm d}^3\vec{\rho}\, u(||\vec{\rho}||)$, where $n = N/V$ is the mean density. Hence

$$\langle U \rangle_{\substack{\text{available} \\ \text{volume}}} \simeq \frac{N}{2}\, n \int_{\rho > r_0} {\rm d}^3\vec{\rho}\, u(||\vec{\rho}||) = -N\, n\, a\,, \tag{6.9}$$

[32] write $\ln Q_N = \sum_{n=0}^{N-1} \ln(V - n\,v) \simeq N\, \ln(V - N\,v/2)$.

where the 1/2 avoid double counting. We have introduced the second parameter of the van der Waals equation :

$$\boxed{a \stackrel{\text{def}}{=} -2\pi \int_{r_0}^{\infty} \mathrm{d}\rho\, \rho^2\, u(\rho)} \tag{6.10}$$

Note that, in terms of the two microscopic parameters, we have $a \sim u_0\, r_0^3$.

Conclusion : VdW partition function.— We conclude that

$$Z_N^{(\mathrm{VdW})} \simeq \frac{1}{N!} \left(\frac{V - Nb}{\lambda_T^3} \right)^N \mathrm{e}^{\beta N^2 a / V} \tag{6.11}$$

Although the approximations leading to $Z_N^{(\mathrm{VdW})}$ seem a bit crude and out of control, we will see that the model qualitatively describes all the phenomena introduced above.

Thermodynamic properties.— The corresponding free energy is

$$\boxed{F(T,V,N) = -N k_{\mathrm{B}} T \left\{ 1 + \ln\left(\frac{V - Nb}{N\lambda_T^3} \right) \right\} - \frac{N^2 a}{V}} \tag{6.12}$$

In the VdW model, the energy is only sensitive to the attraction (but not to the effect of the excluded volume)

$$\overline{E}^{\mathrm{c}} = \underbrace{\frac{3N k_{\mathrm{B}} T}{2}}_{=\overline{E}^{\mathrm{c}}_{\mathrm{kin}}} \underbrace{-\frac{N^2 a}{V}}_{=\overline{U}^{\mathrm{c}}}, \tag{6.13}$$

while the entropy is only sensitive to the excluded volume effect, but not to the weak attraction

$$S^{\mathrm{c}} = N k_{\mathrm{B}} \left\{ \frac{5}{2} + \ln\left(\frac{V - Nb}{N\lambda_T^3} \right) \right\} . \tag{6.14}$$

The equation of state is the well-known van der Waals equation

$$\boxed{p = \frac{n k_{\mathrm{B}} T}{1 - nb} - n^2 a} \tag{6.15}$$

In the limit of low density, we recover pressure for the ideal gas, $p \simeq n k_{\mathrm{B}} T$, as it should. The first term of (6.15) is monotonously increasing with n, from 0 for $n = 0$, to ∞ for $n \to 1/b$, while the second is monotonously decreasing. Writing the expansion in powers of the density (virial expansion)

$$p \simeq n k_{\mathrm{B}} T \Big(1 + \underbrace{(b - \beta a)}_{=B_2(T)}\, n + (b\, n)^2 + \mathcal{O}(n^3) \Big) \tag{6.16}$$

reveals that the curvature changes in sign at $k_{\mathrm{B}} T = a/b \sim u_0$ ($B_n(T) = b^{n-1} - \beta a\, \delta_{n,2}$ are the virial coefficients). Because the weight of the first term is the temperature, we expect that it is dominant at high T, while the second term is important at low T and *the isotherm may become a non monotonic function* of the density n. This is indeed what we observe by plotting the isotherms for different temperatures, Fig. 35.

✍ ***Exercice 6.2 :*** *Find the coordinates (V_c, p_c, T_c) of the critical point, defined as the point where $\frac{\partial p}{\partial V}\big|_C = 0$ and $\frac{\partial^2 p}{\partial V^2}\big|_C = 0$. Deduce the value of $p_c V_c / N k_B T_c$. Compare to the values obtained experimentally for Helium (0.30) and dioxygen (0.29).*

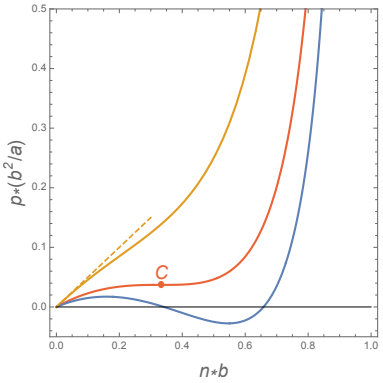


Figure 35: *VdW isotherms* (6.15) *for* $k_BT = 0.5a/b$, $8a/27b$ *and* $0.225a/b$.

The main problem revealed by the figure is the non-monotoneous behaviour observed for low temperatures, say $T < T_c$. Indeed, for stability reasons, the isothermal compressibility of the fluid must be positive

$$\chi_T \overset{\text{def}}{=} -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T = \frac{1}{n}\left(\frac{\partial n}{\partial p}\right)_T > 0 \tag{6.17}$$

Remember the study of the relaxation of a piston between two gases exchanging volume, cf. [48] : stability demands $\partial^2 F/\partial V^2 = -\partial p/\partial V > 0$. This is a very general property of thermodynamic potentials, which are convex functions of their arguments (more precisely : it can be convex or concave, depending on the potential and the parameter, but the convexity cannot change).

Therefore, the van der Waals model predicts that, in certain parameter range, the isotherms (6.15) may present a non-monotonic behaviour, which is non physical (this corresponds to an unstable state, which is incompatible with equilibrium statistical physics).

Phase separation.— This apparent difficulty of the van der Waals model is related to an interesting physical phenomenon. To circumvent the difficulty, we should relax the assumption, implicitly made above, of a homogeneous fluid. Let us explain this. At this stage, it is helpful to study the evolution of the free energy. Since $p = -\frac{\partial F}{\partial V}$, integration of $p(V)$ gives the free energy $F(T, V)$ up to a function of T (Fig. 36).

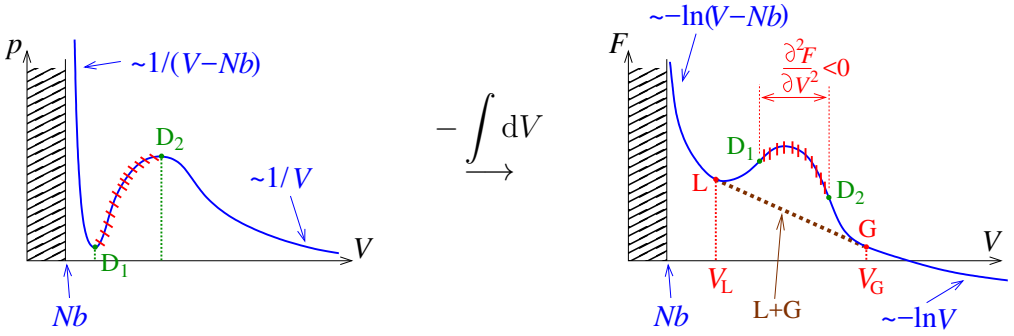


Figure 36: *Integration of the VdW isotherm gives the free energy (hatched part between points* D_1 *and* D_2 *is the forbidden part, which would describe an unstable fluid). Figures from chapter 10 of* [48].

Remember that *each point corresponds to a specific thermodynamic state* of the fluid. The figure makes clear that the existence of a (unphysical) concave part allows us to find a path with lower free energy (remember the principle of minimization of the free energy). For $V \in$

$[V_L, V_G]$, a **mixing** of the two states L and G is characterized by a volume fraction of liquid $x = (V - V_L)/(V_G - V_L) \in [0,1]$ and $1 - x = (V_G - V)/(V_G - V_L)$ of gas. Denoting by $F_L \equiv F(T, V_L)$ the free energy of the liquid phase and $F_G \equiv F(T, V_G)$ the free energy of the gas phase, we conclude that the free energy of the mixed state is $F = x\, F_L + (1-x)\, F_G$ for $x \in [0,1]$, or more explicitly :

$$F(T,V) = \frac{F(T,V_L)\,(V_G - V) + F(T,V_G)\,(V - V_L)}{V_G - V_L} \qquad \text{for } V \in [V_L, V_G] \tag{6.18}$$

This corresponds to a plateau

$$p = -\frac{\partial F}{\partial V} = -\frac{F_G - F_L}{V_G - V_L} \equiv p_s(T) \qquad \text{for } V \in [V_L, V_G] \tag{6.19}$$

(remember that V_L and V_G also depend on T). We interpret the two points as the liquid state (point L) and the gaseous state (point G). Hence, the branch of the isotherm ending at L corresponds to the *liquid phase*, while the branch starting at G is the *gaseous phase*. In between is the liquefaction plateau at the "*saturation vapor pressure*" $p_s(T)$.

Maxwell's construction.— Next question is to find (in practice) the two points L and G. We first turn the van der Waals isotherm by $\pi/2$ and then integrate the curve $V(p)$ over p (Fig. 37). We get the Gibbs free energy $G(T,p,N)$, up to a function $\psi(T,N)$. The Gibbs free energy is a concave function of p. In this representation, the mixed state (the liquefaction plateau) is just a point where $G_G = G_L$. We can give a geometrical interpretation : the plateau is obtained by writing

$$\int_{G\to L} \mathrm{d}p\, V(p) = 0 \tag{6.20}$$

i.e. the two areas between the isotherm and the plateau must be equal : this is the "*Maxwell's construction*", see Fig. 38.

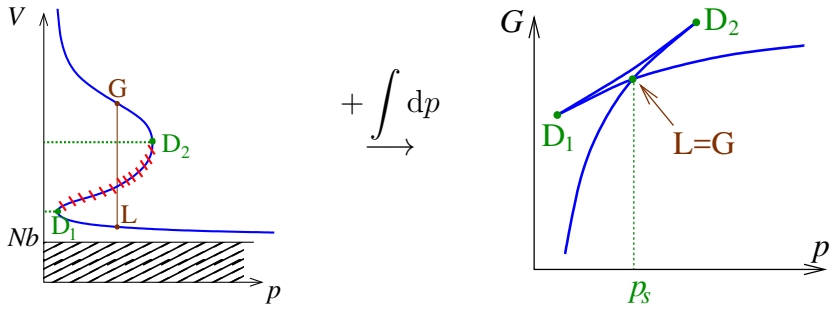


Figure 37: *Construction of the Gibbs free energy $G(T,p,N)$ from the rotated isotherm.*

We can also give a thermodynamic interpretation to the construction. Because $G(T,p,N) = N\,\mu(T,p)$ (from extensivity) the plateau corresponds to

$$\mu_L = \mu_G\,, \tag{6.21}$$

which is the usual equilibrium condition for coexistence of two phases exchanging particles.

We can also write the Maxwell construction

$$\int_{L\to G} \mathrm{d}V \left[p_{\mathrm{VdW}}(V) - p_s\right] = 0 \quad \text{or in short} \quad \oint \mathrm{d}V\, p_{\mathrm{VdW}}(V) = 0 \tag{6.22}$$

where $p_{\mathrm{VdW}}(V)$ is the van der Waals isotherm (including the non physical increasing part) ; in the second expression, the intergration is performed along the closed circuit from L to G through the VdW isotherm and backward through the liquefaction plateau. This equation provides V_L, V_G and p_s (which are all functions of T).

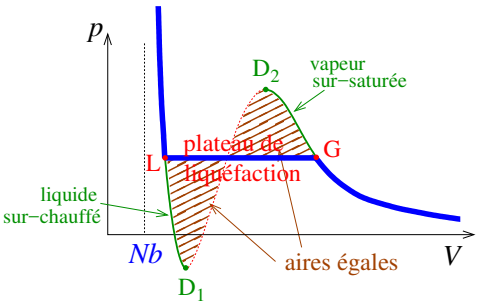


Figure 38: *Maxwell construction ; figure from [48].*

Discontinuities.— We have stressed that the liquid-gas transition is a discontinuous (1st order) phase transition as the density of the fluid presents a discontinuity $n_L > n_G$. Another discontinuity with important consequence is the jump of entropy, which can be written with the help of the above expression

$$\Delta S = S(T, V_G) - S(T, V_L) = N k_{\rm B} \ln\left(\frac{V_G - Nb}{V_L - Nb}\right) > 0\,. \tag{6.23}$$

The positive jump of entropy corresponds to a transition between an "ordered" phase to a "disordered" one. We introduce the **latent heat**

$$L_{\rm vap} = T\,\Delta S = N k_{\rm B} T \ln\left(\frac{V_G - Nb}{V_L - Nb}\right) \tag{6.24}$$

which quantifies the heat required to convert all the liquid into gas (with a reversible transformation). The existence of a latent heat is a general property of first order phase transitions.

✍ ***Exercice 6.3 :*** *We consider a reversible transformation from L to G (on the isotherm). The fluid receives the heat $L_{\rm vap}$. What is the work received ? Study the limit close to the critical point (i.e. for $V_G - V_L = \delta V$ "small").*

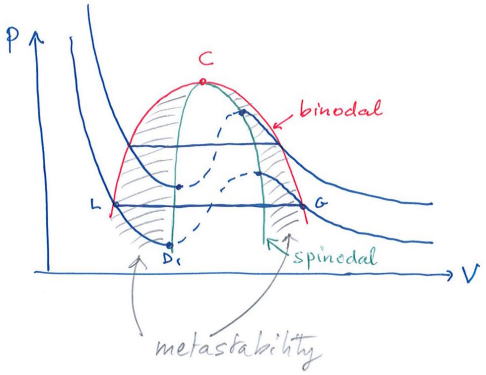


Figure 39: *Binodal, spinodal and metastability region.*

Metastability.— Before the Maxwell construction, we have stressed that the part of the VdW isotherm corresponding to a negative compressibility corresponds to an unstable fluid (unphysical). However, the two branches out of the liquefaction plateau (arcs L-D_1 and D_2-G in Fig. 38) are not forbidden as $\chi_T > 0$. Nevertheless, the Figs. 36 and 37 show that the two arcs correspond to states with a larger free energy than in the mixed state (liquid+gas).

Hence, these states correspond to *metastable states* where the fluid is in a *local* minimum of the free energy which is less favorable energetically, but not forbidden : the system can leave the metastable state due to a thermal fluctuation and fall into the two-phase state (L+G) with a lower free energy. The curve delimiting the coexistence zone in the Clapeyron diagram is called the **binodal** (dashed line on the left part of Fig. 32 or red curve in Fig. 39). The set of points D_1 and D_2 define another curve inside, called the **spinodal**. The zone between the two curves is the metastability region (where metastability is *possible*) : cf. Fig. 39.

✍ ***Exercice 6.4 Binodal and spinodal :*** *We introduce the reduced variables* $v \stackrel{def}{=} (V-V_c)/V_c$, $\pi \stackrel{def}{=} (p-p_c)/p_c$ *and* $t \stackrel{def}{=} (T-T_c)/T_c$.

a) Show that, in the vicinity of the critical point, the VdW isotherm takes the simple form

$$\pi \simeq 4t - 6vt - \frac{3}{2}v^3 \tag{6.25}$$

(justifiy that we can stop at order v^3 *and neglect the term* $v^2 t$ *and higher).*

b) For $t < 0$ *(i.e.* $T < T_c$*), discuss explicitly the Maxwell construction with the simplified isotherm. What are the values of the volume of the liquid* v_L *and of gas* v_G*, defining the two ends of the liquefaction plateau ? What is the value of the saturation pressure* $\pi_s(t)$ *?*

c) In the Clapeyron diagram (π, v)*, the region where liquid and gas coexist is delimited by the "binodal" curve (i.e. the two values* $v_L(t)$ *and* $v_G(t)$ *as a function of* $\pi = \pi_s(t)$*). Give the expression of the binodal curve.*

d) The spinodal is the curve corresponding to the end of metastability (i.e. the set of points where $\frac{\partial \pi}{\partial v} = 0$ *in the Clapeyron diagram). Deduce the expression of the spinodal curve.*

e) Plot neatly the phase diagram in the Clapeyron representation and indicate the region of metastability.

c) Criticality in the liquid-gas transition

We have emphasized above that the liquefaction plateau disappears at a "critical temperature" T_c : cf. Figs. 32, 33 and 35. The critical point C is the place of a second order phase transition. The term "critical" refers to the fact that, approching the point C, the correlation length of the fluid diverges (we will discuss this later) and that the vicinity of the point is characterised by power laws, i.e. scale invariance, and universality. A stricking manifestation of the divergence of the correlation length in the fluid is the phenomenon of "*critical opalescence*". As the point C is approached, the interface between liquid and gas broadens and the fluid becomes cloudy, due to the fact that fluctuations take place at increasing large scale, eventually exceeding the wave length of light.

In 1945, Guggenheim has collected the data for eight different fluids (noble gases –Ne, Ag, Xe, Kr– and also molecular gases –N_2, O_2, CO and CH_4) : he has studied the width of the liquefaction plateau, starting at the gas density $n_G(T) = N/V_G(T)$ and ending at the liquid density $n_L(T) = N/V_L(T)$, as a function of the temperature. To make comparison between the fluids of different natures possible, he plotted the ratios n_G/n_c and n_L/n_c, where n_c is the density at the critical point, as a function of the ratio T/T_c. Although n_c and T_c are different for each fluid, after this proper rescaling, it is remarkable that *all data fall onto a universal curve*, which is shown in Fig. 40. "**Universality**" means that we have obtain a property which is common to many systems (here different fluids).

A careful study of the data shows that, close to C, the difference of densities $\delta n = n_L - n_G$ presents a power law behaviour with temperature

$$\boxed{\delta n \propto (T_c - T)^{\beta}} \tag{6.26}$$

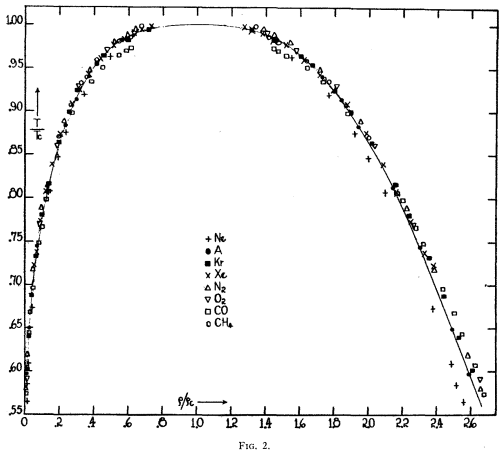


Figure 40: *For different fluids, the ratios $n_G(T)/n_c$ and $n_L(T)/n_c$ are plotted as a function of T/T_c. For all eight fluids, the data fall on a universal curve.* Figure from : E. A. Guggenheim, "*The principles of corresponding states*", J. Chem. Phys. **13**(7), p. 253 (1945).

where β is known as the "*critical exponent for the order parameter*". Analysing the experimental data, Guggenheim gave $\beta \simeq 1/3$; more recent measurements in CO_2 have given $\beta \simeq 0.324$. This power law is not the only one :

- Close to the critical point, the heat capacity presents the behaviour

$$\boxed{C_V \propto |T - T_c|^{-\alpha}} \tag{6.27}$$

  Experiments on CO_2 gives $\alpha \simeq 0.111$.
- The critical isotherm : we have seen on the figures above that the critical point is an inflexion point of the isotherm, which has a flat slope. It presents the behaviour

$$\boxed{p - p_c \propto |n - n_c|^{\delta} \, \mathrm{sign}(n - n_c)} \tag{6.28}$$

  I have not found a direct measurement of the exponent δ, however, as we will see later, it is related to other exponents by the Widom relation $\delta = 1 + \gamma/\beta$ (see below § 7.4). Using the value $\beta \simeq 0.324$ and $\gamma \simeq 1.246$ obtained for CO_2 and Xe, respectively, we get $\delta \simeq 4.846$.
- Approaching the critical temperature from above, the slope of the isotherm eventually vanishes at T_c, corresponding to a divergence of the isothermal compressibility (inverse of the slope of the isotherm). A careful study shows that

$$\boxed{\chi_T \propto |T - T_c|^{-\gamma}} \tag{6.29}$$

  Experiments in xenon gives $\gamma \simeq 1.246$. Other experimental data can be found in [33, 14].

The notations for the four critical exponents are standard.

✍ ***Exercice 6.5 Critical exponents of the VdW equation :*** *Expanding the VdW isotherms around the critical point, show that the van der Waals model predicts the following set of critical exponents $\beta = 1/2$, $\delta = 3$ and $\gamma = 1$.*

6.2 The phenomenological Landau's approach

The study of the critical point within the van der Waals model is possible, however, instead of considering a specific microscopic model, we prefer to follow the phenomenological Landau's approach which provides a very simple description of the vicinity of second order phase transitions. The Landau's approach is a "*mean field approximation*", as will be clarified later.

We expose below the main ideas of Landau's approach in the context of the Ising model for the paramagnetic/ferromagnetic transition.

a) Ising model

The Ising model is of fundamental importance in statistical physics and has applications in many problems involving *binary variables* :

- The Ising model for the Para/Ferro transition, where dynamical variables are "Ising spins" $\sigma_i = \pm 1$ attached to the sites of a lattice.
- The *lattice gas* : space is divided into elementary cells, which are either empty, $n_i = 0$ or occupied by one atom at most, $n_i = 1$. The fact that $n_i = 1$ at most mimmic hard core repulsion between atoms.
- Binary alloys : crystalline structure with two species of atoms which can migrate from site to site.
- etc, etc.

The Ising Hamiltonian is

$$\boxed{H_{\text{Ising}} = -\frac{1}{2}\sum_{i,\,j=1}^{N} J_{ij}\,\sigma_i\sigma_j - B\sum_{i=1}^{N}\sigma_i} \tag{6.30}$$

where J_{ij} is the interaction between the two spins on sites i and j. A natural choice is

$$J_{ij} = \begin{cases} J & \text{for } i \text{ and } j \text{ neighbours} \\ 0 & \text{otherwise} \end{cases} \tag{6.31}$$

Here $J > 0$ is a ferromagnetic interaction and the magnetic field B is expressed in appropriate (energy) unit.

Figure 41: *Ernst Ising (1900-1998).*

✍ ***Exercice 6.6 Mapping Ising—Lattice gas :*** *We consider the lattice gas model defined above, with N cells (i.e. N plays the role of the volume). We denote by $\mathcal{N} = \sum_{i=1}^{N} n_i$ the number of particles. Atoms cannot be two in the same cell (hard core repulsion). They also attract themselves with a short range interaction : when two atoms occupy two adjacent cells, they have an energy $E_{2\text{atoms}} = -\varepsilon < 0$ (the energy is zero when the two atoms are more distant). Write $H_{\text{LG}} - \mu\mathcal{N}$ in terms of the occupation numbers n_i, where μ is the chemical potential. Discuss precisely the mapping between the Ising model for N spins in a magnetic field, and the lattice gas.*

Weiss local field and mean field solution.— In the absence of interaction, $J = 0$, the solution follows from independence of spins : partition function of a spin is $z_{\rm spin} = 2\cosh(\beta B)$ from which one gets the magnetization

$$m \stackrel{\rm def}{=} \overline{\sigma_i} = \tanh(\beta B)\,. \tag{6.32}$$

The mean field solution is obtained by replacing the field B in this equation by the mean field seen by a spin. The local field at site i is by definition the variable conjugated to the spin

$$B_i^{(\rm loc)} \stackrel{\rm def}{=} -\frac{\partial H_{\rm Ising}}{\partial \sigma_i} = B + \sum_j J_{ij}\,\sigma_j \tag{6.33}$$

Assuming that the magnetization is uniform in the lattice, the averaged field is

$$\overline{B}^{(\rm loc)} = B + zJm \tag{6.34}$$

where z is the coordination number of the lattice, i.e. the number of neighbours of a given spin. As a result, we obtain the *self consistent equation* $m = \tanh(\beta \overline{B}^{(\rm loc)})$, explicitly

$$m = \tanh\beta(B + zJm)\,. \tag{6.35}$$

One can expect that this approximation is correct if the number of neighbours z is very large, i.e. when the fluctuations of the local field are small compare to the mean value (central limit theorem).

