

# **Models of Theoretical Physics**

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Lecture Notes of the course *Models of Theoretical Physics* at the *Physics* and *Physics of Data* degrees of the University of Padova. The course and the notes are by Amos Maritan and Marco Baiesi. They are based on an initial version by Vincenzo Maria Schimmenti. A good part of the chapter on disordered systems is by Giacomo Gradenigo, who is teaching 8 hours in the course.



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# Useful Mathematical Tools

## 1.1. Gaussian Integrals

**1.1.1. Multidimensional Gaussian Integrals.** Gaussian integrals are ubiquitous in theoretical physics and constitute the basis of many calculations. Moreover, they allow us to introduce the formalism of generating functions.

We begin by remembering the simplest of those integrals:

$$(1.1) \quad \int_{-\infty}^{\infty} dx e^{-\frac{ax^2}{2}} = \sqrt{\frac{2}{a}} \pi$$

which can be proven by considering the square of the integral and switching to polar coordinates. The argument of the exponent can be regarded