✍ ***Exercice 6.7 An exact relation :*** *In the Ising Hamiltonian, you can isolate the terms which depend on a given spin σ_i from all other terms : $H_{\rm Ising}(\{\sigma_j\}) = -B_{\rm eff}(\sigma')\,\sigma_i + H'(\sigma')$ where "σ'" is a notation for all σ_j's with $j \neq i$. Write explicitly $\langle\sigma_i\rangle$ (with the Gibbs measure). Deduce the exact relation*

$$\langle\sigma_i\rangle = \left\langle \tanh\beta\Big(B + J\sum_{j\in v(i)}\sigma_j\Big)\right\rangle \tag{6.36}$$

where $v(i)$ is the set of z neighbours of the spin σ_i.

✍ ***Exercice 6.8 Mean field solution of the Ising model and critical exponents :***

a) Show that the nature of the solution(s) of the self consistent equation (6.35) for $B = 0$ changes at the temperature $T_c = zJ$ (set $k_B = 1$).

b) Deduce the behaviour $m(T,0) \propto (T_c - T)^{1/2}$ for $T \to T_c^-$.

c) Study the critical isotherm and show that $m(T_c, B) \propto \mathrm{sign}(B)\,|B|^{1/3}$ for $B \to 0$.

d) Using a perturbative method, solve (6.35) for $B \to 0$ and deduce the magnetic susceptibility (i.e. write $m_*(T,B) = m_*(T,0) + \delta m$ with $\delta m \simeq \chi B$).

e) Compare these behaviours with the van der Waals theory for the liquid-gas transition (exercise 6.5).

✍ ***Exercice 6.9 Free energy of the Ising model (mean field) :*** *Write $\sigma_i = m + \delta\sigma_i$ in (6.30), where $m = \langle\sigma_i\rangle$. Neglecting fluctuations, deduce the partition function. Show that the free energy per spin is $f(T,B) = \frac{1}{2}T_c m_*^2 - \frac{1}{2}T\,\ln\left(\frac{1-m_*^2}{4}\right)$, where m_* solves (6.35).*

b) Origin of the Landau's approach : mean field approximation

Consider in this paragraph the case $B = 0$ for simplicity. The Graal would be to compute the Ising partition function

$$Z_{\rm Ising} = \sum_{\{\sigma_i\}} \mathrm{e}^{-\beta H_{\rm Ising}(\{\sigma_i\})} \tag{6.37}$$

where the sum runs over the 2^N configurations (each spin is $\sigma_i = \pm 1$). Due to the interaction, this is however not possible in general. The known results are

- In dimension $d = 1$, the partition is rather easy to compute, either by recursion or using a transfer matrix method (possibly for finite B). The solution was obtained by Ising in 1925.
- In $d = 2$, the calculation of $Z_{\rm Ising}$ was achieved in 1944 by Lars Onsager (Nobel prize in Chemistry in 1968) at $B = 0$. It is considered as a "tour de force".
- In $d \geqslant 3$, only numerical results are available.

Incomplete partition function.— As the aim is here to provide a general presentation of Landau theory, from now on, I will denote by ϕ the **order parameter** and h the conjugate field [for the Para/Ferro transition, $(\phi, h) \to (m, B)$]. $\phi = 0$ in the disordered (paramagnetic) phase, while $\phi \neq 0$ in the ordered (ferromagnetic) phase. Let us introduce the incomplete (or "reduced") partition function (I drop the index "$_{\rm Ising}$" everywhere)

$$Z_L(\phi; T, N) = \sum_{\{\sigma_i\} \text{ with } \sum_i \sigma_i = N\,\phi} \mathrm{e}^{-\beta H(\{\sigma_i\})} \tag{6.38}$$

where the sum is constrained only to (micro)states with a given magnetization $\phi = \frac{1}{N}\sum_i \sigma_i$. The partition function is obviously

$$Z(T, N) = \sum_{\phi} Z_L(\phi; T, N) \tag{6.39}$$

In principle ϕ takes value from $+1$ to -1 with steps $2/N$, thus, in the thermodynamic limit $N \to \infty$, we can rewrite the sum as an integral $\sum_\phi \simeq \frac{N}{2}\int_{-1}^{+1} \mathrm{d}\phi$. The incomplete partition function provides the distribution of the magnetization

$$P(\phi) = \frac{Z_L(\phi; T, N)}{Z(T, N)} \tag{6.40}$$

being the motivation of the concept [48].

For short range interaction, the system exhibits the extensivity property

$$\lim_{N\to\infty} \frac{\ln Z(T, N)}{N} = -\beta\, f(T) \tag{6.41}$$

where f is the free energy per spin. This is also true for the incomplete partition function so that we can write [33]

$$Z_L(\phi; T, N) \simeq \mathrm{e}^{-N\beta f_L(\phi;T)} \quad \text{and} \quad \boxed{P(\phi) \propto \mathrm{e}^{-N\beta f_L(\phi;T)}} \tag{6.42}$$

Thus

$$Z(T, N) \simeq \frac{N}{2}\int_{-1}^{+1} \mathrm{d}\phi\, \mathrm{e}^{-N\beta f_L(\phi;T)} \tag{6.43}$$

In the thermodynamic limit, the summation is dominated by the minimum of the function $f_L(\phi; T)$ (steepest descent method)

$$Z(T, N) \simeq \sqrt{\frac{\pi N}{2\beta f_L''(\phi_*; T)}}\, \mathrm{e}^{-N\beta f_L(\phi_*;T)} \tag{6.44}$$

[33] I do not account for possible sub-exponential prefactor, cf. exercise 6.11.

where

$$\frac{\partial}{\partial\phi} f_L(\phi;T)\Big|_{\phi_*} = 0 \tag{6.45}$$

(here I assume the existence of a unique minimum). We stress that (6.42) in the thermodynamic limit $N \to \infty$ implies that $P(\phi)$ is sharply peaked at ϕ_* so that it has also the meaning of the mean magnetization

$$\overline{\sigma_i} = \phi_*(T)\,. \tag{6.46}$$

Finally we deduce the free energy

$$F(T,N) = -\frac{1}{\beta}\ln Z(T,N) \simeq N\, f_L(\phi_*;T) + \frac{1}{2}k_{\rm B}T \ln\left(\frac{2\beta f_L''(\phi_*;T)}{\pi N}\right) \tag{6.47}$$

hence, in the thermodynamic limit, the free energy per spin is

$$\boxed{f(T) = f_L(\phi_*(T);T)} \tag{6.48}$$

This is the fundamental function encoding the thermodynamic properties.

✍ ***Exercice 6.10 :*** *In the presence of a magnetic field, $f_L(\phi;T,h)$ contains a term $-h\phi$ and the saddle point solution $\phi_*(T,h)$ carries the field dependence. A general property in statistical physics is that the mean value of an observable can be obtained by derivating the thermodynamic potential with respect to the conjugate variable. Check that $\overline{\sigma_i} = -\frac{\partial}{\partial h} f(T,h)$ coincides with ϕ_*.*

Idea of the Landau theory.— The main idea of Landau is to propose a form for the function $f_L(\phi;T)$, based on general principles, rather than derive it from a microscopic model. The incomplete free energy $f_L(\phi;T)$ is called the "**Landau free energy**". Given this function, the problem reduces to finding its minimum. Before following this strategy, which is the conventional Landau's approach, we examine a model where $f_L(\phi;T)$ can be derived. This analysis will bring some ideas on the origin of the general principles allowing to construct $f_L(\phi;T)$ in general.

c) The fully connected Ising model

Consider the case where all spins interact with each other, $J_{ij} = J/N\ \forall i,\, j$ (the $1/N$ is introduced in order to deal with an extensive energy $E \sim N$). In this case the energy takes the form

$$H(\{\sigma_i\}) = -\frac{J}{2N}\sum_{i,j}\sigma_i\sigma_j = -\frac{NJ}{2}\phi^2 \qquad \text{with } \phi = \frac{1}{N}\sum_i \sigma_i\,. \tag{6.49}$$

This model is also known as the "*Curie-Weiss model*". We write can write $H = N\varepsilon(\phi)$ where $\varepsilon(\phi) \overset{\rm def}{=} -J\phi^2/2$ is an energy per spin. Thanks to the fact that the energy depends only on ϕ, the incomplete partition function can be obtained explicitly :

$$Z_L(\phi;T,N) = \sum_{\{\sigma_i\}} \delta_{\frac{1}{N}\sum_i \sigma_i,\phi}\, \mathrm{e}^{-\beta H(\{\sigma_i\})} = \mathrm{e}^{-N\beta\varepsilon(\phi)} \sum_{\{\sigma_i\}} \delta_{\frac{1}{N}\sum_i \sigma_i,\phi} = \Omega(\phi)\,\mathrm{e}^{-N\beta\varepsilon(\phi)} \tag{6.50}$$

where

$$\Omega(\phi) = \frac{N!}{n_+!n_-!} \tag{6.51}$$

is the number of configurations for fixed magnetization ($n_\pm$ is the number of spins up/down). The related entropy (per spin) is the well-known expression

$$s(\phi) = \lim_{N\to\infty}\frac{1}{N}\ln\Omega(\phi) = -\frac{1+\phi}{2}\ln\left(\frac{1+\phi}{2}\right) - \frac{1-\phi}{2}\ln\left(\frac{1-\phi}{2}\right) \tag{6.52}$$

thus

$$Z_L(\phi;T,N) \sim \mathrm{e}^{-N\beta f_L(\phi;T)} \tag{6.53}$$

with

$$f_L(\phi;T) = \varepsilon(\phi) - T\, s(\phi) \tag{6.54}$$

or more explicitly

$$f_L(\phi;T) = -T\ln 2 - \frac{J}{2}\phi^2 + \frac{T}{2}\left[(1+\phi)\ln(1+\phi) + (1-\phi)\ln(1-\phi)\right] . \tag{6.55}$$

The most important feature appears more clearly on the expansion for $\phi \to 0$

$$f_L(\phi;T) \simeq -T\ln 2 + \frac{T-J}{2}\phi^2 + \frac{T}{12}\,\phi^4 + \mathcal{O}(\phi^6) . \tag{6.56}$$

It shows that at the temperature $T_c = J$, the nature of the solutions of (6.45) changes : Fig. 42.

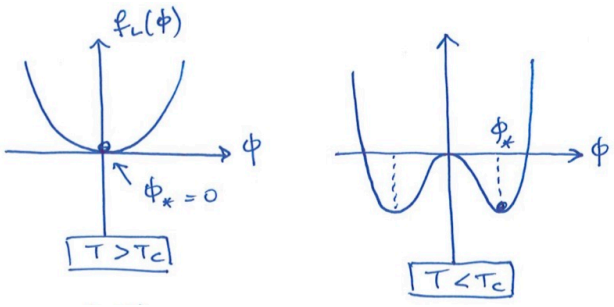


Figure 42: *Landau free energy.*

- For $T > T_c$, the Landau free energy has a unique minimum $\phi_* = 0$. This corresponds to the *paramagnetic* phase (no spontaneous magnetization).
- For $T < T_c$, the Landau free energy has a double well shape (Fig. 42) and eq. (6.45) has two solutions $\phi_* \neq 0$, interpreted as a finite spontaneous magnetization ("spontaneous" means "in the absence of an external magnetic field"). This corresponds to the *ferromagnetic* phase, where interactions between spins dominate thermal fluctuations.

It is straightforward to derive the order parameter for the fully connected model :

$$\phi_*(T) \begin{cases} = 0 & \text{for } T > T_c \\ \simeq \pm\sqrt{3(T_c - T)/T_c} & \text{for } T < T_c \end{cases} \tag{6.57}$$

showing that the fully connected model predicts the value $\beta = 1/2$ for the order parameter critical exponent, see Eq. (6.26).

✍ ***Exercice 6.11 :*** *The aim is here to determine the subleading term (pre-exponential factor) of $Z_L(\phi;T,N)$ for the fully connected model. $\Omega(\phi)$ is the number of available microstates for magnetization ϕ.*
a) What is the value of $\sum_\phi \Omega(\phi)$? Show that $\Omega(\phi) \simeq A_N\, \mathrm{e}^{Ns(\phi)}$, where $s(\phi)$ is the entropy per spin.
Indication : two possible methods : (1) use Stirling formula $\ln N! \simeq N\ln N - N + \frac{1}{2}\ln(2\pi N)$ or (2) use the expansion $s(\phi) \simeq \ln 2 - \phi^2/2$ and the sum rule for $\Omega(\phi)$.
b) Deduce the pre-exponential term in $Z_L(\phi;T,N) \simeq B_N\, \mathrm{e}^{-N\beta f_L(\phi;T)}$.

Spontaneous symmetry breaking.— A generic feature of second order phase transitions is "*spontaneous symmetry breaking*" : although the problem (the *model*) is symmetric with respect to $\phi \to -\phi$, the so-called $\mathbb{Z}_2$ symmetry, the system "chooses" a state that breaks this symmetry below T_c : in the ferromagnetic phase, the magnetization is *either* $\phi_* > 0$ or $\phi_* < 0$ (think at every day life magnets, which have a well defined magnetization). The *state* breaks the symmetry, although the model and the set of all possible states is symmetric.

Ergodicity breaking.— For $T < T_c$, the distribution $P(\phi) \propto \exp\{-N\beta f_L(\phi;T)\}$ presents two symmetric peaks and the partition function in principle involves a sum over the two minima $\pm|\phi_*|$. However, if the system is in the minimum $\phi_* > 0$, going to the minimum $\phi_* < 0$ would require to overcome a very high free energy barrier $\Delta F_N = N\left[f_L(0;T) - f_L(\phi_*;T)\right]$, which cannot occur if $k_{\rm B}T \ll \Delta F_N$ (extensivity prevents the system from jumping the barrier). Hence, spontaneous symmetry breaking is accompanied by *ergodicity breaking* : in practice, the system cannot explore all the available phase space, but is stuck in a region of phase space due to high free energy barrier(s).

✍ ***Exercice 6.12 Incomplete partition function for the Ising model (mean field) :***
The aim of the exercise is to propose a mean field treatment for the calculation of $Z_{\rm Ising}$, in the same spirit as the calculation of $Z_N^{\rm (VdW)}$ in § b) page 83. We consider the Ising model with nearest neighbour couplings on a lattice of N sites : $H = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j$ where the sum runs over all the bonds. We denote z the coordination number of the lattice (number of neighbours of a site) : the number of bonds is thus $N_{\rm bonds} = zN/2$.
In the analysis of the VdW model, we have considered a fixed volume, which plays the role of the order parameter. Here, the equivalent calculation for the Ising model requires to compute the partition function for fixed magnetization, i.e. the incomplete partition function, denoted above $Z_L(\phi)$. Here, ϕ is the magnetization per spin.

a) Give the number $n_\pm$ of spins in state $|\pm\rangle$, as a function of ϕ. Deduce the probability $P_\pm$ for a spin to be in state $|\pm\rangle$.

b) $\Omega(\phi)$ is the number of available microstates for fixed magnetization. Compute it and deduce the entropy per spin $s(\phi)$ in the thermodynamic limit.

c) We denote by N_{++}, N_{+-} and N_{--}, the number of bonds $(++)$, $(+-)$ and $(--)$, respectively. Justify that their averaged values are $\overline{N}_{++} = P_+^2 zN/2$, $\overline{N}_{+-} = P_+P_-zN$ and $\overline{N}_{++} = P_-^2 zN/2$. Deduce the average energy $\overline{E}$ of the lattice, as a function of ϕ. Introduce $\varepsilon(\phi) \stackrel{\rm def}{=} \overline{E}/N$.

d) We can interpret the incomplete partition function as

$$Z_L(\phi) = \Omega(\phi)\left\langle \mathrm{e}^{-\beta H}\right\rangle_{\text{available states}} \tag{6.58}$$

The mean field approximation corresponds to write $\left\langle \mathrm{e}^{-\beta H}\right\rangle \approx \mathrm{e}^{-\beta\langle H\rangle}$, i.e.

$$Z_L^{\rm mf}(\phi) = \Omega(\phi)\,\mathrm{e}^{-\beta\overline{E}} \tag{6.59}$$

This is equivalent to (6.8). Deduce $f_L(\phi)$.

d) Principles of the Landau's approach

Landau's approach aims at studying the vicinity of second order phase transitions (although it is sometimes used out of this range). The general scheme is the following

Low temperature	High temperature
$T < T_c$	$T > T_c$
ordered phase	disordered phase
$\phi \neq 0$	$\phi = 0$
broken symmetry	symmetric state

Because Landau's approach focuses on a regime where the order parameter is "small" $\phi \to 0$ ("close" to T_c), the idea is to *propose* the Landau free energy $f_L(\phi; T)$ under the form of an expansion, constrained by several points :

- *Order parameter* : one must first determine the nature of the order parameter (scalar, vector,..)
- *Stability* : f_L should have a minimum.
- *Symmetry* : use the symmetries of the problem.
- *Analyticity* : $f_L(\phi; T)$ is expected to be an analytic function of ϕ.

Given the expansion, the Landau free energy is minimized

$$\boxed{\frac{\partial}{\partial \phi} f_L(\phi; T)\Big|_{\phi_*} = 0} \tag{6.60}$$

which provides, in an extremely simple manner, the order parameter as a function of temperature and other parameters. The free energy of the problem is then $f(T) = f_L(\phi_*(T); T)$, which contains all thermodynamic properties.

Order parameter.— The order parameter is the observable allowing to distinguish the two phases ($\phi = 0$ for the high T disordered phase and $\phi \neq 0$ for the low T ordered phase). The first step of the Landau's approach is the determination of the *nature* of the order parameter, which can be a difficult question : think at the case of antiferromagnet, where magnetization is zero in the presence of Néel order (alternate spins), or the case of supraconductivity, where the identification of the nature of the order parameter has taken a long time.

- The Ising model has provided a situation where the order parameter is a *real scalar*, $\phi \in [-1, +1]$.
- The metal/supraconducting transition is an example of phase transition with *complex* order parameter $\phi \in \mathbb{C}$ (the wave function for the condensate of Cooper pairs).
- Magnetization is due to local moments which are vectors. Hence the paramagnetic/ferromagnetic transition should rather involves a *vectorial* order parameter $\vec{M}$. This is important when couplings are isotropic.
- Isotropic-nematic transition in liquid crystal : orientational order is characterised by a tensorial order parameter.

Symmetry.— The discussion of the symmetries is another crucial aspect of the Landau's approach, in the same way as particle physicists build effective models constrained by fundamental symmetries of nature. It is important to have in mind the "*symmetry breaking scheme*".

- For the **Ising universality class** discussed so far, it is pretty simple : the theory has the $\mathbb{Z}_2$ symmetry, which is fully broken in the ferromagnetic state :

$$\begin{aligned} \text{Para} &\longrightarrow \text{Ferro} \\ \mathbb{Z}_2 &\longrightarrow \varnothing \, . \end{aligned}$$

- Let us now consider the case of the **Heisenberg model** for vectorial spins

$$H_{\text{Heisenberg}} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \tag{6.61}$$

where $\sum_{\langle i,j \rangle}$ is a sum over all pairs of neartest neighbout sites of the lattice (i.e. a sum over the links). $\vec{S}_i$ is a *three* components vector with fixed modulus (the model where the spin is a two-dimensional vector on the circle is called the XY-model). The *model* is symmetric under spin rotation, i.e. under the transformations of the group SO(3) (careful : the lattice partly breaks the rotational symmetry in space, however the interaction $\vec{S}_i \cdot \vec{S}_j$ is invariant under rotation of spins). The paramagnetic state is characterized by $\langle \vec{S}_i \rangle = 0$, thus it is also symmetric under the group SO(3). If the system enters the ferromagnetic phase, with $\langle \vec{S}_i \rangle = \vec{M} \neq 0$, the symmetry is partly broken : there remains a rotational symmetry in the plane perpendicular to the vector $\vec{M}$. The *symmetry breaking scheme* is in this case

$$\begin{aligned} \text{Para} &\longrightarrow \text{Ferro} \\ \text{SO(3)} &\longrightarrow \text{SO(2)} \, . \end{aligned}$$

e) Landau theory for the Ising universality class

We construct the Landau free energy for the Ising problem (we have in mind a magnet with local ferromagnetic interaction) : The order parameter is a real scalar in this case, $\phi_*(T,h) = \overline{\sigma_i}$. It is a function of the temperature and the magnetic field h. In the absence of the magnetic field, the $\mathbb{Z}_2$ symmetry holds, thus $f_L(-\phi;T,0) = f_L(\phi;T,0)$ and we should retain only terms of a series with even powers in ϕ : $f_L(\phi;T,0) = \sum_{k=0}^{\infty} a_{2k}(T)\, \phi^{2k}$. The coupling to the conjugate field h is linear, hence we add a term $-h\,\phi$:

$$f_L(\phi;T,h) \simeq f_0(T) - h\,\phi + \frac{a(T)}{2}\,\phi^2 + \frac{b}{4}\,\phi^4 \tag{6.62}$$

The study of the fully connected model has shown that a change in sign of $a(T)$ induces a change in the nature of the solution. We write

$$a(T) = \tilde{a}\ (T - T_c)\,, \tag{6.63}$$

with $\tilde{a} > 0$. We have chosen the coefficient $b > 0$ and independent of T for simplicity : we can stop the expansion at order four. Although the starting point is extremely simple, we will see that the outcome are not trivial.

✍ ***Exercice 6.13 :*** *What are the parameters f_0, a and b corresponding to the fully connected model discussed above ?*

Field equation .— The equation for the order parameter, Eq. (6.60), takes the explicit form

$$b\,\phi^3 + a(T)\,\phi = h\,. \tag{6.64}$$

We denote $\phi_*(T,h)$ the solution of the equation.

Solution at $h = 0$.— For $h = 0$, Eq. (6.64), $(b\,\phi^2 + a)\,\phi = 0$ has different types of solutions, depending on the sign of a.

- $a > 0$ (i.e. $T > T_c$) : $\phi_*(T,0) = 0$. This is the paramagnetic phase.
- $a < 0$ (i.e. $T < T_c$) : $\phi_*(T,0) = \pm\sqrt{-a/b}$ (the system chooses one solution). This is the ferromagnetic phase.

We write

$$\boxed{\phi_*(T,0) = \begin{cases} 0 & \text{for } T > T_c \\ \pm\sqrt{\frac{\tilde{a}}{b}(T_c - T)} & \text{for } T < T_c \end{cases}} \tag{6.65}$$

This shows that the mean field critical exponent for the order parameter is

$$\boxed{\beta_{\rm mf} = 1/2} \tag{6.66}$$

We can now derive the free energy. For $T > T_c$ we find $f(T,0) = f_L(\phi_*;T,0) = f_0(T)$ while for $T < T_c$ we get $f(T,0) = f_0(T) + \frac{1}{2}a\,\phi_*^2 + \frac{1}{4}b\,\phi_*^4 = f_0(T) - a^2/(4b)$ thus

$$f(T,0) = f_0(T) - \begin{cases} 0 & \text{for } T > T_c \\ \frac{\tilde{a}^2}{4b}(T - T_c)^2 & \text{for } T < T_c \end{cases} \tag{6.67}$$

The free energy is lower in the ferromagnetic phase. With this in hand, we can deduce the heat capacity $c(T) = -T\frac{\partial^2 f}{\partial T^2}$:

$$c(T) = -T\frac{\partial^2 f_0(T)}{\partial T^2} + \begin{cases} 0 & \text{for } T > T_c \\ \frac{\tilde{a}^2 T}{2b} & \text{for } T < T_c \end{cases} \tag{6.68}$$

thus the heat capacity makes a jump at the transition

$$\boxed{\Delta c_{\rm mf} \stackrel{\rm def}{=} c(T_c^-) - c(T_c^+) = \frac{\tilde{a}^2 T_c}{2b}} \tag{6.69}$$

The discontinuity is interpreted in terms of the heat capacity critical exponent, defined by $c(T) \sim |T - T_c|^{-\alpha}$, by writing $\boxed{\alpha_{\rm mf} = 0}$.

Solution at $h \neq 0$: isotherm.— The isotherm (the curve of the magnetization ϕ_* as a function of the field h) is easy to analyze : we can simply plot the field as a function of ϕ, which is the elementary function Eq. (6.64), and perform a rotation. For $T > T_c$, this gives the monotoneous function (Fig. 43). For $T < T_c$, this would give the "multivalued" function ; with our experience of the van der Waals theory, we understand however that the branch with positive magnetisation for negative field is metastable (Fig. 43). Let us now study few properties of the isotherms.

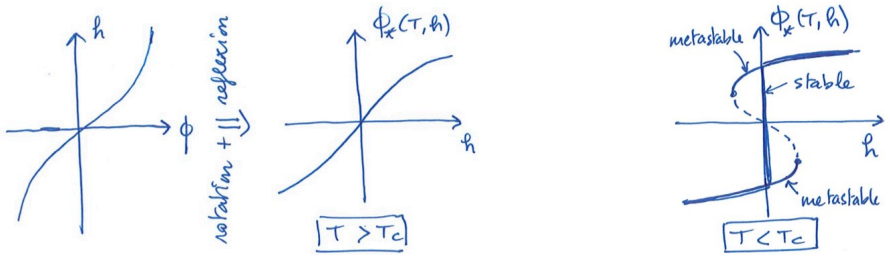


Figure 43: *Ising isotherms.*

It is pretty easy to study the critical isotherms, for $T = T_c$, i.e. $a = 0$:

$$\phi_*(T_c,h) = \text{sign}(h)\,|h/b|^{1/3} \tag{6.70}$$

corresponding to the generic behaviour $\phi \sim h^{1/\delta}$. We identify the mean field prediction for the critical exponent $\boxed{\delta_{\rm mf} = 3}$.

We can also derive the magnetic susceptibility χ, which controls the linear response of the magnetization to an external field. We write

$$\phi_*(T,h) = \phi_*(T,0) + \delta\phi \qquad \text{with } \delta\phi \simeq \chi\, h \tag{6.71}$$

We can obtain $\delta\phi$ by a perturbative method. Denote $\phi_{*0} = \phi_*(T,0)$. Injecting the form in (6.64) and keeping only linear order terms in h we have

$$(3b\,\phi_{*0}^2 + a)\,\delta\phi \simeq h \tag{6.72}$$

so that

$$\chi = \frac{1}{3b\phi_{*0}^2 + a} = \begin{cases} \frac{1}{a} = \frac{1}{\tilde{a}\,(T-T_c)} & \text{for } T > T_c \\ \frac{1}{-2a} = \frac{1}{2\tilde{a}\,(T_c-T)} & \text{for } T < T_c \end{cases} \tag{6.73}$$

thus we have the behaviour $\chi(T) \simeq A_\pm\,|T-T_c|^{-\gamma}$ where the (universal) critical exponent is $\boxed{\gamma_{\rm mf} = 1}$ and the non universal constant $A_\pm$ differs above and below the transition : $A_-/A_+ = 1/2$.

Remark : transition between low field to high field regimes.— we have just analysed the low field regime, for which $\phi_*(T,h) \simeq \phi_*(T,0) + \chi\, h$ for $h \to 0$. The study the high field regime corresponds to neglect the second term in $b\phi^3 + a\phi = h \to b\phi^3 \simeq h$, leading to $\phi_*(T,h) \simeq (h/b)^{1/3}$ for $h \to \infty$. The crossover field separating the two regimes is clearly

$$h_c = \frac{|a|^{3/2}}{\sqrt{b}} \propto |T-T_c|^{3/2}\,. \tag{6.74}$$

$h \lesssim h_c$ is the "small field regime" and $h \gtrsim h_c$ is the "high field regime".

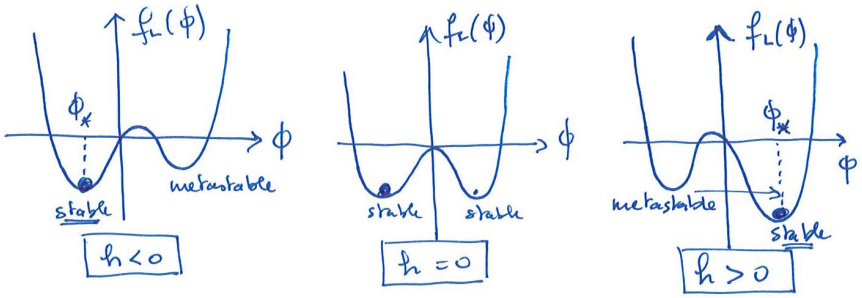


Figure 44: *Evolution of the Landau free energy for $T < T_c$ as a function of h.*

2nd order and 1st order phase transitions in the Ising universality class.– Our presentation of the Landau theory of phase transition is adapted to problems in the "Ising universality class". Setting $h = 0$, the temperature T drives a **second order** phase transition, i.e. $\phi_*(T,0)$ is continuous. If now we consider a different protocol and consider $T < T_c$ fixed and vary the field, i.e. study $\phi_*(T,h)$ as a function of h, Fig. 43 shows that the magnetization is discontinuous at $h = 0$, i.e. the phase transition is now **first order**. The difference is extremely easy to understand by studying the Landau free energy : in the first case, we have the scenario represented in Fig. 42, which makes clear that ϕ_* is continuous when the concavity of f_L at $\phi = 0$ changes in sign. In the second situation, the evolution of the free energy as the conjugated field changes from negative to positive is represented in Fig. 44 : this makes clear that the order parameter is discontinuous around $h = 0$ (cf. Fig. 43).

It is insteresting to plot the free energy as a function of the conjugated field (Fig . 45). The existence of the spontaneous magnetization corresponds to the singular behaviour of the free energy around $h = 0$ for $T < T_c$.

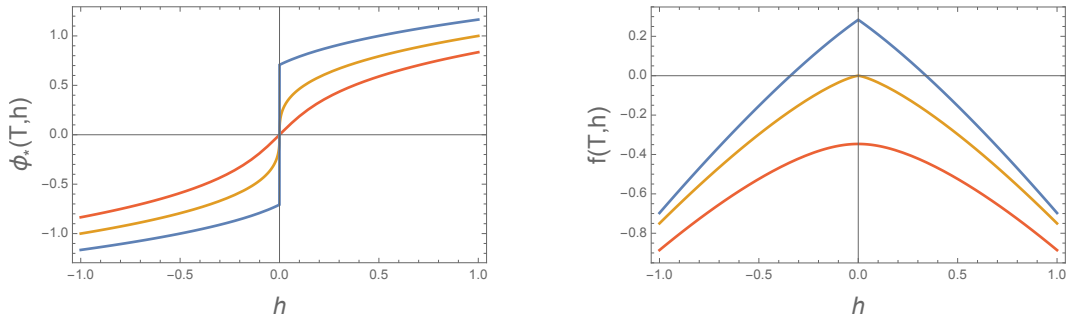


Figure 45: *Magnetization and free energy for* $t = 0.5$, $t = 0$ *and* $t = -0.5$ *(where* $t = (T - T_c)/T_c$*).*

✍ ***Exercice 6.14 Non analyticity of*** $f(T,h)$***:*** *Consider the Landau free energy* $f_L(\phi) = f_0(T) - h\phi + \frac{a}{2}\phi^2 + \frac{b}{4}\phi^4$*. Deduce the behaviour of the free energy* $f(T,h)$ *and analyze its analyticity for* $T \to T_c$ *and* $h \to 0$*.*

Hint: use the limiting behaviours of $\phi_*(T,h)$.

✍ ***Exercice 6.15 Helium-4 / helium-3:*** *Liquid helium-4 presents a second order phase transition between a normal fluid phase and a superfluid phase. The situation is more complicated if helium-3 is added. For a small concentration of helium-3, the second order phase transition is weakly affected. However, a high concentration of helium-3 makes possible the coexistence between a superfluid phase, rich in helium-4, and a normal fluid, rich in helium-3, hence the transition becomes first order.*
A simple model is to consider the Landau free energy

$$f_L(\phi) \simeq f_0 + \frac{a}{2}\,\phi^2 + \frac{b}{4}\,\phi^4 + \frac{c}{6}\,\phi^6 \tag{6.75}$$

with $c > 0$*. Compare the situation when* a *changes in sign with* $b > 0$ *and the one where* b *changes in sign with* $a > 0$*. Argue that the transition is first order in one case and second order in the other case. Find the first order line in the plane* (a,b)*.*

Two remarks :
∗ *In the plane* (a,b)*, the point* $(0,0)$ *is the intersection of three transition lines : it is called a tri-critical point.*
∗ *Blume-Emery-Griffiths have proposed a microscopic model within which it is possible to justify the form (6.75). The coefficients* a *and* b *are controlled by the temperature* T *and the concentration* x *in helium-3, hence there is a mapping from* (a,b) *to* (T,x)*.*

Ising model and VdW model : the discussions made clear the perfect analogy between the liquid/gas and para/ferro transitions. If the isotherms $\phi_*(T,h)$ of Fig. 43 are rotated by 90 °, we recover exactly the same behaviour as the VdW isotherms : compare the Figs. 32 and 43.

	liquid/gas		para/ferro
order parameter ϕ :	$\delta n = n_L - n_G$	$\leftrightarrow$	m (magnetization)
conjugated field h:	p (pressure)	$\leftrightarrow$	B (magnetic field)

6.3 The case of inhomogeneous systems : Ginzburg-Landau's approach

The situation where the order parameter is inhomogeneous is relevant in several physical situations :

- it is possible to act on the order parameter by imposing a non-uniform conjugate field $h(\vec{r})$, which will induces a spatial dependence $\phi(\vec{r})$.

- In a finite size system, boundary conditions can act as a constraint on the value of the field. For example, studying a piece of superconductor in contact with a normal metal imposes that the order parameter of superconductivity vanishing at the interface.

Developping a more elaborate theory for spatial-dependent order parameter will be important for the following and the discussion of fluctuations.

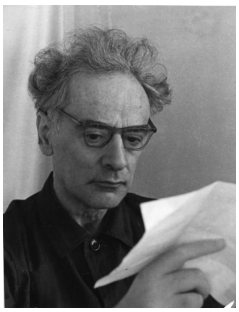
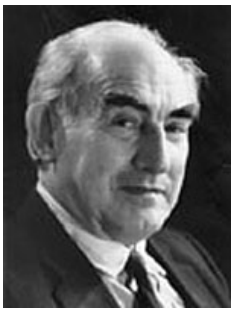



Figure 46: *Lev Davidovich Landau (1908-1968), Nobel prize 1962, and Vitaly Lazarevitch Ginzburg (1916-2009), Nobel prize 2003.*

a) Landau-Ginzburg functional

Coarse-graining.— Our starting point is again the Ising model for nearest neighbour interaction, Eqs. (6.30,6.31). We divide the lattice of N sites into blocks of $n_\ell = \ell^d$ spins, with $\ell \gg 1$ (many spins in each block) and $N/n_\ell \gg 1$ (many blocks), cf. Fig 47.

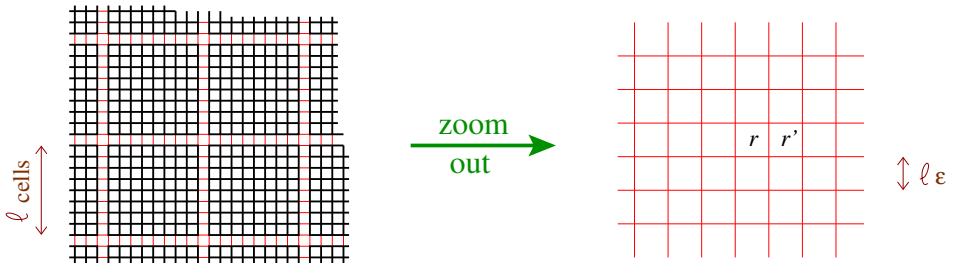


Figure 47: We consider blocks, each of $n_\ell = \ell^d$ lattice sites.

The size of the block is chosen such that we can assume that the order parameter is almost uniform in each block, say ϕ_r in the block around r (I omit the arrow on the vector). We introduce an incomplete partition function, constrained by the value of the order parameter in each block :

$$\mathscr{Z}_L(\{\phi_r\}) = \sum_{\{\sigma_i\}} \mathrm{e}^{-\beta H(\{\sigma_i\})} \prod_r \delta_{\phi_r, \frac{1}{n_\ell}\sum_{i\in \text{block } r}\sigma_i} \tag{6.76}$$

and

$$Z(T,N) \simeq \left(\frac{n_\ell}{2}\right)^{N/n_\ell} \int \prod_r \mathrm{d}\phi_r \; \mathscr{Z}_L(\{\phi_r\}) \tag{6.77}$$

(in a block, the magnetization varies by step $2/n_\ell$). We can split the Ising Hamiltonian as

$$H = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j = \sum_{\text{block } r} H_r + \sum_{\langle r,r'\rangle} H_{r,r'} \tag{6.78}$$

where H_r is the Ising Hamiltonian for block r (i.e. gathers all the interaction terms corresponding to links inside the block) and $H_{r,r'}$ the interface energy between two adjacent blocks (links joining the two blocks), cf. Fig 47. All spins belong to one block, therefore

$$\mathscr{Z}_L(\{\phi_r\}) = \prod_r \Big(\sum_{\{\sigma_i \in \text{block } r\}} \mathrm{e}^{-\beta H_r} \delta_{\phi_r, \frac{1}{n_\ell}\sum_{i\in\text{block } r}\sigma_i} \Big) \prod_{\langle r,r'\rangle} \mathrm{e}^{-\beta H_{r,r'}} \tag{6.79}$$

In the parenthesis, we recognize the incomplete partition function for the homogeneous problem associated with a block of n_ℓ spins, $Z_L(\phi_r; T, n_\ell) \sim \mathrm{e}^{-n_\ell \beta f_L(\phi_r)}$. The product over the blocks is

$$\Big(\cdots\Big) = Z_L(\phi_r; T, n_\ell) \sim \exp\Big\{ -\beta \ell^d f_L(\phi_r) \Big\} \tag{6.80}$$

We can treat the two products in (6.79) only if we neglect the dependency of the $H_{r,r'}$ terms in the spin variables, i.e. if we replace in the terms in $H_{r,r'}$ the spins by their averaged $\sigma_i \to \overline{\sigma_i} = \phi_r$. We justify this by the fact that H_r contains a larger number of terms, ℓ^d (volume), compared to $H_{r,r'}$ which contains ℓ^{d-1} terms (surface). Thus we write

$$H_{r,r'} = +\frac{J}{2} \sum_{\substack{\langle i,j\rangle \text{ between} \\ \text{blocks } r \,\&\, r'}} (\sigma_i - \sigma_j)^2 + \text{cste} \simeq \frac{J\ell^{d-1}}{2} (\phi_r - \phi_{r'})^2 + \text{cste} \tag{6.81}$$

where ℓ^{d-1} is the number of links between the two blocks. Finally

$$\mathscr{Z}_L(\{\phi_r\}) \sim \exp\Big\{ -\beta \frac{J\ell^{d-1}}{2} \sum_{\langle r,r'\rangle} (\phi_r - \phi_{r'})^2 - \beta \ell^d \sum_r f_L(\phi_r) \Big\} . \tag{6.82}$$

After summation over all the pairs of neighbouring blocks, for a smooth order parameter, we have

$$\sum_{\langle r,r'\rangle} (\phi_r - \phi_{r'})^2 = \frac{1}{2} \sum_r \sum_{r'\in v(r)} (\phi_r - \phi_{r'})^2 \simeq (\ell\epsilon)^2 \int \frac{\mathrm{d}^d r}{(\ell\epsilon)^d} (\nabla\phi_r)^2 \tag{6.83}$$

where ϵ is the lattice spacing and $\ell\epsilon$ is the block size. $v(r)$ the set of $2d$ neighbouring blocks. Thus

$$\mathscr{Z}_L(\{\phi_r\}) \sim \exp\Big\{ -\beta \frac{J\ell\epsilon^{2-d}}{2} \int \mathrm{d}^d r\, (\nabla\phi_r)^2 - \beta\epsilon^{-d} \int \mathrm{d}^d r\, f_L(\phi_r) \Big\} \tag{6.84}$$

We now adopt notations for a continuous field $\phi(r)$. The incomplete partition function becomes a *functional* $\mathscr{Z}_L[\phi]$. Setting $g = J\ell\epsilon^{2-d}/2$ and absorbing the factor ϵ^{-d} in a redefinition of the coefficients of the Landau free energy, we conclude that

$$\boxed{\mathscr{Z}_L[\phi] \sim \mathrm{e}^{-\beta F_L[\phi]} \quad \text{where} \quad F_L[\phi] = \int \mathrm{d}^d r \left[g\,(\nabla\phi(r))^2 + f_L(\phi(r)) \right]} \tag{6.85}$$

is the **Ginzburg-Landau functional**.

The partition function is given by a "*path integral*", i.e. a summation in the space of functions $\phi(r)$ defined inside the volume V of the system,

$$Z(T) = \int \mathcal{D}\phi\, \mathrm{e}^{-\beta F_L[\phi]} \tag{6.86}$$

where $\mathcal{D}\phi$ should be understood as the limit of $\prod_r \mathrm{d}\phi_r$. The exponential controls the canonical weight of a field configuration :

$$P[\phi] = \frac{1}{Z}\, \mathrm{e}^{-\beta F_L[\phi]} . \tag{6.87}$$

Another point of view on the Ginzburg-Landau functional : here, I have made an attempt to justify the Landau functional from the microscopic model. There is another point of view, more phenomenological : assuming the existence of such a functional, we propose an expansion (assume analyticity) and use the symmetries. For $h = 0$ it must be symmetric under $\phi \to -\phi$. The simplest assumption is to assume *locality* and expand in powers of gradients :

$$F_L[\phi] = \int \mathrm{d}^d r \left\{ \frac{1}{2} a\, \phi^2 + \frac{1}{4} b\, \phi^4 + \cdots + g^1_{ij}\, \partial_i\phi\partial_j\phi + g^2_{ij}\, \phi^2\, \partial_i\phi\partial_j\phi + g^3_{ijkl}\, \partial_i\phi\partial_j\phi\partial_k\phi\partial_l\phi + \cdots \right\}$$

Isotropy constrains the gradient terms, $g^1_{ij} = g\,\delta_{ij}$, etc. As for the Landau free energy, the expansion is stopped as soon as possible. Here we will only keep the first term involving the gradient, $g(\nabla\phi)^2$, which already describes interesting effects as we will see.

✍ ***Exercice 6.16 :*** *Consider the functional* $F_L[\phi] = \int \mathrm{d}^d r \left[g_1 (\nabla\phi)^2 + g_2 (\nabla^2\phi)^2 + f_L(\phi) \right]$ *with* $f_L(\phi) = \frac{1}{2} a\phi^2 + \frac{1}{4} b\phi^4$, $g_2 > 0$ *and* $b > 0$. *Argue that the optimal configuration may present spatial modulations for* $g_1 < 0$.

Hint: compare the free energy of a flat configuration $\phi_f(x) = \phi_0$ with those of a modulated configuration $\phi_m(x) = \phi_q \cos(qx + \varphi_0)$ (in this second case, both q and ϕ_q should be understood as variational parameters to be determined).

We now have to minimize the functional $F_L[\phi]$ in order to find the configuration of the field which minimizes the free energy and dominates the calculation of the partition function, i.e. with maximal probability weight :

$$Z(T) \sim \mathrm{e}^{-\beta F_L[\phi_*]} \,. \tag{6.88}$$

In order to determine ϕ_*, we study a variation of the functional due to a variation of the field $\phi \to \phi + \delta\phi$:

$$\begin{aligned} F_L[\phi + \delta\phi] &\simeq F_L[\phi] + \int \mathrm{d}^d r \left[2g\, \nabla\phi\, \nabla\delta\phi + f'_L(\phi)\, \delta\phi \right] + \mathcal{O}(\delta\phi^2) \qquad (6.89) \\ &= F_L[\phi] + \int \mathrm{d}^d r \left[-2g\, \Delta\phi(r) + f'_L(\phi(r)) \right] \delta\phi(r) = F_L[\phi] + \int \mathrm{d}^d r\, \frac{\delta F_L[\phi]}{\delta\phi(r)}\, \delta\phi(r) \end{aligned}$$

where we have introduced the "functional derivative"

$$\frac{\delta F_L[\phi]}{\delta\phi(r)} = -2g\, \Delta\phi(r) + f'_L(\phi(r)) \,. \tag{6.90}$$

Functional derivation.— Consider a function F of a vector $\vec{\phi} = (\cdots \phi_r \cdots)$. We write the Taylor expansion :

$$F(\vec{\phi} + \delta\vec{\phi}) = F(\vec{\phi}) + \sum_r \frac{\partial F(\vec{\phi})}{\partial \phi_r}\, \delta\phi_r + \frac{1}{2} \sum_{r,r'} \frac{\partial^2 F(\vec{\phi})}{\partial\phi_r \partial\phi_{r'}}\, \delta\phi_r\, \delta\phi_{r'} + \cdots$$

Note the relation $\partial\phi_x / \partial\phi_y = \delta_{x,y}$, useful to perform derivations.

Consider now a *functional* $F[\phi(r)]$ (an application from a space of functions to $\mathbb{R}$ or $\mathbb{C}$). Considering $\phi(r)$ as the "component" of the "vector" ϕ, we write the expansion

$$F[\phi + \delta\phi] = F[\phi] + \int \mathrm{d}^d r\, \frac{\delta F[\phi]}{\delta\phi(r)}\, \delta\phi(r) + \frac{1}{2} \int \mathrm{d}^d r \mathrm{d}^d r'\, \frac{\delta^2 F[\phi]}{\delta\phi(r)\delta\phi(r')}\, \delta\phi(r)\delta\phi(r') + \cdots \tag{6.91}$$

A useful formula is

$$\boxed{\frac{\delta\phi(r)}{\delta\phi(r')} = \delta(r - r')} \tag{6.92}$$

This relation with the usual rules for derivation allows to compute any functional derivative.

Examples : $\frac{\delta}{\delta\phi(r)} \int \mathrm{d}^d x\, \phi(x)^n = n\, \phi(r)^{n-1}$, $\frac{\delta}{\delta\phi(r)} \int \mathrm{d}^d x\, \mathrm{e}^{\lambda\phi(x)} = \lambda\, \mathrm{e}^{\lambda\phi(r)}$, etc.

The equation for the optimal configuration ϕ_* of the order parameter is now

$$\boxed{\left.\frac{\delta F_L[\phi]}{\delta\phi(r)}\right|_{\phi_*(r)} = 0} \tag{6.93}$$

or more explicitely

$$-2g\,\Delta\phi_*(r) + f_L'(\phi_*(r)) = 0\,. \tag{6.94}$$

Let us now consider the case introduced above, with $f_L(\phi) = -h\,\phi + \frac{a}{2}\phi^2 + \frac{b}{4}\phi^4$. We can also consider a non uniform conjugated field : in this case $F_L[\phi]$ contains a term $-\int \mathrm{d}^d r\, h(r)\phi(r)$. We obtain finally the equation for the optimal field configuration :

$$-2g\,\Delta\phi_*(r) + a\,\phi_*(r) + b\,\phi_*(r)^3 = h(r) \tag{6.95}$$

This is a non linear partial differential equation : such equations are in general extremely difficult to solve. Still, two situations can be analyzed :

- The case of a problem effectively one-dimensional, for example invariant by translation in two directions : $\phi_*(\vec{r}) \to \phi_*(x)$ and the field equation is an ordinary (nonlinear) differential equation $-2g\,\phi_*''(x) + f_L'(\phi_*(x)) = 0$ which can be solved. We can study the interface problem and answer to the interesting question of the related energy cost.
- Assuming a small field, we can look for solutions which are small perturbations around the uniform solution : $\phi_*(r) = \phi_0 + \varphi(r)$ where $f_L'(\phi_0) = 0$ and $\varphi \to 0$ (ϕ_0 was denoted ϕ_* above). Then we can linearize the differential equation and apply standard techniques.

b) Perturbation on the top of a uniform solution

We study solutions of (6.95) of the form

$$\phi_*(r) = \phi_0 + \overbrace{\varphi(r)}^{\text{"small" modulation}} \tag{6.96}$$

where $\phi_0 = 0$ for $T > T_c$ and $\phi_0 = \sqrt{-a/b}$ for $T < T_c$ is the uniform solution (6.65). Linearization of the field equation (6.94) gives the linear differential equation

$$-2g\Delta\varphi(r) + f_L''(\phi_0)\,\varphi(r) \simeq h(r) \tag{6.97}$$

Correlation length.— We identify an important length scale ξ

$$\boxed{\frac{1}{\xi^2} \stackrel{\text{def}}{=} \frac{f_L''(\phi_0)}{2g}} = \frac{a + 3b\phi_0^2}{2g} = \begin{cases} \frac{a}{2g} & \text{for } T > T_c \\ \frac{-a}{g} & \text{for } T < T_c \end{cases} \tag{6.98}$$

Clearly the new length scale is a direct consequence of the introduction of the elastic term in the Landau functional. Dimensional analysis indeed that the dimensions of the various parameters are

$$[h] = \frac{E}{L^d[\phi]} \qquad [a] = \frac{E}{L^d[\phi]^2}\,, \qquad [b] = \frac{E}{L^d[\phi]^4}\,, \qquad [g] = \frac{E}{L^{d-2}[\phi]^2}\,, \tag{6.99}$$

where I used that f_L has dimension of an energy density. With the introduction of g, we can now introduce the length scale $\sqrt{g/|a|}$. Being the unique length scale involved in the differential equation for φ, it coincides with the typical length over which the field varies, hence it can

be interpreted as the *correlation length* (this will become more clear when we will analyze the correlation of the field, below). Explicitly it presents the temperature dependence

$$\xi(T) = \begin{cases} \sqrt{\frac{2g}{\tilde{a}(T-T_c)}} & \text{for } T > T_c \\ \sqrt{\frac{g}{\tilde{a}(T_c-T)}} & \text{for } T < T_c \end{cases} \tag{6.100}$$

The most important feature is its divergence for $T \to T_c$: correlations manifest at larger and larger scales as the critical point is reached. In general we write

$$\boxed{\xi(T) \propto |T - T_c|^{-\nu}} \tag{6.101}$$

in terms of a new critical exponent. The mean field (Landau-Ginzburg) theory thus gives $\boxed{\nu_{\rm mf} = 1/2}$.

Green's function and response function.— We now come back to the differential equation

$$(-\Delta + \xi^{-2})\, \varphi(r) \simeq \frac{1}{2g} h(r)\,. \tag{6.102}$$

Such equation is conveniently solved by introducing the Green's function G of the equation, i.e. the solution of

$$(-\Delta + \xi^{-2})\, G(r) = \delta(r)\,. \tag{6.103}$$

Given G, we can write the solution as a convolution

$$\varphi(r) = \int \mathrm{d}^d r'\, G(r - r')\frac{h(r')}{2g}\,. \tag{6.104}$$

This shows that the Green's function coincides here with the "response function" which characterizes the linear response due to the introduction of the field

$$\phi_*(r) = \phi_0 + \int \mathrm{d}^d r'\, \chi(r - r')\, h(r') + \mathcal{O}(h^2) \tag{6.105}$$

with

$$\boxed{\chi(r) = \frac{1}{2g}\, G(r)} \tag{6.106}$$

in the same spirit as in the first part of the course, with now some additional spatial dependence.

Calculation of the Green's function.— Let us start with the $d = 1$ case : $-G''(x) + \xi^{-2}G(x) = \delta(x)$ is pretty easy to solve. The solution decaying at infinity is $G(x) = A_\pm \mathrm{e}^{\mp x/\xi}$ for $x \in \mathbb{R}^\pm$. The solution must be continuous at the origin, $A_+ = A_-$ and should satisfy the matching condition $-G'(0^+) + G'(0^-) = 1$. Hence

$$G(x) = \frac{\xi}{2}\, \mathrm{e}^{-|x|/\xi} \qquad \text{in } d = 1\,. \tag{6.107}$$

This makes clear that the value of the order parameter at x, $\varphi(x) = \frac{\xi}{4g}\int \mathrm{d}x'\, \mathrm{e}^{-|x-x'|/\xi}\, h(x')$ involves only the field at distance $|x' - x| \lesssim \xi$, hence the interpretation of ξ as a correlation length.

In order to derive the general expression for G (in any dimension), it is more convenient to use Fourier transform, leading to :

$$G(\vec{r}) = \int \frac{\mathrm{d}^d \vec{q}}{(2\pi)^d}\, \frac{\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}}}{\vec{q}^{\,2} + \xi^{-2}} \tag{6.108}$$

The multiple integral can be made separable with the following trick : introduce

$$\frac{1}{\vec{q}^{\,2}+\xi^{-2}} = \int_0^\infty \mathrm{d}y\, \mathrm{e}^{-y(\vec{q}^{\,2}+\xi^{-2})} \tag{6.109}$$

then the integral over $\vec{q}$ is a simple Gaussian multiple integral and we are left with the integral representation

$$G(\vec{r}) = \frac{1}{(4\pi)^{d/2}} \int_0^\infty \frac{\mathrm{d}y}{y^{d/2}}\, \mathrm{e}^{-y/\xi^2 - \vec{r}^{\,2}/(4y)}\,. \tag{6.110}$$

This representation is convenient to analyze the limiting behaviours.

✍ ***Exercice 6.17 :*** *Deduce the limiting behaviours of the Green's function (for $r \ll \xi$ and $r \gg \xi$) from asymptotic analysis on the integral representation (6.110).*

However a little knowledge on special functions shows that the integral corresponds to the MacDonald function K_ν for $\nu = (d-2)/2$ (modified Bessel function of third kind) :

$$\boxed{G(\vec{r}) = \frac{1}{(2\pi)^{d/2}(r\xi)^{\frac{d}{2}-1}} K_{\frac{d}{2}-1}(r/\xi)} \tag{6.111}$$

where $r = ||\vec{r}||$. Using the limiting behaviours [15, 1]

$$K_\nu(z) \simeq \frac{\Gamma(\nu)}{2}\left(\frac{z}{2}\right)^{-\nu} \quad \text{for } z \to 0 \text{ with } \nu \neq 0 \tag{6.112}$$

$$K_\nu(z) \simeq \sqrt{\frac{\pi}{2z}}\, \mathrm{e}^{-z} \quad \text{for } z \to \infty \tag{6.113}$$

$$K_0(z) \simeq \ln(2/z) - \mathbf{C} \quad \text{for } z \to 0 \tag{6.114}$$

where $\mathbf{C} = 0.577...$ is the Euler-Mascheroni constant, we conclude that

$$G(\vec{r}) \underset{r\to 0}{\sim} \begin{cases} \xi & \text{for } d = 1 \\ \ln(\xi/r) & \text{for } d = 2 \\ r^{-d+2} & \text{for } d > 2 \end{cases} \tag{6.115}$$

and

$$G(\vec{r}) \underset{r\to\infty}{\sim} \frac{1}{r^{\frac{d-2}{2}}}\, \mathrm{e}^{-r/\xi}\,. \tag{6.116}$$

Using the limiting behaviour of the MacDonald function, we get the behaviour of the Green's function at the critical point (i.e. for $\xi \to \infty$) :

$$G(\vec{r}) = \frac{\Gamma(\frac{d}{2}-1)}{4\pi^{d/2}} \frac{1}{r^{d-2}} \qquad \text{for } T = T_c\,. \tag{6.117}$$

In $d = 2$ we obtain [34] $G(\vec{r}) = -\frac{1}{2\pi}\ln r$.

c) Summary of critical exponents in the mean field approximation

We summarize in all the critical exponents introduced above. Introducing the rescaled temperature, $t = (T - T_c)/T_c$, the scaling behaviour with mean field exponents are given in table 1 below (page 117).

[34] The 2D result can be deduced from (6.117) by *dimensional regularization* : write $d = 2+\epsilon$ and let $\epsilon \to 0$ in in the expression (use $\Gamma(z) \simeq 1/z$ for $z \to 0$. The infinite term is a constant and can be disregarded as the Green's function is defined up to a constant.

7 Beyond mean field

The development of the Ginzburg-Landau theory has led to the representation of the partition function in terms of a path integral over the order parameter :

$$Z = \int \mathcal{D}\phi \, \mathrm{e}^{-\beta F_L[\phi]} \qquad \text{with } F_L[\phi] = \int \mathrm{d}^d r \left[g \left(\nabla \phi(r) \right)^2 + f_L(\phi(r); h(r)) \right] , \tag{7.1}$$

where $f_L(\phi; h) = f_0 - h\phi + \frac{1}{2} a\phi^2 + \frac{1}{4} b\phi^4$ is the Landau free energy. Correspondingly, the (canonical) weight of a field configuration is

$$P[\phi] = \frac{\mathscr{Z}_L[\phi]}{Z} \propto \mathrm{e}^{-\beta F_L[\phi]} . \tag{7.2}$$

This representation of Z was deduced from the coarse graining procedure, by assuming that the field $\phi(r)$ is smooth (at the scale of the lattice). In a more precise presentation, the passage from the original Ising partition function (6.37) to (7.1) means that we have "integrated over the short scale fluctuations" to get a representation of Z involving only large scale fluctuations.

7.1 Fluctuation-response relation

In this paragraph, we first discuss how we can characterize, in practice, the fluctuations/correlations. The continuous formulation is quite interesting : the partition function Z is a *functional* of the conjugated field configuration $h(r)$, which allows to obtain a formula for the mean value of the field. The field $h(r)$ is conjugated to the order parameter, hence $F_L[\phi]$ contains the term $-\int h\phi$ and thus :

$$\frac{\delta F_L[\phi]}{\delta h(r)} = -\phi(r) . \tag{7.3}$$

Using this relation, we find

$$\frac{\delta}{\delta h(r)} \ln Z = \frac{1}{Z} \frac{\delta}{\delta h(r)} \int \mathcal{D}\phi \, \mathrm{e}^{-\beta F_L[\phi]} = \frac{\beta}{Z} \int \mathcal{D}\phi \, \phi(r) \, \mathrm{e}^{-\beta F_L[\phi]} \tag{7.4}$$

i.e. the canonical average of the field is

$$\boxed{\langle \phi(r) \rangle = \frac{1}{\beta} \frac{\delta}{\delta h(r)} \ln Z = -\frac{\delta F}{\delta h(r)}} , \tag{7.5}$$

which is the *local* version of the well known formula $\overline{M}^{\mathrm{c}} = -\frac{\partial F}{\partial B}$. In the same way we can write the correlation function as

$$\left\langle \phi(r) \phi(r') \right\rangle = \frac{1}{\beta^2 Z} \frac{\delta^2 Z}{\delta h(r) \delta h(r')} \tag{7.6}$$

etc. One can easily check that the connex correlation function is

$$C_h(r, r') = \left\langle \phi(r) \phi(r') \right\rangle_c \overset{\text{def}}{=} \left\langle \phi(r) \phi(r') \right\rangle - \langle \phi(r) \rangle \langle \phi(r') \rangle = \frac{1}{\beta^2} \frac{\delta^2}{\delta h(r) \delta h(r')} \ln Z \tag{7.7}$$

This relation shows that the correlator can be written as a derivative of the averaged value

$$C_h(r, r') = \frac{1}{\beta} \frac{\delta}{\delta h(r')} \langle \phi(r) \rangle \tag{7.8}$$

The mean value of the field $\langle \phi(r) \rangle$ can be expanded in powers of the conjugated field as follows

$$\langle \phi(r) \rangle \big|_h = \langle \phi(r) \rangle \big|_0 + \int \mathrm{d}^d r' \, \chi(r - r') \, h(r') + \mathcal{O}(h^2) \tag{7.9}$$

where $\chi(r)$ is the (linear) response function introduced above. This follows from the fact that the measure $P[\phi]$ is strongly concentrated around $\phi_*(r)$ (assumption of the Ginzburg-Landau approach), hence $\langle\phi(r)\rangle = \phi_*(r)$ where $\phi_*(r)$ solves (6.93). The above equation is nothing else but the expansion (6.105). This shows that

$$\frac{\delta\,\langle\phi(r)\rangle\,\big|_h}{\delta h(r')} = \chi(r-r') + \mathcal{O}(h) \tag{7.10}$$

and thus we obtain the important "*fluctuation-response*" relation

$$\chi(r-r') = \beta\, C(r-r') \tag{7.11}$$

where $C(r-r') = C_{h=0}(r,r')$ is the correlator for $h=0$. [35] This relation is a "fluctuation-response" relation, as it relates the response function, controlling how the field "responds" to the introduction of an external field, and the fluctuations. This is also called the "fluctuation-dissipation theorem" (although dissipative phenomena in principle involve the dynamic response function, and not the static one, as we have seen in the first part of the lectures).

Note that (7.11) is the local version of the relation $\chi = -\frac{\partial^2 F}{\partial B^2}\big|_{B=0} = \langle\delta M^2\rangle/(k_{\rm B}T)$ [48].

We have analyzed in great detail the Green's function above. All functions can thus be related :

$$\boxed{\chi(r) = \beta\, C(r) = \frac{1}{2g}\, G(r)} \tag{7.12}$$

where G is given by (6.111). The Green's function decay exponentially as $C(r) \sim G(r) \sim \exp\{-||r||/\xi\}$, hence the field is only correlated over length scales smaller than ξ, which provides a more direct definition of ξ as a correlation length.

A last critical exponent : The result obtained above for the Green's function characterizes the correlations of the field $C(r) = \langle\delta\phi(r)\delta\phi(0)\rangle$, where $\delta\phi(r) = \phi(r) - \langle\phi(r)\rangle$. Away from the critical point, the correlations are short range and decay over the scale ξ. Exactly at the critical point ($T = T_c$ and $h = 0$), we rather obtain the power law behaviour

$$\boxed{C(\vec{r}) \sim \frac{1}{r^{d-2+\eta}} \qquad \text{for } T = T_c} \tag{7.13}$$

with a critical exponent η. The mean field approximation (behaviour $C(r) = \frac{T_c}{2g}G(r) \sim ||r||^{-d+2}$ at $T = T_c$ given above) thus predicts $\boxed{\eta_{\rm mf} = 0}$.

7.2 The Gaussian approximation and the "one-loop" correction

Preliminary (technical) : steepest descent approximation : We have used above the formula

$$\int \mathrm{d}\phi\, \mathrm{e}^{-k f(\phi)} \underset{k\to\infty}{\simeq} \sqrt{\frac{2\pi}{k f''(\phi_*)}}\, \mathrm{e}^{-k\, f(\phi_*)} \tag{7.14}$$

where ϕ_* is the minimum of $f(\phi)$ (assumed to have a unique minimum).

The generalization to an integral over $\mathbb{R}^D$ is not difficult (still assuming the existence of a unique minimum). It requires a Gaussian integration in $\mathbb{R}^D$

$$\int \mathrm{d}^D\vec{\phi}\, \mathrm{e}^{-k\, f(\vec{\phi})} \underset{k\to\infty}{\simeq} \frac{(2\pi/k)^{D/2}}{\sqrt{\det(\partial_i\partial_j f|_{\vec{\phi}_*})}}\, \mathrm{e}^{-k\, f(\vec{\phi}_*)} \quad \text{with} \quad \frac{\partial f}{\partial\phi_i}\Big|_{\vec{\phi}_*} = 0\ \forall\, i\,. \tag{7.15}$$

[35] In the presence of the conjugated field $h(r)$, the correlator $C_h(r,r')$ is not translation invariant. However when $h(r) \to 0$ (or uniform in space), translation invariance is restored, as shown by the calculation of $\chi(r-r')$.

Denoting by $\lambda_i > 0$ the eigenvalue of the $D \times D$ Hessian matrix $\mathcal{H}_{ij} = \partial_i \partial_j f|_{\vec{\phi}_*}$, we can rewrite the formula as

$$\int \mathrm{d}^D \vec{\phi}\, \mathrm{e}^{-k\, f(\vec{\phi})} \underset{k\to\infty}{\simeq} \frac{1}{\sqrt{\prod_{i=1}^{D} \frac{k\,\lambda_i}{2\pi}}}\, \mathrm{e}^{-k\, f(\vec{\phi}_*)} = \frac{1}{\sqrt{\det\left[\frac{k}{2\pi}\mathcal{H}\right]}}\, \mathrm{e}^{-k\, f(\vec{\phi}_*)}\,. \tag{7.16}$$

a) Effect of fluctuations on the thermodynamic properties

Start first with the formulation developped in § 6.2 : Eq. (6.47) can be rewritten as

$$\frac{F(T,N)}{N} \simeq \underbrace{f_L(\phi_*;T)}_{\text{mean field}} + \underbrace{\frac{1}{N}\,\frac{T}{2}\,\ln\left(\frac{2\beta f_L''(\phi_*;T)}{\pi N}\right)}_{\text{uniform fluctuations}} \tag{7.17}$$

where the second contribution originates from the Gaussian integration around ϕ_*, i.e. the effect of the fluctuations of ϕ around its average in the calculation of (6.43). Of course, this fluctuation term disappears in the thermodynamic limit $N \to \infty$. This approach is however very schematic : the system is not characterized by a single degree of freedom (the spatial average of the local magnetization $\phi = \frac{1}{N}\sum_i \sigma_i$), but by a macroscopic number of degrees of freedom N_{df}. Hence, we expect rather the structure

$$\frac{F(T,N)}{N} \simeq \underbrace{f_L(\phi_*;T)}_{\text{mean field}} + \underbrace{\frac{N_{\mathrm{df}}}{N}\,\frac{T}{2}\,\ln(\cdots)}_{\text{fluctuations of } N_{\mathrm{df}} \text{ modes}} \tag{7.18}$$

Because $N_{\mathrm{df}} \sim N$, the contribution of fluctuations has no reason to vanish in the thermodynamic limit.

b) Calculation of the "one-loop" correction

The path integral formulation provides a simple way to formulate the calculation of the contribution of fluctuations. Let us expand the free energy functional around the optimal solution as

$$F_L[\phi_* + \eta] \simeq F_L[\phi_*] + g \int \mathrm{d}^d r\, \eta(r)(-\Delta + \xi^{-2})\eta(r) \tag{7.19}$$

where $\eta(r)$ is a fluctuation. The calculation of the partition function is reduced to a Gaussian path integral

$$Z = \int \mathcal{D}\phi\, \mathrm{e}^{-\beta F_L[\phi]} \simeq \mathrm{e}^{-\beta F_L[\phi_*]} \int \mathcal{D}\eta\, \mathrm{e}^{-\beta g \int \mathrm{d}^d r\, \eta(r)(-\Delta+\xi^{-2})\eta(r)} \tag{7.20}$$

(Jacobian is one, $\mathcal{D}\phi = \mathcal{D}\eta$ since $\phi = \phi_* + \eta$ is a translation). Remembering that the original problem was defined on a lattice, we extend the formula for Gaussian integration in $\mathbb{R}^D$ to the path integration and write

$$Z \simeq \underbrace{\frac{1}{\sqrt{\det[\frac{\beta g}{\pi}(-\Delta+\xi^{-2})]}}}_{\text{fluctuations}} \underbrace{\mathrm{e}^{-\beta F_L[\phi_*]}}_{\text{mean field}} \tag{7.21}$$

where the only remaining difficulty is to give a precise meaning to the determinant of the operator. This provides the first correction to the mean field solution :

$$F = F_L[\phi_*] + \frac{1}{2\beta}\ln\det\left[\frac{\beta g}{\pi}(-\Delta+\xi^{-2})\right] \equiv F_L[\phi_*] + \delta F_{1\,\mathrm{loop}}\,. \tag{7.22}$$

This correction is known as the "one-loop correction" (this terminology comes from the diagrammatic methods).

The determinant can be expressed as a product over the eigenvalues of the operator : here the spectrum of eigenvalues of the Laplace operator Δ is simply $-\vec{q}^2$:

$$\delta F_{1\,\mathrm{loop}} = \frac{T}{2} \ln \left(\prod_{\vec{q}} \left[\frac{g}{\pi T} (\vec{q}^2 + \xi^{-2}) \right] \right) \tag{7.23}$$

We have obtained a simple formula, however the problem comes from the infinite product

$$\prod_{\vec{q}} \left[\frac{g}{\pi T} (\vec{q}^2 + \xi^{-2}) \right] = \infty \tag{7.24}$$

as the spectrum of $-\Delta$ is not bounded from above. Let us now see how one can solve this problem.

Cutoffs.— We should remember that the original model is a lattice model for a finite volume (finite number of spins). The continuous Laplace operator arises here only due to the continuous description. Coming back to the lattice model would have mostly produced a "discrete Laplacian".

- Large scale ("infrared") cutoff : the existence of a finite volume $V = L^d$ implies that summation over $\vec{q}$ is discrete (wave vectors are quantized) and the smaller allowed wave length is $q \sim 1/L$.
- Small scale ("UV") cutoff : the existence of a lattice with lattice spacing ϵ implies that the largest wave length is $q \sim 1/\epsilon$ (in principle wave vectors belong to the Brillouin zone, of size $\sim 1/\epsilon$).

In conclusion

$$\frac{1}{V} \sum_{\vec{q}} \to \int_{1/L<q<1/\epsilon} \frac{\mathrm{d}^d \vec{q}}{(2\pi)^d} \tag{7.25}$$

We now consider the correction to the free energy per unit volume, $\delta f_{1\,\mathrm{loop}} \overset{\mathrm{def}}{=} \delta F_{1\,\mathrm{loop}}/V$,

$$\boxed{\delta f_{1\,\mathrm{loop}} = \frac{T}{2} \int_{q<1/\epsilon} \frac{\mathrm{d}^d \vec{q}}{(2\pi)^d} \ln \left[\frac{g}{\pi T} (\vec{q}^2 + \xi^{-2}) \right]} \tag{7.26}$$

where we have forgotten the IR cutoff, which is now played by the correlation length ξ, as we will see clearly. As anticipated, we have obtained that the fluctuations give a finite contribution to the free energy in the thermodynamic limit, as the number of degree of freedom is extensive.

✍ ***Exercice 7.1 Regularization : lattice of blocks :*** *The original model is a lattice model. Starting from (6.82) we can come back to the discrete formulation and replace the Ginzburg-Landau function by*

$$F_L(\{\phi_r\}) = \frac{J \ell^{d-1}}{2} \sum_{\langle r,r' \rangle} (\phi_r - \phi_{r'})^2 + \ell^d \sum_{\text{block } r} f_L(\phi_r) \tag{7.27}$$

where (ϕ_r is the field in block r. The blocks form a square lattice with lattice spacing $\ell\epsilon$. Assuming a finite size (a finite number of spins), derive a formula for $\delta f_{1\,\mathrm{loop}} = \delta F_{1\,\mathrm{loop}}/V$, the correction to the free energy per unit volume due to field fluctuations. Compare with (7.26).

The most interesting property is the heat capacity. Because the correlation length diverges as $T \to T_c$, we anticipate that the most important temperature dependency is those of ξ. Hence, we simplify the calculation by doing $T \to T_c$ for the temperature in factor in (7.26). We introduce the rescaled temperature

$$t \stackrel{\text{def}}{=} \frac{T - T_c}{T_c} \tag{7.28}$$

thus the one-loop correction to the heat capacity is

$$\delta c_{1\,\text{loop}}(t) = -T \frac{\partial^2 \delta f_{1\,\text{loop}}}{\partial T^2} \simeq -\frac{1}{T_c} \frac{\partial^2 \delta f_{1\,\text{loop}}}{\partial t^2} \tag{7.29}$$

leading to

$$\boxed{\delta c_{1\,\text{loop}}(t) \simeq \frac{1}{2} \left(\frac{\partial \xi^{-2}}{\partial t} \right)^2 \int_{q<1/\epsilon} \frac{\mathrm{d}^d \vec{q}}{(2\pi)^d} \frac{1}{(\vec{q}^2 + \xi^{-2})^2}} \tag{7.30}$$

If we want to study the case $\xi = \infty$, then we have to reintroduce the IR cutoff $\xi \to L$.

We write Eq. (6.98) as

$$\frac{1}{\xi^2} = \frac{\tilde{a} T_c}{2g} \begin{cases} t & \text{for } T > T_c \\ -2t & \text{for } T < T_c \end{cases} \tag{7.31}$$

leading to

$$\frac{\partial \xi(t)^{-2}}{\partial t} = \xi(1)^{-2} \begin{cases} 1 & \text{for } T > T_c \\ -2 & \text{for } T < T_c \end{cases} \tag{7.32}$$

where $\xi(1) = \sqrt{2g/\tilde{a}T_c}$. Performing the integration as

$$\int_{q<1/\epsilon} \frac{\mathrm{d}^d \vec{q}}{(2\pi)^d} \frac{1}{(\vec{q}^2 + \xi^{-2})^2} \sim \int_0^{1/\epsilon} \mathrm{d}q \, \frac{q^{d-1}}{(q^2 + \xi^{-2})^2} \simeq \int_{1/\xi}^{1/\epsilon} \mathrm{d}q \, q^{d-5} \tag{7.33}$$

we conclude that

$$\delta c_{1\,\text{loop}}(t) \sim \left(\frac{\partial \xi^{-2}}{\partial t} \right)^2 \times \begin{cases} \frac{1}{4-d} \left(\xi^{4-d} - \epsilon^{4-d} \right) & \text{for } d \neq 4 \\ \ln(\xi/\epsilon) & \text{for } d = 4 \end{cases} \tag{7.34}$$

The most interesting feature is the dependency in the dimension, which we discuss below.

✍ ***Exercice 7.2 :*** *Show that the derivation of (7.30) has neglected a contribution to* $\delta c_{1\,\text{loop}}(t)$

$$\delta c_{1\,\text{loop}}^{\text{forgotten}} = -\left(\frac{\partial \xi^{-2}}{\partial t} \right) \int_{q<1/\epsilon} \frac{\mathrm{d}^d \vec{q}}{(2\pi)^d} \frac{1}{\vec{q}^2 + \xi^{-2}} \tag{7.35}$$

Argue that it is negligible.

Case $d > 4$ **:** above dimension four the integral is dominated by the UV cutoff, thus the correction

$$\delta c_{1\,\text{loop}}(t) \sim \xi(1)^{-4} \epsilon^{4-d} \times \begin{cases} 1 & \text{for } T > T_c \\ 4 & \text{for } T < T_c \end{cases} \tag{7.36}$$

where I have reintroduced the factor $(\frac{\partial \xi^{-2}}{\partial t})^2$. Hence the correction is independent of the temperature (apart for the jump around T_c).

Case $d = 4$ **:** this is called the "marginal" case. In general logarithmic corrections appear. Here we have obtained

$$\delta c_{1\,\text{loop}}(t) \sim -\xi(1)^{-4} \ln |t| \,. \tag{7.37}$$

Case $d < 4$: In this case the correction is dominated by the large scales and we get a temperature dependence

$$\delta c_{1\,\mathrm{loop}}(t) \sim \left(\frac{\partial \xi^{-2}}{\partial t}\right)^2 \xi(t)^{4-d} \tag{7.38}$$

The mean field correlation length diverges at T_c, as $\xi(t) = \xi(1)|t|^{-1/2}$ (for $t > 0$), thus we get a diverging correction

$$\boxed{\delta c_{1\,\mathrm{loop}}(t) \sim \xi(1)^{-d}\,|t|^{-\frac{4-d}{2}} \times \begin{cases} 1 & \text{for } T > T_c \\ 4 & \text{for } T < T_c \end{cases}} \tag{7.39}$$

The critical exponent of the heat capacity, $c(t) \sim A_\pm |t|^{-\alpha}$, has thus changed from $\alpha_{\mathrm{mf}} = 0$ (mean field) to

$$\alpha_{1\,\mathrm{loop}} = \frac{4-d}{2}\,. \tag{7.40}$$

We have also : $A_+/A_- = 1/4$.

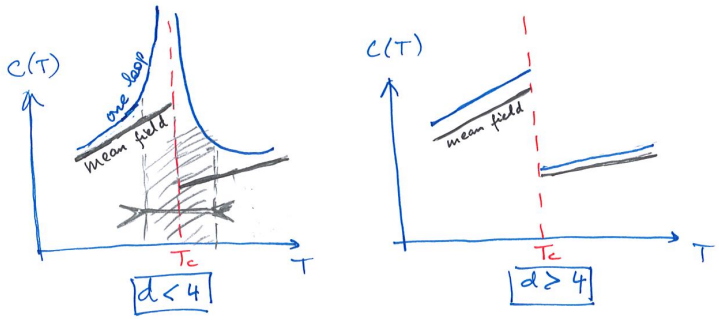


Figure 48: *The specific heat with the one-loop correction. The shaded region corresponds to the region where mean field breaks down.*

7.3 The Ginzburg criterion

a) From the one-loop correction

We have just analysed a first correction $\delta f_{1\,\mathrm{loop}}$ to the mean field solution $f_{\mathrm{mf}}(t) = F_L[\phi_*]/V$ which arises from the fluctuations of the field around ϕ_* in the path integral (7.21). The justification for such an expansion is therefore that fluctuations should remain "small" and therefore corrections to thermodynamic property should remain small as well :

$$f_{\mathrm{mf}}(t) \gg \delta f_{1\,\mathrm{loop}}(t) \tag{7.41}$$

For the heat capacity, we should compare $\delta c_{1\,\mathrm{loop}}$ to the jump of the heat capacity obtained above, Δc_{mf}, thus, using the expression for $d < 4$, we conclude that the validity of the mean field treatment requires

$$\boxed{|t|^{\frac{4-d}{2}} \gg \frac{1}{\xi(1)^d\,\Delta c_{\mathrm{mf}}}} \tag{7.42}$$

This condition is called the "*Ginzburg criterion*". It is fulfilled as $t \to 0$ for $d > 4$, which means that the mean field approximation correctly describes the vicinity of the second order phase transition only when $d > 4$ (for the Ising universality class). For $d < 4$, the condition get violated as one gets closer to the critical point. The dimension where the transition occur is called the **upper critical dimension** : for the Ising university class we have

$$d_u = 4\,. \tag{7.43}$$

b) The Ginzburg estimate

A more direct derivation of the Ginzburg criterion is provided by comparing the field fluctuations and the averaged field. We introduce the **Ginzburg estimate**

$$E_{\rm G} \stackrel{\rm def}{=} \frac{\int_V {\rm d}^d r \int_V {\rm d}^d r' \ \langle \delta\phi(r)\delta\phi(r')\rangle}{\Big[\int_V {\rm d}^d r \ \langle\phi(r)\rangle\Big]^2} \tag{7.44}$$

where $\delta\phi(r) = \phi(r) - \langle\phi(r)\rangle$. We recognize the connex correlation $C(r-r')$ in the numerator. In the denominator we can write $\langle\phi(r)\rangle = \phi_*$, thus, using translation invariance

$$\boxed{E_{\rm G} \simeq \frac{\int_V {\rm d}^d r\, C(r)}{V\,\phi_*^2}} \tag{7.45}$$

We have to consider the situation with largest fluctuations, hence we choose the volume to be $V = \xi^d$: Using that $\phi_* = \sqrt{\tilde{a}T_c(-t)/b}$ for $t<0$, we see that the denominator is

$$\xi^d\,\phi_*^2 = \xi^d\,\frac{\tilde{a}T_c}{b}(-t)\,. \tag{7.46}$$

The numerator is estimated by using (7.12) and the expression of the Green's function (6.115,6.116) :

$$\int_V {\rm d}^d r\, C(r) \sim \frac{T}{g}\int_0^\xi \frac{{\rm d}r\, r^{d-1}}{r^{d-2}} \sim \frac{T_c}{g}\xi^2 \tag{7.47}$$

Finally the Ginzburg estimate is

$$E_{\rm G} \sim \frac{b\,\xi(t)^{2-d}}{\tilde{a}\,g\,(-t)} \tag{7.48}$$

Using the expression (6.69), we get $\tilde{a}\,g/b = \Delta c_{\rm mf}\,\xi(1)^2$. Finally the Ginzburg criterion takes the form

$$\boxed{E_{\rm G} \sim \frac{|t|^{(d-4)/2}}{\Delta c_{\rm mf}\,\xi(1)^d} \ll 1} \tag{7.49}$$

This is equivalent to (7.42) (however we did not have to assume that $d<4$).

c) The upper critical dimension d_u

Let us summarize the situation :

- In $d > 4 = d_u$, the Ginzburg estimate gets smaller as $t \to 0$, thus the singular behaviours close to T_c, predicted by the mean field picture, are not modified by accounting for the fluctuations. As mentioned above, the justification for the mean field approximation is that each particle is surrounded by many neighbours, so that the effect of neighbouring interactions is dominated by the average rather than the fluctuations. As a result, it would have been natural that the mean field approximation hold for high dimension, being only asymptotically exact for $d \to \infty$. This is indeed what physicists thought until the seventies. At this point, it is important to distinguish "*universal properties*" (like the critical exponents) and "*non universal properties*" (like the expression of T_c as a function of microscopic parameters). What shows the analysis is that universal properties are correctly predicted by the mean field approximation above $d_u = 4$, while the non universal properties are quantitavely predicted by the mean field only asymptotically for $d \to \infty$. Still, the existence of the upper critical dimension $d_u = 4$ is remarkable.

- In $d < 4$, we expect that the fluctuations are not dominant away from the critical point, as the correlation length is "small", thus the mean field approximation is correct sufficiently far from T_c, however it does not correctly describe the vicinity of the critical point. There exists a domain in temperature $[T_c - \delta T_*, T_c + \delta T_*]$, where (7.42) is violated, however mean field approximation provides a correct picture out of this region. The window has width

$$\delta t_* = \delta T_*/T_c = \left[\Delta c_{\rm mf}\, \xi(1)^d\right]^{-\frac{2}{4-d}} . \tag{7.50}$$

  The breakdown of the mean field approximation for $t \to 0$ shows that the correct critical exponents are *not* those given by the mean field approximation, although the system is expected to remain critical (because $\xi \to \infty$ as $T \to T_c$).
- In $d = 4$, the mean field results are corrected by logarithmic corrections.

In practice, mean field is however still broadly used in many situations as it provides a good description, although sometimes only qualitative.

It might also be that the region where mean field breaks down is small in practice, i.e. that δT_* is so small that the breakdown of mean field is irrelevant from a practical point of view. This is for example the case in the theory of superconductivity (BCS theory).

d) The Ginzburg estimate in the general case

The upper critical dimension depends on the nature of the problem (nature of order parameter, etc). However we can formulate the calculation of the Ginzburg estimate in a more general case. Using (7.12), we write the numerator of the Ginzburg estimate as $\int \mathrm{d}^d r\, C(r) = T \int \mathrm{d}^d r\, \chi(r) = T\,\chi \sim |t|^{-\gamma}$ [the susceptibility χ introduced at first is the response coefficient for a uniform field, hence it is the integral of the response function $\chi(r)$]. The denominator is $\xi^d\, \phi_*^2 \sim |t|^{-d\nu+2\beta}$. We get

$$E_{\rm G} \sim |t|^{-\gamma+d\nu-2\beta} \tag{7.51}$$

The upper critical dimension is the dimension for which the exponent changes in signs, thus

$$\boxed{d_u = \frac{2\beta+\gamma}{\nu}} \tag{7.52}$$

where the three critical exponents are calculated in the mean field approximation.

e) The lower critical dimension d_l

In the lectures, we are discussing systems in the "Ising universality class", i.e. for a real scalar order parameter. In $d = 2$, it was demonstrated by Onsager in 1940 that the model presents a PARA/FERRO transition. However it is well known that the Ising model for short range interaction does not exhibit a phase transition in $d = 1$: the exact calculation of the free energy is performed in Exercise 8.1 where it is shown that the free energy is a perfectly regular function, cf. Eq. (A.156). The reason is that the effect of thermal fluctuations is stronger in low dimensions and, as dimension diminishes, it eventually prevents the existence of a stable ordered (ferromagnetic) phase. This occurs when the dimension is lower that the "*lower critical dimension* d_l", which is this $d_l = 1$ for the Ising universality class.

7.4 Scaling laws

We have seen that although it is often a good starting point, the mean field approximation does not provide the accurate description for $T \to T_c$ (for $d < d_u$). However, despite it is

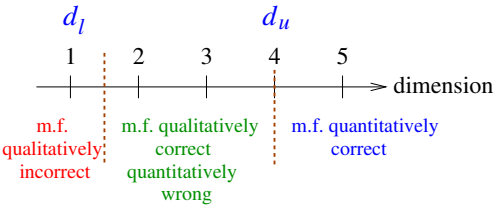


Figure 49: *Below the lower critical dimension d_l, the fluctuations do not allow the existence of an ordered phase. Between d_l and the upper critical dimension d_u, the mean field provides the qualitative picture, although it fails to predict the critical exponents. Above d_u, the mean field provide the critical exponents (universal properties).*

quantitatively wrong, the mean field provides the good qualitative description when $d > d_l$. In particular it predicts that

$$\xi \to \infty \quad \text{for} \quad T \to T_c \,,$$

i.e. the system is *critical* close to T_c. Leaving to a later discussion the question of the determination of the critical exponents, we want now to discuss here the consequence of the critical behaviour (existence of scaling laws). The aim of the paragraph is to show that despite we have introduced several (six) critical exponents, these exponents are constrained by "super-universal" relations. This has a very practical consequence : it is sufficient to measure few of them to get all exponents, characterizing all scaling properties. The question is thus : what is the minimal number of exponents which fully characterize the universal properties of a system ?

a) Scaling in the free energy

At this step, it is interesting to come back on the mean field free energy for the Ising model. The result is $f = \frac{1}{2}T_c\,\phi_*^2 + \frac{1}{2}T\ln((1-\phi_*^2)/4)$ where the order parameter solves the self-consitent equation $\phi_* = \tanh((T_c\phi_* + B)/T)$ (cf. Exercise 6.9). Introducing $h = B/T_c$ and $t = (T - T_c)/T_c$, we get

$$f(t,h) = \frac{1}{2}T_c\left\{-(1+t)\ln 4 + \phi_*^2 + (1+t)\ln(1-\phi_*^2)\right\} \qquad \text{where } \phi_* = \tanh\left(\frac{\phi_* + h}{1+t}\right) \tag{7.53}$$

is the self-consistent equation for the order parameter. Its expansion for $h \to 0$ near the critical point takes the form :

$$\frac{1}{T_c}f(t,h) \underset{h\to 0}{\simeq} \begin{cases} -(1+t)\ln 2 - \frac{3t^2}{4} + \cdots - |h|\sqrt{-3t}\left(1 + \frac{2t}{5} + \cdots\right) + h^2\,\frac{1}{4t}\left(1 + \frac{9t}{5} + \cdots\right) & \text{for } t < 0 \\ -\ln 2 - \frac{1}{4}\,(3|h|)^{4/3} + \cdots & \text{for } t = 0 \\ -(1+t)\ln 2 - h^2\,\frac{1}{2t} + \cdots & \text{for } t > 0 \end{cases}$$

(see Fig. 45). Although the problem (the calculation of the partition function) is controlled by three dimensional parameters, T, J and B, there exists a point $(T = T_c, B = 0)$ around which the free energy exhibits power law behaviours, in both arguments h and t.

Numerical results (Table 1) and experiments show that we expect in general the following behaviours

$$f(t,h) \underset{h\to 0}{\simeq} f_{\rm reg}(t,h) - \begin{cases} a_-\,(-t)^{2-\alpha} + b|h|\,(-t)^{\beta} + c_-h^2\,(-t)^{-\gamma} & \text{for } t < 0 \\ d\,|h|^{1+1/\delta} & \text{for } t = 0 \\ a_+\,t^{2-\alpha} + c_+h^2\,t^{-\gamma} & \text{for } t > 0 \end{cases}$$

where $a_\pm$, b, $c_\pm$ and d are non universal constants and α, β, γ and δ a set of four universal critical exponents. The aim of the paragraph is to show that there exists super-universal relations between the critical exponents.

exponent	quantity	behaviour	Ising 2D	Ising 3D	mean field
α	specific heat	$c(t) \sim \lvert t\rvert^{-\alpha}$	0 (log.)	0.110 ± 0.001	0 (discont.)
β	order parameter	$\phi(t,0) \sim (-t)^{\beta}$	1/8	0.3265 ± 0.0003	1/2
γ	susceptibility	$\chi(t) \sim \lvert t\rvert^{-\gamma}$	7/4	1.2372 ± 0.0005	1
δ	critical isotherm	$\phi(0,h) \sim h^{1/\delta}$	15	4.789 ± 0.002	3
ν	correlation length	$\xi(t) \sim \lvert t\rvert^{-\nu}$	1	0.6301 ± 0.0004	1/2
η	GF at T_c	$G(r) \sim r^{-d+2-\eta}$	1/4	0.0364 ± 0.0005	0

Table 1: Critical exponents of the Ising university class. Exponents for Ising 3D are given in the review by Pelissetto & Vicari [34].

b) Anomalous dimensions

Many scaling laws simply follow from dimensional analysis : a rather simple example is the Kepler's law. [36] Hence, let us start with a bit of dimensionless analysis. We base again the discussion on the Ising universality class. The Ginzburg-Landau's approach, is based on the continuous formulation with the functional

$$F_L[\phi] = \int \mathrm{d}^d r \, \left[g \, (\nabla\phi)^2 - h \, \phi + \frac{1}{2} a \, \phi^2 + \frac{1}{4} b \, \phi^4 \right] . \tag{7.54}$$

For convenience, we now rescale the various quantities as follows :

$$\phi = \frac{\varphi}{\sqrt{\beta \, g}} , \quad h = \tilde{h} \sqrt{g/\beta} , \quad a = g \, A , \quad b = \beta \, g^2 \, B \tag{7.55}$$

we obtain the dimensionless functional

$$\boxed{\widetilde{F}[\varphi] \stackrel{\text{def}}{=} \beta F_L[\phi] = \int \mathrm{d}^d r \, \left[(\nabla\varphi)^2 - \tilde{h} \, \varphi + \frac{1}{2} A \, \varphi^2 + \frac{1}{4} B \, \varphi^2 \right]} \tag{7.56}$$

where all dimensions are express in terms of length

$$[\varphi] = L^{1-d/2} , \quad [\tilde{h}] = L^{-1-d/2} , \quad [A] = L^{-2} , \quad [B] = L^{d-4} . \tag{7.57}$$

The canonical weight of a field configuration $\varphi(r)$ is now $\mathrm{e}^{-\widetilde{F}[\varphi]}$. The partition function seems a function of the three parameters

$$Z(A, B, \tilde{h}) = \int \mathcal{D}\varphi \, \mathrm{e}^{-\widetilde{F}[\varphi]} , \tag{7.58}$$

hence all properties extracted from it should combine the three parameters. Let us construct several quantities with the three parameters :

[36] Since the gravitational constant G has dimension $[G] = M^{-1} L^3 T^{-2}$, given a mass M, an orbit radius R and a period T, the three quantities should obey a scaling law $R^3/T^2 = \alpha \, GM$, where α is dimensionless. Of course, this requires an additional assumption of scaling, which is natural as the Newton's force is a power law.

(i) At $h = 0$, we construct a characteristic length scale from the parameters A and B : the only possibility is $\xi \sim |A|^{-1/2} \propto |t|^{-1/2}$, hence we recover $\nu = 1/2$.

(ii) At $h = 0$, we construct a characteristic scale for the field : $\varphi \sim \sqrt{|A|/B}$, corresponding to $\beta = 1/2$.

(iii) At $A = 0$ ($T = T_c$), we construct another scale for the field : obviously $\varphi \sim (|\tilde{h}|/B)^{1/3}$, hence $\delta = 3$.

(iv) Finally, assuming the scaling form $C(r) = \langle \varphi(r)\varphi(0) \rangle \propto r^{-d+2-\eta}$ at $T = T_c$, dimensional analysis imposes $\eta = 0$.

With simple dimensional arguments and without any calculation, we have recovered the mean field exponents, which could lead us to the (incorrect) conclusion that these values are constrained by dimensional analysis. Indeed, we have mentioned that the mean field values of the critical exponents are not correct for $d < 4$: cf. table 1 ! This raises the interesting question : if scaling laws are expected, and they are indeed observed in experiments, how can we understand that the values of the critical exponents deviate from their mean field values ? The answer lies in the existence of a length scale which is "hidden" in the continuous formulation. The Ginzburg-Landau theory suggests that the only relevant length scale is the correlation length ξ, however this is deeply wrong : close to the critical point, **fluctuations are important at all length scales**, down to the microscopic cutoff (lattice spacing ϵ). This implies that the correct scaling functions should also involve the UV cutoff. In other terms, the formulation (7.58) is misleading : being purely continuous, whatever means the path integral, it disregards the importance of the UV cutoff when $T \to T_c$. [37]

With this observation in mind, tet us now discuss a plausible scenario to explain the deviation of the critical exponents from the mean field exponents. For example, consider the correlation length, which could thus be constructed from the *two* characteristic lengths ϵ and $1/\sqrt{|A|}$:

$$\xi(t) = |A|^{-1/2} f(|A|\epsilon^2) \qquad \text{with } A \propto t \,, \tag{7.59}$$

where f is a scaling dimensionless function. The scaling assumption then authorizes a correlation length exponent different from $1/2$: imagine that $f(x) \sim x^{-\theta}$ for $x \to 0$, then we have $\xi \propto |t|^{-\theta-1/2}$, i.e.

$$\nu = 1/2 + \theta \,. \tag{7.60}$$

This gives a plausible explanation for the deviation from the mean field exponent. The difference θ between the mean field exponent and the "real" exponent is called the "*anomalous dimension*".

c) Scale invariance

Now that we have identified a plausible origin for the non trivial critical exponents, let us examine the consequence of the scaling assumption. Scale invariance implies the absence of a characteristic length scale, so that properties are the same at all scales. A standard example is a fractal object. Let us consider a quantity function of a parameter $f(x)$. Scale invariance requires that the property at scales x and λx are similar :

$$f(\lambda\, x) = g(\lambda)\, f(x) \quad \forall\ \lambda > 0 \,, \tag{7.61}$$

where g is a given function of the dilatation factor. This condition is extremely restrictive : it requires that the function is a power law

$$f(x) = f(\pm 1)\, |x|^{a_\pm} \,, \tag{7.62}$$

where the exponents are $a_\pm = \pm f'(\pm 1)/f(\pm 1)$.

[37] We could also write the path integral as an integration over the Fourier modes $\tilde{\varphi}_q$ of the field $\int \mathcal{D}\varphi \to \int \prod_q \mathrm{d}\tilde{\varphi}_q$. In this case it is more clear how to encode the presence of the cutoff : integration should only runs over Fourier modes with $||q|| < 1/\epsilon$.

Proof : get rid of the function $g(\lambda)$ by considering

$$\frac{\mathrm{d}}{\mathrm{d}x}\ln\left[f(\lambda\,x)/f(x)\right]=0 \qquad \Rightarrow \qquad \lambda\,\frac{f'(\lambda\,x)}{f(\lambda\,x)}=\frac{f'(x)}{f(x)} \tag{7.63}$$

- For $x>0$, set $\lambda=1/x$ and integrate : get $f(x)=f(1)\,x^{a_+}$ with $a_+=f'(1)/f(1)$.
- For $x<0$, set $\lambda=1/(-x)$ and integrate : get $f(x)=f(-1)\,(-x)^{a_-}$ with $a_-=-f'(-1)/f(-1)$.

Remark : the result shows that $g(\lambda)=\lambda^{a_\pm}$, i.e. we should introduce *two* functions $g_\pm(\lambda)$.

✍ ***Exercice 7.3 :*** *Check that another form of scale invariance is* $f(x)/f(y)=\psi(x/y)\ \forall\, x,\, y$.

The property $f(\lambda x)=\lambda^a\,f(x)$, $\forall\lambda>0$, defines a *homogeneous function* of degree a. The generalization to functions of several arguments is convenient if we start from the form $f(\lambda^{1/a}x)=\lambda\,f(x)$, which leads to introduce generalized homogeneous function of n arguments as $f(\lambda^{1/a_1}x_1,\cdots,\lambda^{1/a_n}x_n)=\lambda\,f(x_1,\cdots,x_n)$.

d) Scaling relations

We now consider the fundamental function encoding thermodynamic properties : the free energy per unit volume. We expect that it is splitted as the sum of a regular part and a singular part,

$$f(t,h)=f_{\rm reg}(t,h)+f_s(t,h)\,, \tag{7.64}$$

where the latter exhibits scaling properties (remember that a phase transition manifests mathematically through non analyticity in f). For the function with two arguments, the scaling property introduced above should be generalized as $f_s(\lambda^{1/a}\,t,\lambda^{1/b}\,h)=\lambda\,f_s(t,h)$. In the following, we prefer to write this property under the form

$$\boxed{f_s(t,h)=\ell^{-d}\,f_s(\ell^{y_t}\,t,\ell^{y_h}\,h)} \tag{7.65}$$

where ℓ is a factor of dilatation of space ; the factor ℓ^{-d} is related to the fact that f is the free energy per unit volume. Eq. (7.65) is called the **scaling assumption**. At this stage, it is sufficient to accept the existence of such a scaling relation, which expresses that f_s is a generalized homogeneous function, written in a convenient form for the following. The relation defines the exponents y_t and y_h, which characterize the rescaling of the temperature and the conjugated field, respectively, against dilatation of space with factor ℓ. In the following, we will see that the two fundamental exponents y_t and y_h have a precise meaning in the renormalization group analysis :

$$\Lambda_t=\ell^{y_t} \qquad \text{and} \qquad \Lambda_h=\ell^{y_h} \tag{7.66}$$

(or the exponents y_t and y_h) are called "*eigenvalues of the renormalization group*". To the two arguments of the free energy, we have associated two exponents, hence we expect that the six exponents α, β, γ, δ, ν and η introduced above are not independent from each other.

Let us examine the consequences of assuming the scaling form (7.65). Choosing the scaling factor as $\ell=|t|^{-1/y_t}$ we have

$$f_s(t,h)=|t|^{d/y_t}\,f_s(\pm1,|t|^{-y_h/y_t}\,h)\equiv|t|^{d/y_t}\,F_\pm(|t|^{-y_h/y_t}\,h) \tag{7.67}$$

where $\pm=\mathrm{sign}(t)$. The two functions $F_\pm(x)$ should be symmetric. Similarly, we could set $\ell=|h|^{-1/y_h}$, leading to the form

$$f_s(t,h)=|h|^{d/y_h}\,f_s(|h|^{-y_t/y_h}\,t,\pm1)\equiv|h|^{d/y_h}\,G(|h|^{-y_t/y_h}\,t) \tag{7.68}$$

there is only one scaling function $G(x)$ as $f(t,h)$ is a symmetric function of h. However $G(x)$ has no reason to be a symmetric function.

- Heat capacity : we differentiate (7.67) with respect to t :

$$c(t) \sim -\frac{\partial^2 f(t,0)}{\partial t^2} \sim |t|^{\frac{d}{y_t}-2} \tag{7.69}$$

This assumes that $F_\pm(0)$ is finite, with $F_+(0) \neq F_-(0)$ *a priori*. This shows that

$$\boxed{\alpha = 2 - \frac{d}{y_t}} \tag{7.70}$$

- Order parameter : using (7.67) we write

$$\phi \sim -\left.\frac{\partial f}{\partial h}\right|_{h=0^+} = -|t|^{\frac{d-y_h}{y_t}}\, F'_\pm(0^+)\,. \tag{7.71}$$

Because the order parameter is non zero below T_c and vanishes above T_c, we expect $F'_+(0^+) = 0$ and $F'_-(0^+)$ finite. Inspection of the power law gives

$$\boxed{\beta = \frac{d-y_h}{y_t}} \tag{7.72}$$

- Magnetic susceptibility : we differentiate once more

$$\chi \sim -\left.\frac{\partial^2 f}{\partial h^2}\right|_{h=0} = -|t|^{\frac{d-2y_h}{y_t}}\, F''_\pm(0^+) \tag{7.73}$$

i.e., assuming $F''_\pm(0^+)$ finite, with $F''_+(0^+) \neq F''_-(0^+)$ *a priori*, we get

$$\boxed{\gamma = \frac{2y_h - d}{y_t}} \tag{7.74}$$

- Critical isotherm : we now start from (7.68). Setting $t = 0$ we have $f_s(0,h) = |h|^{d/y_h}\, G(0)$. Assuming $G(0)$ finite and differentiating, we deduce

$$\boxed{\delta = \frac{y_h}{d-y_h}} \tag{7.75}$$

- Similar arguments on the Green's function give

$$\boxed{\nu = \frac{1}{y_t}} \tag{7.76}$$

and

$$\boxed{\eta = d + 2 - 2y_h} \tag{7.77}$$

The six relations show that the six exponents are controlled by the two independent exponents y_t and y_h. These constraints between the exponents can be written under the form of *four* relations, which are now easy to prove :

$$\alpha + 2\beta + \gamma = 2 \qquad \text{(Rushbrooke relation)} \tag{7.78}$$
$$\beta\delta = \beta + \gamma \qquad \text{(Widom)} \tag{7.79}$$
$$2 - \alpha = d\,\nu \qquad \text{(Josephson)} \tag{7.80}$$
$$\gamma = \nu\,(2 - \eta) \qquad \text{(Fisher)}\,. \tag{7.81}$$

Of course, the determination of the two exponents y_t and y_h is still open at this stage.

✍ ***Exercice 7.4*** *: Check the four scaling relations (7.78,7.79,7.80,7.81).*

These four relations are very important and useful in practice. For example : if one measures the specific heat critical exponent α, one gets immediatly y_t and thus also ν, the correlation length critical exponent. This is a beautiful surprise : *a thermodynamic property* at $h = 0$, the behaviour $c(t) \sim |t|^{-\alpha}$, provides some information about the divergence of the correlation length, i.e. a property of the correlations between spins $\langle \sigma_i \sigma_j \rangle \sim \langle \phi(r)\phi(0) \rangle$ where r is the distance between spins i and j, which would be much more difficult to obtain by a direct measurement in experiments.

✍ ***Exercice 7.5 Proof of*** *(7.76)* ***:*** *In general the correlation length is a function of both t and h. Hence, rescaling by a factor ℓ leads to*[38]

$$\xi(t,h) = \ell\, \xi(\ell^{y_t}\, t, \ell^{y_h}\, h) \tag{7.82}$$

Deduce (7.76).

✍ ***Exercice 7.6 Critical exponents of the 2D Ising model:*** *In 1944, Lars Onsager has found an alytically expression for the free energy of the 2D Ising model on the square lattice for zero magnetic field [31]*

$$f(t,0) = -\frac{1}{\hat\beta}\ln 2 - \frac{1}{2\hat\beta}\int_{-\pi}^{+\pi} \frac{\mathrm{d}k_x \mathrm{d}k_y}{(2\pi)^2} \ln\left[\cosh^2(2\hat\beta J) - \sinh(2\hat\beta J)\,(\cos k_x + \cos k_y)\right] \tag{7.83}$$

where $\hat\beta = 1/T$ (note that f can be related to an elliptic integral). The critical temperature solves $\sinh(2\hat\beta_c J) = 1$, i.e. $T_c = 2J/\ln(1+\sqrt{2})$. The analysis of the $t \to 0$ behaviour shows that the specific heat exhibits a logarithmic divergence $c(t) \sim -\ln|t|$, i.e. $\alpha = 0$. Few years later, in a conference, he announced an expression for the spontaneous magnetization [32],

$$m(t,0) = \left[1 - 1/\sinh^4(2\hat\beta J)\right]^{1/8} \tag{7.84}$$

without giving the details of the proof. The expression was eventually proved by C. N. Yang [50] (the case of the triangular lattice was studied by Potts [38] the same year). Argue that this behaviour corresponds to the critical exponent $\beta = 1/8$.
Deduce all other critical exponents (including y_t and y_h).

✍ ***Exercice 7.7 Divergence of the correlation length:*** *Study the correlation length at $T = T_c$ and small field. Give the critical exponent controlling the divergence for $h \to 0$. Apply the formula to the 2D Ising model.*

8 Introduction to the renormalization group

The previous chapters have left unanswered several questions :

- Is there a method to determine the critical exponents ?
- Scaling leads to the behaviour (7.62), hence, in the three following cases, one could expect the behaviour : $c(t) \sim |t|^{-\alpha_\pm}$ (with α_+ for $t > 0$ and α_- for $t < 0$), $\chi(t) \sim |t|^{-\gamma_\pm}$ and $\xi(t) \sim |t|^{-\nu_\pm}$. However it is observed that exponents coincide $\alpha_+ = \alpha_-$, $\gamma_+ = \gamma_-$ and $\nu_+ = \nu_-$.
- Can we understand the origin of universality ? (and maybe of universality classes)

[38] Although it is not essential at this stage, let us point out that this relation corresponds to a RG transformation, introduced later, Eqs.(8.19,8.27,8.76,)

The answer to these questions lies in the renormalization group (RG) method.

The renormalization group first appeared in quantum electrodynamics with the work of Gell-mann and Low (1954), in order to cure the divergences of the field theory. Later, Leo Kadanoff introduced the concept of block spin and renormalization transformation (1966), however the precise connection with the critical properties was only understood in 1971 by Kenneth Wilson (Nobel prize winner in 1982). Another important contribution is the ϵ-expansion by Michael Fisher, which provides nowadays the most accurate theoretical predictions for critical exponents.

8.1 The Ising chain

A good starting point is to consider the Ising chain

$$H_N = -J \sum_{n=1}^{N-1} \sigma_{n+1}\sigma_n \tag{8.1}$$

(here with open boundary conditions). The model is exactly solvable : in a first step I recall the calculation of the partition function (next paragraph), then the problem is reanalysed with the RG method.

a) Reminder : the exact solution

There exist two simple methods to solve the problem (calculate the partition function *exactly*).

- A recursive approach (at $h = 0$ and for an open chain)
- A transfer matrix approach (at $h \neq 0$, irrespectively of the boundary conditions)

Let us follow the first approach (which is a bit faster), which is sufficient for our purposes here. Aiming at calculating the correlation function $\langle \sigma_n \sigma_m \rangle$, we generalize the problem and consider the Hamiltonian

$$\widehat{H}_N = -\sum_{n=1}^{N-1} J_n \sigma_{n+1}\sigma_n \tag{8.2}$$

with position dependent couplings. The partition function is

$$\widehat{Z}_N = \sum_{\sigma_1,\cdots,\sigma_N} \mathrm{e}^{\sum_{n=1}^{N-1} K_n \sigma_n \sigma_{n+1}} \qquad \text{where } K_n = \beta J_n \, . \tag{8.3}$$

Using that

$$\sum_{\sigma_N} \mathrm{e}^{K_{N-1}\sigma_N\sigma_{N-1}} = 2\cosh(K_{N-1}\sigma_{N-1}) = 2\cosh(K_{N-1}) \tag{8.4}$$

we deduce the recursion $\widehat{Z}_N = 2\cosh(K_{N-1})\,\widehat{Z}_{N-1}$ hence

$$\widehat{Z}_N = 2^N \prod_{n=1}^{N-1} \cosh(K_n) \, . \tag{8.5}$$

In particular, setting all coupling equals, we get $Z_N = 2^N \left[\cosh(\beta J)\right]^{N-1}$ and the free energy per spin $f(T) = -T \, \ln[\cosh(J/T)]$, from which we can deduce thermodynamic properties.

The interest of the generalization lies in the fact that it allows a simple determination of the correlation function. Remark that

$$\langle \sigma_n \sigma_{n+1} \rangle = \frac{\partial}{\partial K_n} \ln \widehat{Z}_N = \tanh(K_n) \tag{8.6}$$

We have also

$$\frac{1}{\widehat{Z}_N}\frac{\partial^\ell \widehat{Z}_N}{\partial K_n \partial K_{n+1}\cdots\partial K_{n+\ell-1}} = \langle(\sigma_n\sigma_{n+1})(\sigma_{n+1}\sigma_{n+2})\cdots(\sigma_{n+\ell-1}\sigma_{n+\ell})\rangle = \langle\sigma_n\sigma_{n+\ell}\rangle \tag{8.7}$$

Using the expression of $\widehat{Z}_N$ and eventually setting $J_n = J\ \forall\, n$ in this relation, we get

$$\langle\sigma_n\sigma_{n+\ell}\rangle = [\tanh(K)]^\ell = \mathrm{e}^{-\ell/\tilde{\xi}} \tag{8.8}$$

where

$$\tilde{\xi}(K) = \frac{1}{-\ln\tanh(K)} \simeq \begin{cases} 1/\ln(T/J) & \text{for } T \gg J \\ \frac{1}{2}\,\exp\{J/T\} & \text{for } T \ll J \end{cases} \tag{8.9}$$

is the correlation length in lattice spacing unit (hence the ˜). The correlation length diverges as $T \to 0$ (i.e. going to the "ferromagnetic phase" at $T = 0$).

✍ ***Exercice 8.1 Ising chain and transfer matrices :*** *We consider an Ising chain submitted to a finite magnetic field B in the ring geometry (which will be slightly more easy to deal with).*

a) Use the transfer matrix method to compute the partition function, i.e. write $Z_N = \mathrm{Tr}\left\{T^N\right\}$ where T is a 2×2 transfer matrix.

Hint: start from the form $Z_N = \sum_{\sigma_1,\cdots,\sigma_N} \mathrm{e}^{-\beta H_N} = \sum_{\sigma_1,\cdots,\sigma_N} T_{\sigma_1,\sigma_2}T_{\sigma_2,\sigma_3}\cdots T_{\sigma_N,\sigma_1}$.

b) compute the free energy per spin $f(T,B)$ in the thermodynamic limit $N\to\infty$. Check your result by comparing with the result given above for $B = 0$.

c) Use the method to derive the correlation function.

b) Decimation and the renormalization group transformation

The general idea of the renormalization group is to perform the "integration" over a fraction of degrees of freedom and study the new problem emerging. To simplify the discussion, we consider now the Ising chain with the ring geometry

$$Z_N = \sum_{\sigma_1,\cdots,\sigma_N} \mathrm{e}^{K\sum_{n=1}^N \sigma_n\sigma_{n+1}} \qquad \text{with } \sigma_{N+1} \equiv \sigma_1 \tag{8.10}$$

for $N = 2^p$ so that we can "decimate" half of the spins at each step. One can perform an integration over half of the spins (all spins with even index) by using

$$\sum_{\sigma_2} \mathrm{e}^{K\sigma_2(\sigma_1+\sigma_3)} = 2\cosh[K(\sigma_1+\sigma_3)] = \begin{cases} 2\cosh(2K) & \text{for } (\sigma_1,\sigma_3) = (++) \text{ or } (--) \\ 2 & \text{for } (\sigma_1,\sigma_3) = (+-) \text{ or } (-+) \end{cases} \tag{8.11}$$

It takes two different values corresponding to aligned spins or anti-aligned spins, like $\mathrm{e}^{K'\sigma_1\sigma_3}$. Hence we can write

$$2\cosh[K(\sigma_1+\sigma_3)] = \mathrm{e}^{K'_0 + K'\sigma_1\sigma_3} \tag{8.12}$$

by setting $\mathrm{e}^{2K'} = \cosh(2K)$, or more elegantly

$$\boxed{\tanh K' = (\tanh K)^2} \tag{8.13}$$

and

$$\mathrm{e}^{K'_0} = 2\sqrt{\cosh(2K)}\,. \tag{8.14}$$

In conclusion we have $\sum_{\sigma_2} \mathrm{e}^{K\sigma_2(\sigma_1+\sigma_3)} = \mathrm{e}^{K_0'+K'\sigma_1\sigma_3}$. If we use this identity for all even spins $\sigma_2, \sigma_4, \cdots$ in the partition function, we get rid of half of the sums and we obtain the *exact* identity

$$\boxed{Z_N(K) = \mathrm{e}^{(N/2)K_0'}\, Z_{N/2}(K')} \tag{8.15}$$

By "integrating over half of the degrees of freedom" (i.e., performing the summation over half of the spin variables), the decimation has related the problem with N spins for coupling K to the problem with $N/2$ spins with coupling K', *for the same hamiltonian*, up to the shift K_0'.

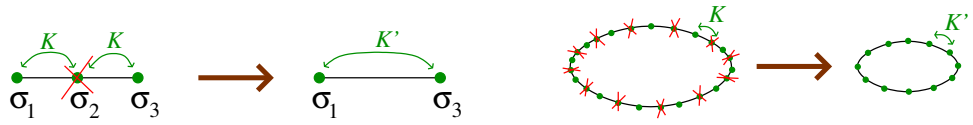


Figure 50: *Decimation : one "integrates" over half of the spins (i.e. the "small scale degrees of freedom") in order to relate the original problem with N spins for coupling K to the same problem with $N/2$ spins and coupling K'.*

If we define the "free energy" per spin (here without the $1/\beta$, i.e. $f = \tilde{f}/\beta$),

$$\tilde{f}(K) \stackrel{\text{def}}{=} -\lim_{N\to\infty} \frac{\ln Z_N(K)}{N} \tag{8.16}$$

we get

$$\tilde{f}(K) = \frac{1}{2}\left[\tilde{f}(K') - K_0'\right] . \tag{8.17}$$

The correlation length should be the same with $Z_N(K)$ or $Z_{N/2}(K')$, as they describe the same problem. One should however pay attention to the fact that (8.9) is measured in units of the lattice spacing

$$\xi = \epsilon\, \tilde{\xi}(K) = 2\epsilon\, \tilde{\xi}(K') \tag{8.18}$$

from which we get

$$\boxed{\tilde{\xi}(K') = \frac{1}{2}\, \tilde{\xi}(K)} \tag{8.19}$$

The relation also obviously follows from (8.13), given the knowledge of the exact expression (8.9).

The set of transformations (8.13,8.15,8.17,8.19) is called a RG transformation.

We have now to understand why these formal manipulations, which seem purely technical at the level of the partition function $Z_N(K)$, can have some interest for the study of critical phenomena. This has to do with the existence of *fixed points*.

8.2 Fixed points

a) Case of the Ising chain

We now identify some values of the "coupling" $K = J/T$ invariant under the RG transformation (8.13) : such values are called "*fixed points*". It is more clear if we introduce $x = \tanh K \in [0, 1]$: the RG transformation (8.13) takes the form $x' = x^2$, which makes clear that it presents two fixed points $x = 0$ or $x = 1$ (cf. Fig. 51). They correspond to :

- the point $K = 0$: paramagnetic (trivial) fixed point.
- the point $K = \infty$: ferromagnetic fixed point.

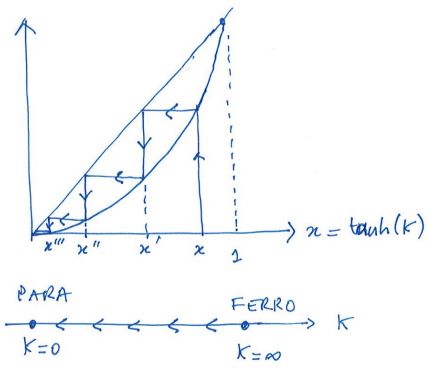


Figure 51: *RG flow for the 1D Ising model*

Starting from any value of K, iterations of the RG transformation lead to a decrease of the coupling, which eventually vanishes :

$$K \to K' \to K'' \to \cdots \to 0\,.$$

In other terms, the ferromagnetic fixed point is *repulsive*, while the paramagnetic fixed point is *attractive*. The RG transformation drives the system towards the point describing the large scale physics. Hence, the interpretation is here that *the system is disordered at any temperature*, as it is always driven towards the *paramagnetic phase* with $\tilde{\xi} \to 0$.

b) Case of the 2D Ising model

Imagine now that the RG transformation accompagnying the transformation $N \to N' = N/\ell^d$ and $Z_N(K) = \mathrm{e}^{N'K_0} Z_{N'}(K')$ are

$$K' = \psi(K) \qquad \text{with} \qquad \tilde{\xi}(K') = \frac{1}{\ell}\tilde{\xi}(K) \tag{8.20}$$

involves a function of the form represented in Fig. 52. It is shown below that this corresponds to the 2D Ising model, which is known to exhibit a second order phase transition. Here we have introduced the scaling factor $\ell \geqslant 1$, which depends on the precise nature of the RG transformation (it was $\ell = 2$ for the Ising chain ; below it will be taken equal to $\ell = \sqrt{2}$ for the square lattice and $\ell = \sqrt{3}$ for the triangular lattice).

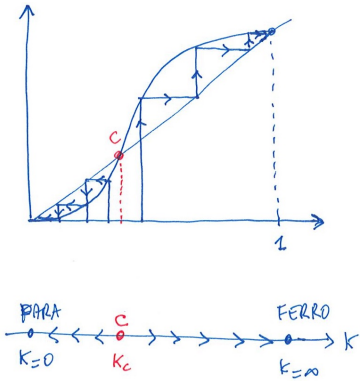


Figure 52: *RG flow for the 2D Ising model : function* $K' = \psi(K)$.

A fixed point of the RG transformation is defined as $K_* = \psi(K_*)$. The function of Fig. 52 has three fixed points :

- $K = 0$: the paramagnetic *attractive* fixed point.
- $K_c = J/T_c$ such that $K_c = \psi(K_c)$. This fixed point is *repulsive*.
- $K = \infty$: the ferromagnetic fixed point, which is *attractive*.

The existence of a repulsive fixed point at K_c has now made the ferromagnetic fixed point attractive. By elimination of degrees of freedom characterizing the physics on small scale (lattice spacing $\epsilon \to \epsilon' = \ell\,\epsilon$), the RG transformation drives the system towards the state describing the problem on large scale. Depending on the initial point we have : for an initial $K < K_c$ (i.e. $T > T_c = J/K_c$) the system flows towards the paramagnetic state, while for $K > K_c$ (i.e. $T < T_c$) it flows towards the ferromagnetic state. The *repulsive* fixed point separating these two situations is the critical point as we now show.

The critical exponent from the RG transformation.— The only way the transformation of the correlation length (8.20) can be consistent with the existence of fixed points, $\tilde{\xi}(K_*) = \frac{1}{\ell}\tilde{\xi}(K_*)$, is that it is zero or infinite :

- $\tilde{\xi}(0) = 0$ for the paramagnetic fixed point.
- $\tilde{\xi}(K_c) = \infty$ for the *critical* fixed point.
- $\tilde{\xi}(\infty) = 0$ for the ferromagnetic fixed point.

Let us perform an expansion in the neighbourhood of K_c. We linearize the transformation

$$K' - K_c \simeq \psi'(K_c)\,(K - K_c) \tag{8.21}$$

Assume the standard behaviour $\xi \sim |T - T_c|^{-\nu} \propto |K - K_c|^{-\nu}$, as $K = \beta J$. Thus, if we combine

$$\tilde{\xi}(K) \sim |K - K_c|^{-\nu} \qquad \text{for } K \sim K_c \tag{8.22}$$

with $\tilde{\xi}(K') = \tilde{\xi}(K)/\ell$, we have $|K' - K_c|^{\nu} \sim \ell |K - K_c|^{\nu}$, i.e. combined with the above equation we get the critical exponent

$$\nu = \frac{\ln \ell}{\ln \psi'(K_c)}\,. \tag{8.23}$$

Of course, this leaves entire the problem of the determination of $\psi(K)$! However, this shows how the study of the RG transformation, a very formal operation, can provide a practical tool to determine the critical exponent ν (and other exponents).

This discussion emphasizes the critical nature of the repulsive fixed point. Indeed, in general denoting by K_* the fixed point, we have :

- For $\psi'(K_*) > 1$ (repulsive fixed point), we find $\nu > 0$, hence $\tilde{\xi}(K) \to \infty$ for $K \to K_*$. The **repulsive fixed point is critical**.
- However if $\psi'(K_*) < 1$ (attractive fixed point, see figure), the same formula gives $\nu < 0$, leading to $\tilde{\xi}(K) \to 0$ for $K \to K_*$, corresponding to a trivial fixed point.

✍ ***Exercice 8.2 :*** *Argue that the "thermal eigenvalue of the RG", $\Lambda_t = \ell^{y_t}$, is*

$$\boxed{\Lambda_t = \left.\frac{\partial K'}{\partial K}\right|_{K_c}} \tag{8.24}$$

and recover the expression of the critical exponent ν in terms of $\psi(K)$.

✍ ***Exercice 8.3 Two-dimensional Ising model for triangular lattice :*** *Consider the Ising model on the triangular lattice. The RG transformation replaces the three spins on each triangular plaquette by one effective spin, correspondly the number of spins is reduced as* $N \to N' = N/3$ *and thus the correlation length in lattice spacing unit is* $\tilde{\xi}(K') = \frac{1}{\sqrt{3}}\tilde{\xi}(K)$. *The renormalization transformation of the coupling is controlled by a function,* $K' = \psi(K)$, *which is approximatively given by*

$$\psi(K) \simeq 2K \left(\frac{1 + \mathrm{e}^{-4K}}{1 + 3\,\mathrm{e}^{-4K}} \right)^2 \tag{8.25}$$

(it is derived below).

a) Find the fixed points. Discuss their stability (attractive/repulsive).

b) Deduce the value of the critical exponent ν. *Using the scaling relations, give the heat capacity critical exponent* α.

c) Compare ν *and* α *with the exact results : the Onsager solution corresponds to* $\alpha = 0$.

Imposrtant remark : long-range order *versus* longe-range-correlations.— One should distinguish two concepts :

(i) Long range correlations : the correlation length ξ goes to infinity, which characterizes a *critical state*.

(ii) Long range order : characterizes an ordered phase, like the ferromagnetic state.

In $d \geqslant 2$, we have $\langle \sigma_r \rangle = \pm 1$ and $\langle \sigma_r \sigma_{r'} \rangle \simeq 1$ for $T \to 0$ (long range order), however $\langle \sigma_r \sigma_{r'} \rangle_c = \langle \sigma_r \sigma_{r'} \rangle - \langle \sigma_r \rangle \langle \sigma_{r'} \rangle \sim \exp\{-||r - r'||/\xi\}$ with a finite ξ when $T \to 0$ (short range correlations). At $T = T_c$, $\langle \sigma_r \rangle = 0$ (no long range order) and $\langle \sigma_r \sigma_{r'} \rangle \sim ||r - r'||^{-d+2-\eta}$ (long range correlations). Long range correlations are observed in the vicinity of a critical fixed point, which manifests itself in the RG flow by its *repulsive* nature : there $\xi = \infty$ (long range correlations).
Let us now make a remark about the **ferromagnetic fixed point** : in $d \geqslant 2$, the ferromagnetic fixed point is *attractive* and is characterized by a finite correlation length. The one-dimensional case is a bit peculiar as the ferromagnetic fixed point is *repulsive*, which indeed characterizes a critical point with $\xi = \infty$, as demonstrated by the exact calculation. For $d \geqslant 2$, the ferromagnatic fixed point is attractive (with $\xi = 0$)

8.3 RG flow

The renormalization group method is the study of the flow generated by the RG transformation in the parameter space of the Hamiltonian. Note that the parameter space is nothing but the **phase diagram**. This allows (in principle) to identify the fixed points and determine the critical exponents. In the language of the previous paragraph, this amounts to the determination of the function ψ, which is unfortunately a difficult task in general. I discuss few approaches for the 2D Ising model.

a) Decimation for the 2D Ising model on the square lattice

In dimension higher than one, the decimation should be done so that the nature of the lattice is not changed. This is simple on the square lattice since it is a bipartite network made of two intricated square lattices. One can remove half of the spins, $N \to N' = N/2$, as it is represented in Fig. 53. The lattice spacing changes as

$$\epsilon' = \sqrt{2}\,\epsilon\,. \tag{8.26}$$

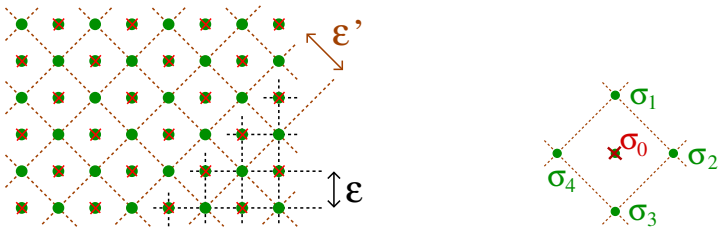


Figure 53: *Decimation on the square lattice. Half of the spins are removed (red crossed), hence the number of spins changes as* $N' = N/2$.

The correlation length is thus renormalized as

$$\tilde{\xi}(K') = \tilde{\xi}(K)/\sqrt{2}\,. \tag{8.27}$$

We are however confronted with a new difficulty : if we "decimate" the spin σ_0 in the middle of four spins, the result cannot be expressed in terms of nearest neighbour (n.n.) couplings only, like in 1D. Indeed, $\sum_{\sigma_0} \mathrm{e}^{K_1\,\sigma_0\,(\sigma_1+\sigma_2+\sigma_3+\sigma_4)} = 2\cosh(K_1 S_{\rm tot})$ where $S_{\rm tot} = \sigma_1+\sigma_2+\sigma_3+\sigma_4 \in \{0,\,\pm 2,\,\pm 4\}$. On the other hand $\widetilde{\mathcal{H}} = \sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_1 \in \{0,\,\pm 4\}$. The problem is that there is no simple correspondence between $S_{\rm tot}$ and $\widetilde{\mathcal{H}}$. Considering the 16 states, we find several situations :

- $S_{\rm tot} = \pm 4$ for $\widetilde{\mathcal{H}} = 4$
- $S_{\rm tot} = \pm 2$ for $\widetilde{\mathcal{H}} = 0$
- $S_{\rm tot} = 0$ for $\widetilde{\mathcal{H}} = 0$ or $\widetilde{\mathcal{H}} = -4$

Hence we cannot relate $\sum_{\sigma_0} \mathrm{e}^{K_1\,\sigma_0\,(\sigma_1+\sigma_2+\sigma_3+\sigma_4)}$ to an effective nearest neighbour interaction between the four spins, of the form $\mathrm{e}^{\frac{1}{2}K_1'\widetilde{\mathcal{H}}}$.

Instead, the exact identity

$$\sum_{\sigma_0} \mathrm{e}^{K_1\,\sigma_0\,(\sigma_1+\sigma_2+\sigma_3+\sigma_4)} = \mathrm{e}^{K_0'}\,\underbrace{\mathrm{e}^{\frac{1}{2}K_1'\,(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_1)}}_{\text{n. n. couplings}}\overbrace{\mathrm{e}^{K_2'\,(\sigma_1\sigma_3+\sigma_2\sigma_4)}}^{\text{n. n. n. couplings}}\,\underbrace{\mathrm{e}^{K_3'\,\sigma_1\sigma_2\sigma_3\sigma_4}}_{\text{quartet couplings}} \tag{8.28}$$

shows that the *decimation generates new types of couplings* (the 1/2 in front of K_1' is introduced for convenience, as each such term will appear twice when decimating the two spins in the two sides of the bond). While the simple decimation leaves the form of the Hamiltonian invariant for the Ising chain (in 1D), this is not the case in 2D : the RG transformation now relates two different Hamiltonians. One could introduce the partition function $Z_N(K_1, K_2, K_3)$ describing the problem with nearest neighbour (n.n.) couplings (K_1), next nearest neighbour (n.n.n.) couplings (K_2), and quartet couplings (K_3), in order to write the RG transformation as

$$Z_N(K_1, 0, 0) = \mathrm{e}^{K_0' N/2}\, Z_{N/2}(K_1', K_2', K_3')\,. \tag{8.29}$$

The relation is exact, however, another RG step will generate further types of couplings. In order to proceed with "reasonable" calculation, one needs to perform approximations, i.e. neglect certain couplings, which is however difficult to justify properly. Copying Brézin [3], "*real space RG transformations of the sort considered here are more an art than a science*" !

✍ ***Exercice 8.4 Decimation for the square lattice :*** *We consider the decimation on the square lattice, Eq. (8.28). Identify four types of 16 states for the four spins* $(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$ *on a square (i.e. classify the states with respect to their symmetries). Comparing the two sides of the*

equation (8.28) *for each of these states, deduce four equations and show that the RG equations corresponding to the decimation are*

$$\mathrm{e}^{4K_0'} = 16\cosh^2(2K_1)\sqrt{\cosh(4K_1)}\,, \tag{8.30}$$

$$\mathrm{e}^{4K_1'} = \cosh(4K_1)\,, \tag{8.31}$$

$$\mathrm{e}^{4K_2'} = \sqrt{\cosh(4K_1)}\,, \tag{8.32}$$

$$\mathrm{e}^{4K_3'} = \sqrt{\cosh(4K_1)}/\cosh^2(2K_1)\,. \tag{8.33}$$

The RG analysis of the Ising model on the square lattice will be discussed at the end of the chapter, with the help of these equations.

b) Block spins and projectors

We describe here a different approach allowing to integrate out a fraction of degrees of freedom, using the idea of "block spin" of Leo Kadanoff. Consider N spins $\{\sigma_i\}$ on a lattice. One introduces blocks gathering each $n_\ell = \ell^d$ spins and to which are attached new spin variables denoted $\{S_b\}$, the "block spins". Here the number of spins is reduced as $N \to N' = N/\ell^d$, hence ℓ is the rescaling factor for the lattice spacing. An example is represented in Fig. 54 which shows the triangular lattice with block spins of $n_\ell = 3$ spins on each plaquette (thus $\ell = \sqrt{3}$). A standard choice for the relation between the original spins and the new variables is

$$S_b = \mathrm{sign}\Big(\sum_{i\in \text{ block } b} \sigma_i\Big) \tag{8.34}$$

so that, if n_ℓ is odd, the new variables are similar to the original one : $S_b = \pm 1$. Note that for an even number of spins per block, there is an ambiguity with the states such that $\sum_{i\in \text{ block } b}\sigma_i = 0$, however it is possible to choose blocks with an odd number of spins : for example, for the square lattice, the smallest natural blocks with $\ell = 2$ contain 4 spins, however choosing $\ell = 3$ leads to $n_\ell = 9$ odd.

The RG transformation corresponds to integrate over the $\{\sigma_i\}$, keeping fixed the values of the $\{S_b\}$. This is conveniently expressed with the help of the *projector* :

$$\Pi\left(\{S_b\},\{\sigma_i\}\right) \stackrel{\text{def}}{=} \prod_b \delta_{S_b\,,\,\mathrm{sign}\left(\sum_{i\in \text{ block } b}\sigma_i\right)} \tag{8.35}$$

so that the RG transformation, also known as the "*Kadanoff transformation*", takes the form

$$\mathrm{e}^{-\beta H'_{N'}(\{S_b\})} = \sum_{\{\sigma_i\}} \Pi\left(\{S_b\},\{\sigma_i\}\right)\mathrm{e}^{-\beta H_N(\{\sigma_i\})} \tag{8.36}$$

where H_N and $H'_{N'}$ are the Hamiltonians before and after the RG transformation, respectively. The renormalization transformation of the partition function convert the sum over spins into a sum over block spins

$$Z_N = \sum_{\{\sigma_i\}_{i=1,\cdots,N}} \mathrm{e}^{-\beta H_N(\{\sigma_i\})} = Z'_{N'} = \sum_{\{S_b\}_{b=1,\cdots,N'}} \mathrm{e}^{-\beta H'_{N'}(\{S_b\})} \tag{8.37}$$

In general the projector should satisfy three properties :

(i) Positivity, $\Pi\left(\{S_b\},\{\sigma_i\}\right) \geqslant 0$, so that the previous expression makes sense.

(ii) $\sum_{\{S_b\}}\Pi\left(\{S_b\},\{\sigma_i\}\right) = 1$.

(iii) The projector should reflect the symmetry of the problem so that H_N and H'_N have the same form (same types of couplings)

To emphasize the third point : for example, for vectorial spins (XY or Heisenberg model), the block spins must also be vectorial, like the original spins [14]. For example, using incorrectly the relation (8.34) for the z component of vectorial spins would change the universality class.

We illustrate the method on the 2D Ising model for a triangular lattice (Fig. 54). The analysis of the paragraph is due to Niemeyer and van Leeuwen [28] (see also § 9.6 of [14]). Each plaquette (three spins) is associated with one block b. Thus

$$N' = N/3 \qquad \text{and} \qquad \ell = \sqrt{3}\,. \tag{8.38}$$

Let us denote by

$$\mathcal{H}_b = K\,(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1) \tag{8.39}$$

the three couplings internal to the block b and by

$$\mathcal{H}_{b,b'} = K\,\sigma_1(\sigma_4 + \sigma_5) \tag{8.40}$$

the interblock couplings (cf. Fig. 54). The Ising Hamiltonian can be splitted as

$$-\beta H_N(\{\sigma_i\}) = \sum_b \mathcal{H}_b + \sum_{\langle b,b'\rangle} \mathcal{H}_{b,b'}\,. \tag{8.41}$$

The implementation of (8.43) can be done by treating first $\mathcal{H}_b$ and then $\mathcal{H}_{b,b'}$ in perturbation. The key observation is that at order 0 in the interblock couplings (i.e. forgetting $\mathcal{H}_{b,b'}$), the blocks are independent :

- $S_b = +1$ corresponds to the four states $(+++)$, $(++-)$, $(+-+)$, $(-++)$. Thus the partition function of the block, constrained by the value of the the spin block, is

$$\sum_{\sigma_1,\sigma_2,\sigma_3} \mathrm{e}^{\mathcal{H}_b(\{\sigma_i\})}\,\delta_{+1\,,\,\mathrm{sign}(\sum_i \sigma_i)} = \mathrm{e}^{3K} + 3\mathrm{e}^{K} \equiv z_b \tag{8.42}$$

  the (unconstrained) partition function of a block being $2z_b$.
- $S_b = -1$ corresponds to the four states $(---)$, $(+--)$, $(-+-)$, $(--+)$. The constrained partition function is also z_b

We now write

$$\mathrm{e}^{-\beta H'_{N'}(\{S_b\})} = (z_b)^{N'} \left\langle \mathrm{e}^{\sum_{\langle b,b'\rangle} \mathcal{H}_{b,b'}} \right\rangle_{\{S_b\}} \tag{8.43}$$

where $\langle\cdots\rangle_{\{S_b\}}$ is the average for a fixed configuration $\{S_b\}$, with the measure $\mathrm{e}^{\sum_b \mathcal{H}_b}$. [39] Then we use $\langle \mathrm{e}^V\rangle = \exp\left\{\langle V\rangle + \frac{1}{2}(\langle V^2\rangle - \langle V\rangle^2) + \cdots\right\}$ (cumulant expansion).

First order in the interblock couplings : we first consider (see labels in Fig. 54)

$$\left\langle \mathcal{H}_{b,b'}\right\rangle_{S_b,S_{b'}} = K\,\langle\sigma_1(\sigma_4+\sigma_5)\rangle_{S_b,S_{b'}} = K\,\langle\sigma_1\rangle_{S_b}\,\langle\sigma_4+\sigma_5\rangle_{S_{b'}} \tag{8.45}$$

where I have used the independence of the blocks for the measure $\mathrm{e}^{\sum_b \mathcal{H}_b}$.

[39] Explicitely

$$\langle\cdots\rangle_{\{S_b\}} = \sum_{\{\sigma_i\}} \cdots \prod_b \frac{1}{z_b} \mathrm{e}^{\mathcal{H}_b}\,\delta_{S_b\,,\,\mathrm{sign}(\sum_{i\in b}\sigma_i)} \tag{8.44}$$

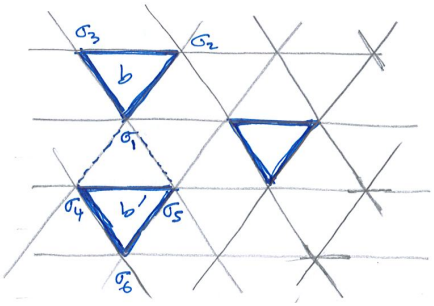


Figure 54: *The 2D Ising model on the triangular lattice. Blue triangles represent the "block spins" and form another triangular lattice with larger lattice spacing.*

Consider $S_b = +1$:

$$\langle \sigma_1 \rangle_{S_b=+1} = \frac{1}{z_b} \left(\mathrm{e}^{3K} + (1+1-1)\mathrm{e}^{-K} \right) = \frac{\mathrm{e}^{3K} + \mathrm{e}^{-K}}{\mathrm{e}^{3K} + 3\mathrm{e}^{K}} \equiv \Phi(K) \tag{8.46}$$

Similarly, for $S_b = -1$:

$$\langle \sigma_1 \rangle_{S_b=-1} = \frac{1}{z_b} \left(-\mathrm{e}^{3K} + (-1-1+1)\mathrm{e}^{-K} \right) = -\Phi(K) \tag{8.47}$$

hence we obtain the useful relation

$$\langle \sigma_1 \rangle_{S_b} = \Phi(K)\, S_b \,. \tag{8.48}$$

Finally we have

$$\left\langle \mathcal{H}_{b,b'} \right\rangle_{S_b, S_{b'}} = 2K \Phi(K)^2 \, S_b \, S_{b'} \tag{8.49}$$

If we truncate the cumulant expansion of (8.43) at the first order in the block couplings, we have

$$\mathrm{e}^{-\beta H'_{N'}(\{S_b\})} \approx (z_b)^{N'} \mathrm{e}^{\left\langle \sum_{\langle b,b' \rangle} \mathcal{H}_{b,b'} \right\rangle_{\{S_b\}}} = \mathrm{e}^{N' K'_0} \mathrm{e}^{K' \sum_{\langle b,b' \rangle} S_b \, S_{b'}} \tag{8.50}$$

where $N' = N/3$, $K'_0 = \ln z_b$ and

$$\boxed{K' = \psi(K) \simeq 2K \Phi(K)^2 = 2K \left(\frac{\mathrm{e}^{3K} + \mathrm{e}^{-K}}{\mathrm{e}^{3K} + 3\mathrm{e}^{K}} \right)^2} \tag{8.51}$$

is the function introduced above, cf. Eq. (8.25). The function is plotted in Fig. 55. The RG transformation of the partition function thus takes the form

$$Z_N(K) \approx \mathrm{e}^{N' K'_0} \, Z_{N'}(K') \tag{8.52}$$

Because the lattice spacing changes as $\epsilon' = \sqrt{3}\,\epsilon$, the correlation length in lattice spacing unit changes as

$$\boxed{\tilde{\xi}(K') = \frac{1}{\sqrt{3}} \tilde{\xi}(K)} \tag{8.53}$$

[this follows from the invariance of the correlation length $\xi = \epsilon \tilde{\xi}(K) = \epsilon' \tilde{\xi}(K')$, as discussed above].

The fixed point, defined by $K_c = \psi(K_c)$, can be found explicitly. Using the approximate form (8.51), one finds

$$K_c \simeq \frac{1}{4} \ln(1 + 2\sqrt{2}) \simeq 0.3556 \,. \tag{8.54}$$

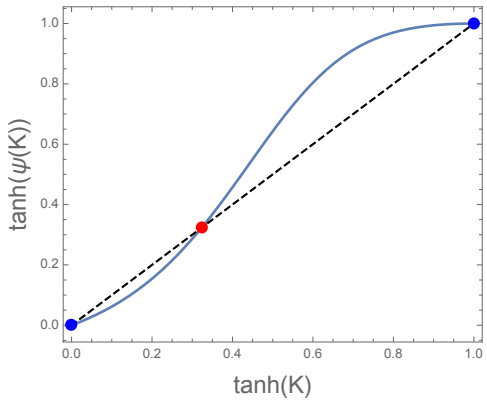


Figure 55: *Function $\psi(K)$ for the triangular lattice, given by Eq. (8.51).*

At first order, only n.n. couplings matter and we can get the critical exponent as explained above, see Eq. (8.23),

$$\nu \simeq \ln(\sqrt{3})/\ln \psi'(K_c) \simeq 1.133 \tag{8.55}$$

(cf. exercise 8.3). I postpone the comparison with the exact results to the end of the section.

Second order in the interblock couplings : We have to consider contributions to the renormalized Hamitonian $-\beta H'_{N'}$ of the form

$$\frac{1}{2}\left[\left\langle \mathcal{H}_{b,b'}\mathcal{H}_{b'',b'''}\right\rangle_{S_b,S_{b'},S_{b''},S_{b'''}} - \left\langle \mathcal{H}_{b,b'}\right\rangle_{S_b,S_{b'}}\left\langle \mathcal{H}_{b'',b'''}\right\rangle_{S_{b''},S_{b'''}}\right] \tag{8.56}$$

Obviously, this vanishes if the blocks b and b' do not have common spins with the blocks b'' and b'''. In fact, at least two blocks must coincide, like $b' = b'''$. Note that $\langle \mathcal{H}^2_{b,b'}\rangle - \langle \mathcal{H}_{b,b'}\rangle^2$ is independent of the spin block variables, and thus only contributes to the term K'_0.

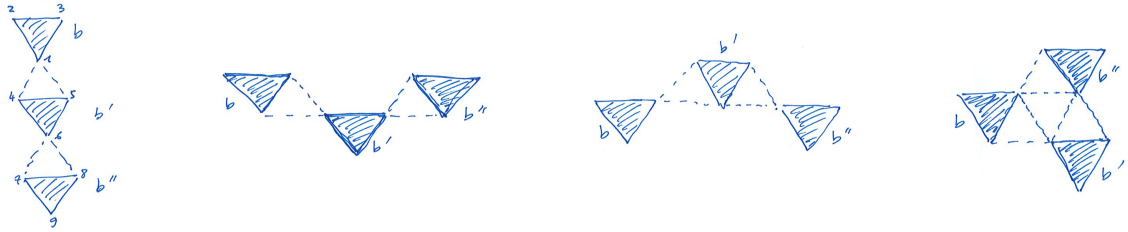


Figure 56: *Different configurations of blocks.*

We have to consider several cases represented on the Fig. 56 :

Case where b, b' and b'' are aligned [(a), (b), or (c)] : this is the case where the three blocks are aligned. We write

$$\left\langle \mathcal{H}_{b,b'}\mathcal{H}_{b',b''}\right\rangle_{S_b,S_{b'},S_{b''}} = K^2\langle \sigma_1(\sigma_4+\sigma_5)\sigma_6(\sigma_7+\sigma_8)\rangle_{S_b,S_{b'},S_{b''}} \tag{8.57}$$

$$= K^2\langle \sigma_1\rangle_{S_b}\langle(\sigma_4+\sigma_5)\sigma_6\rangle_{S_{b'}}\langle\sigma_7+\sigma_8\rangle_{S_{b''}} \tag{8.58}$$

The calculation is similar as above : additionnaly to the rule

$$\langle \sigma_i\rangle_{S_b} = \Phi(K)\, S_b \tag{8.59}$$

obtained above (8.46,8.47), the calculation requires

$$\langle \sigma_i \sigma_j \rangle_{S_b} = \frac{\mathrm{e}^{3K} - \mathrm{e}^{-K}}{\mathrm{e}^{3K} + 3\mathrm{e}^{-K}} = 2\Phi(K) - 1 \qquad \text{for } i \neq j \quad \text{(both in block } b\text{)}\,, \tag{8.60}$$

the result is independent of S_b. Note that $\pm\Phi(K)$ has the interpretation of the average magnetization in the block, constrained by $S_b = \pm 1$, and $3K\,[2\Phi(K) - 1]$ is the average energy. In the configuration (a) or (b) of Fig. 56, one obtains after some simple calculations that

$$\frac{1}{2}\Big[\big\langle \mathcal{H}_{b,b'}\mathcal{H}_{b',b''}\big\rangle_{S_b,S_{b'},S_{b''}} - \big\langle \mathcal{H}_{b,b'}\big\rangle_{S_b,S_{b'}}\big\langle \mathcal{H}_{b',b''}\big\rangle_{S_{b'},S_{b''}}\Big] = -2K^2\Phi(K)^2\,(1-\Phi(K))^2\; S_b\, S_{b''} \tag{8.61}$$

i.e. this produces *next nearest neighbour* couplings, like in the decimation procedure. For the configuration (c) of Fig. 56, one rather gets $-K^2\Phi(K)^2\left(1 - 3\Phi(K) + 2\Phi(K)^2\right)\, S_b\, S_{b''}$. The two contributions (b) and (c) should be added and describe another type of n.n.n. coupling, renormalized in a different manner. Hence, one should introduce two parameters to describe n.n.n. couplings : $K'_{2\|} \simeq -2K^2\Phi(K)^2\big[1-\Phi(K)\big]^2$ the n.n.n. coupling for aligned sites [like (a) for blocks], and $K'_{2\diamond} \simeq -K^2\Phi(K)^2\big[3 - 7\Phi(K) + 4\Phi(K)^2\big]$ the n.n.n. for non aligned sites [like (b+c)].

Case where b, b' and b'' form a triangle [case (d)] : Similar arguments give

$$\frac{1}{2}\Big[\big\langle \mathcal{H}_{b,b'}\mathcal{H}_{b',b''}\big\rangle_{S_b,S_{b'},S_{b''}} - \big\langle \mathcal{H}_{b,b'}\big\rangle_{S_b,S_{b'}}\big\langle \mathcal{H}_{b',b''}\big\rangle_{S_{b'},S_{b''}}\Big] = 2K^2\Phi(K)^3\,(1-\Phi(K))\; S_b\, S_{b''} \tag{8.62}$$

This time however the blocks b and b'' are neighbours, hence this is another contribution to the nearest neighbour couplings. If we consider a triangle of blocks, we have to consider the three couplings

$$\mathcal{H}_{b,b'}\mathcal{H}_{b',b''} + \mathcal{H}_{b',b''}\mathcal{H}_{b'',b} + \mathcal{H}_{b'',b}\mathcal{H}_{b,b'} \tag{8.63}$$

which produce the contribution to $-\beta H'_{N'}$:

$$2K^2\Phi(K)^3\,[1-\Phi(K)]\,(S_b\,S_{b'} + S_{b'}\,S_{b''} + S_{b''}\,S_b) \tag{8.64}$$

Because the bond $\langle b, b'\rangle$ belongs to two such triangles, we conclude that the renormalized coupling between nearest neighbour blocks is

$$K' = \psi(K) \simeq 2K\Phi(K)^2 + 4K^2\Phi(K)^3\,[1-\Phi(K)]\;. \tag{8.65}$$

Note that the results have the form of an expansion in powers of the coupling K. Forgetting the n.n.n. couplings, we can easily find the fixed point numerically : $K_c^{(2)} \simeq 0.2758$ which is closer to the exact value (I recall that the first approximation (8.51) has led to $K_c^{(1)} \simeq 0.3556$). If we apply the formula (8.55) to the new function $\psi(K)$, we get $\nu^{(2)} \simeq 1.1246$. We will compare to the exact results below, and will provide a more precise discussion.

Effect of the magnetic field : the effect of the magnetic field is easy to analyze, at least at the lowest order. We have to account for the term

$$\beta H_N = \cdots - h\sum_i \sigma_i \tag{8.66}$$

(from now on, the temperature is included in the field h for convenience). At lowest order, i.e. writing $\langle \mathrm{e}^{\mathcal{H}_b^{\text{mag.}}}\rangle \approx \mathrm{e}^{\langle \mathcal{H}_b^{\text{mag.}}\rangle}$, this corresponds to add to $-\beta H'_{N'}$

$$+h\Big\langle \sum_i \sigma_i \Big\rangle_{\{S_b\}} = h\sum_b \sum_{i\in \text{ block } b} \langle \sigma_i\rangle_{S_b} = h\sum_b 3\,\Phi(K)\,S_b\,. \tag{8.67}$$

We can interpret this term as a RG equation for the conjugated field

$$\boxed{h' \simeq 3\,\Phi(K)\,h} \tag{8.68}$$

Close to the critical fixed point, the magnetic eigenvalue is [see (8.24)]

$$\Lambda_h = \left.\frac{\partial h'}{\partial h}\right|_{K_c} \simeq 3\,\Phi(K_c) = \frac{3}{\sqrt{2}} > 1\,, \tag{8.69}$$

hence the RG flow drives the system away from the critical fixed point in the direction of the field. The *fixed point is repulsive both in the K direction and the h direction.*

✍ ***Exercice 8.5 Renormalization of the magnetic field:*** *Because the magnetic Hamiltonian does not couple blocks, we can improve the treatment of the magnetic field. Write $\mathcal{H}_b^{\rm mag.} = h\,\widehat{S}_b$ with $\widehat{S}_b = \sum_{i\in b}\sigma_i$, hence $S_b = \mathrm{sign}\big(\widehat{S}_b\big)$, and perform exactly the calculation of $\langle \mathrm{e}^{\mathcal{H}_b^{\rm mag.}}\rangle_{S_b}$. Compare with the above analysis (in particular the RG eigenvalue Λ_h).*

Comparison with the exact results : Many exact results have been obtained for the 2D Ising model. The critical temperature for the triangular lattice is known :

$$K_c^{(\rm triang.)} = \frac{1}{4}\ln(3) \simeq 0.27465\,. \tag{8.70}$$

All the critical exponents in 2D can be deduced from the Onsager and Yang solutions : we have determined the thermal and magnetic critical exponents controlling all critical exponents in the exercise 7.6 : $y_t = 1$ and $y_h = 15/8$. Correspondingly, the two RG eigenvalues are $\Lambda_t = \ell^{y_t} = \sqrt{3} \simeq 1.732$ and $\Lambda_h = \ell^{y_h} = \big(\sqrt{3}\big)^{15/8} \simeq 2.801$ (for the triangular lattice, the scaling factor was chosen to be $\ell = \sqrt{3}$).

Lowest order.— We can compare with the solution for lowest order (for nearest neighbour couplings only) : above, we have obtained the form $K' = \psi(K)$, from which we have deduced $K_c^{(1)} \simeq 0.3556$. Linearization close to the fixed point gives $K' - K_c \simeq \psi'(K_c)\,(K - K_c)$, i.e. writing $K - K_c = (\beta - \beta_c)J \simeq -t\,K_c$

$$t' \simeq \psi'(K_c)\,t \equiv \Lambda_t\,t \tag{8.71}$$

The renormalization of the coupling constant is equivalent to renormalization of the temperature. At lowest order, we can use the expression (8.51) giving

$$\Lambda_t^{(1)} \simeq 1.6235\,. \tag{8.72}$$

Renormalization of the magnetic field close to the fixed point is $h' \simeq 3\,\Phi(K_c)\,h \equiv \Lambda_h^{(1)}\,h$ hence

$$\Lambda_h^{(1)} = 3\,\Phi(K_c) = \frac{3}{\sqrt{2}} \simeq 2.1213\,. \tag{8.73}$$

Considering the simplicity of the analysis and the calculations, the agreement is quite satisfactory.

Second order.— The analysis at second order in the interblock couplings presented above has neglected an important point : starting from the Hamiltonian for n.n. couplings only, we have generated n.n. and n.n.n. couplings after RG transformation. As for the square lattice, the correct analysis requires to consider from the begining of the calculation both the n.n. coupling K_1 and the n.n.n. couplings $K_{2\|}$ (for Fig. 56.a) and $K_{2\diamond}$ (for Fig. 56.b+c). [40] It is a bit long but not difficult in principle. It has been performed in Ref. [28] for $h = 0$. These authors give

$$K_c^{(2)} \simeq 0.251 \tag{8.74}$$

showing a significant improvement, with respect to $K_c^{(1)}$. The RG eigenvalue is

$$\Lambda_t^{(2)} \simeq 1.7835\,, \tag{8.75}$$

which gets closer to the expected value $\sqrt{3}$. Correspondingly one finds the critical exponents $y_t^{(2)} \simeq 1.053$ and $\nu^{(2)} \simeq 0.949$ (this is better than the rough approximation neglecting the n.n.n. couplings discussed above). [41]

c) RG in momentum space

As we have seen on these two examples, the derivation of the RG equations by real space renormalization is not very well controlled, although the block spins technique allows for systematic improvement (the reference [28] also proposes other approximations). Another more systematic approach is the one of renormalization in momentum space. The general idea is to consider the free energy (7.56) as the action of a (statistical) field theory : for the Ising universality class, this is just the φ^4 theory for a real scalar field with Euclidean action in dimension d. The theory is then studied as follows : for $B = 0$, the integral is Gaussian and can be performed exactly (at least for $A > 0$, i.e. $T > T_c$). Then, the φ^4 term is treated in perturbation theory (for $A < 0$, one should rather expand around $\varphi \neq 0$). Renormalization is needed to make the perturbative calculations meaningful. In this case, the RG equations for the coupling constants are obtained by successive integration over momentum shell, i.e. eliminating short scale degrees of freedom. The procedure can be safely defined for the critical dimension $d = d_u = 4$. The dimensions $d < d_u$ are considered by performing "*dimensional regularisation*" and so-called "ϵ-expansion" (where $\epsilon = d_u - d$). Such systematic expansions provide the best theoretical estimates for the critical exponents. If you are interested in this more technical question, see [3] or [17].

8.4 General discussion

We now provide an abstract discussion : we assume that the problem is described by p couplings, thus its partition function is $Z_N(K_1, \cdots, K_p)$. A RG transformation by a factor ℓ is

$$\left\{ \begin{array}{ll} N \to N' = N/\ell^d & \text{(degrees of freedom)} \\ \epsilon \to \epsilon' = \ell\,\epsilon & \text{(lattice spacing)} \\ \tilde{\xi} \to \tilde{\xi}' = \tilde{\xi}/\ell & \text{(correl. length in latt. sp. unit)} \\ K_\alpha \to K'_\alpha = \psi_\alpha(K_1, \cdots, K_p)\,, \quad \alpha = 1, \cdots, p & \text{(couplings)} \\ Z_N(K_1, \cdots, K_p) = \mathrm{e}^{K'_0 N'}\, Z_{N'}(K'_1, \cdots, K'_p) & \text{(parition function)} \end{array} \right. \tag{8.76}$$

where K'_0 represents a shift, which is the contribution to the free energy of integrating out the degrees of freedom on short scale.

[40] In Refs. [28, 14], $K_{2\diamond}$ and $K_{2\|}$ are called "second" and "third" nearest neighbour couplings.

[41] As we will see in the next section, the linearization of the RG transformation leads to consider a 3×3 matrix. Niemeyer and van Leeuwen have found the eigenvalues $\Lambda_1 \simeq 1.7835$, $\Lambda_2 \simeq 0.2286$ and $\Lambda_3 \simeq -0.1156$.

Let us assume that the transformation has a fixed point $(K_1^*, \cdots, K_p^*)$. We can linearize in its neighbourhood

$$K'_\alpha - K^*_\alpha \simeq \sum_\beta M_{\alpha\beta}(\ell)\, \left(K_\beta - K^*_\beta\right) \qquad \text{for } M_{\alpha\beta}(\ell) \stackrel{\text{def}}{=} \left.\frac{\partial \psi_\alpha}{\partial K_\beta}\right|_* \tag{8.77}$$

I have emphasize that the RG transformation depends on the scaling factor ℓ for later convenience. We further assume that the matrix can be diagonalized : it has p eigenvalues $\Lambda_n(\ell)$ corresponding to p directions in the parameter space, given by the (right) eigenvector, $M(\ell)R^{(n)} = \Lambda_n(\ell)\, R^{(n)}$. Because the matrix has no reason to be symmetric, each eigenvalue is related to a pair of right and left eigenvectors, the latter satisfying $M(\ell)^{\mathrm{T}} L^{(n)} = \Lambda_n(\ell)\, L^{(n)}$. They form a bi-orthogonal set, $\left(L^{(n)}\right)^{\mathrm{T}} R^{(m)} = \delta_{n,m}$. We denote by $\widetilde{K}_n$ the new parameters, linear combinations of the original couplings, $\widetilde{K}_n = \sum_\alpha R^{(n)}_\alpha\, (K_\alpha - K^*_\alpha)$.

Combining two RG transformations for two scales ℓ_1 and ℓ_2 corresponds to one RG transformation for scale $\ell_2\ell_1$. This is also true for the linearized transformation

$$M(\ell_2)M(\ell_1) = M(\ell_2\ell_1) \tag{8.78}$$

with $M(1) = \mathbf{1}_p$. I.e. the RG transformations form a *semi-group* (because $\ell \geqslant 1$, there is no inverse transformation). Correspondingly, the eigenvalues present the same property

$$\Lambda_n(\ell_2)\Lambda_n(\ell_1) = \Lambda_n(\ell_2\ell_1) \tag{8.79}$$

leading to the *power law* behaviour

$$\Lambda_n(\ell) = \ell^{y_n} \tag{8.80}$$

where y_n is an exponent characterizing the behaviour of the coupling $\widetilde{K}_n$ upon RG transformation : $\widetilde{K}'_n \simeq \Lambda_n(\ell)\widetilde{K}_n$.

We distinguish three cases :

(i) $y_n < 0$: the corresponding coupling $\widetilde{K}_n$ is said **irrelevant**. The RG transformations drive such a coupling to zero, $\widetilde{K}_n \to \widetilde{K}'_n \to \widetilde{K}''_n \to \cdots \to 0$. Hence it has no effect on the critical behaviour : an irrelevant coupling can be set to zero, without changing the critical properties.

(ii) $y_n > 0$: the corresponding coupling $\widetilde{K}_n$ is said **relevant**. It increases under the effect of successive RG transformations, which eventually drive the system out of the critical region.

(iii) $y_n = 0$: the corresponding coupling $\widetilde{K}_n$ is said **marginal**. The influence of such couplings cannot be determined from the linearized transformation.

The correlation length is infinite at the critical point $\xi = \infty$. Because the irrelevant couplings play no role, on the critical properties, $\xi = \infty$ everywhere in the "surface" spanned by the irrelevant directions : this subspace is called the **critical manifold**. All trajectories on the critical manifold end at the critical point, hence the critical manifold is the *basin of attraction* of the critical point. This is the explanation for **universality** : all points of the critical surface correspond to different Hamiltonians (with different couplings), however under the action of succesive RG transformations they all end at the critical point. As a consequence, the properties of all models living in the critical manifold are controlled by the same set of positive exponents $\{y_n\}_{n=1,\cdots,r}$, where $r \leqslant p$ is the number of relevant directions.

✍ ***Exercice 8.6 RG flow for the square lattice — Wilson solution :*** *This exercise aims at solving the RG equations obtained in the exercise 8.4. Wilson has proposed a solution in 1975, which neglects the quartet couplings $K_3\sigma_1\sigma_2\sigma_3\sigma_4$. Assuming small couplings, the equations*

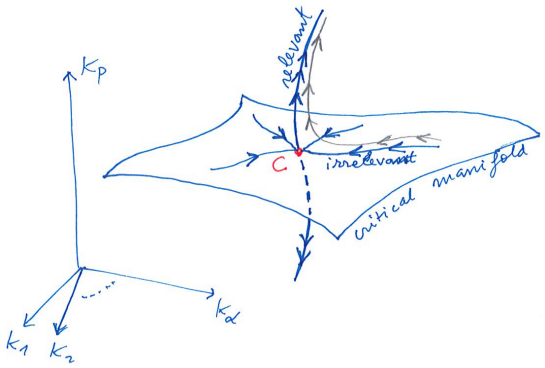


Figure 57: *RG flow in the parameter space. For example, consider the Ising model on the square lattice at $h = 0$. We have seen that the first RG step involves the three couplings : K_1 (nearest neighbours), K_2 (next nearest neighbours) and K_3 (quartet). Assume that one can restrict to these three couplings for the next RG steps. In this case there exists one relevant coupling (associated with the thermal eigenvalue) and two irrelevant couplings : the critical manifold is a 2D surface in the three dimensional space, like on the figure.*

(8.31,8.32) for n.n. and n.n.n. couplings read $K_1' \simeq 2K_1^2$ and $K_2' \simeq K_1^2$. For consitency, one should however introduce the n.n.n. couplings from the begining, i.e. add such terms in the l.h.s. of Eq. (8.28) : this is easy as n.n.n. couplings before decimation is independent of the decimated spin and simply become n.n. couplings after decimation. [42] *We can simply write $K_1' \simeq 2K_1^2 \to K_1' \simeq 2K_1^2 + K_2$ in the previous equation :*

$$\begin{cases} K_1' \simeq 2K_1^2 + K_2 \\ K_2' \simeq K_1^2 \end{cases} \tag{8.81}$$

a) Find the fixed point (K_1^*, K_2^*).

b) Linearize the transformation : $K_i \simeq K_i^* + \kappa_i$ with $\kappa_i \ll 1$. Diagonalize the linearized transformation and plot the RG flow in the neighbourhood of the two fixed points (the trivial paramagnetic fixed point and the non trivial critical fixed point).

c) The critical value K_c for the Ising model with nearest neighbour couplings only corresponds to the point $(K_c, 0)$ on the critical manifold. A rough approximation can be obtained by finding the projection of the fixed point along the irrelevant direction on the n.n. axis. Compute K_c.

d) Compare with the exact result in 2D :

$$K_c^{(\text{square})} = \frac{1}{2}\ln(1+\sqrt{2}) \tag{8.82}$$

Remembering that $\nu = 1$, give the related eigenvalue Λ_t and compare with the approximation found previously.

To learn more about RG

there are plenty of books introducing the RG. This last chapter is inspired by the three following references :

- The excellent book of Édouard Brézin [3].

[42] note that this neglects the n.n.n. couplings of the spin σ_0 with spins outside the square of four spins $(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$.

- The book of Pathria [33] (chapter 14) is detailed and pedagogical.
- Last but not least, I recommend the book of Goldenfeld [14].

I can also mention the little book of Cardy [5] or the book of Ma [26].

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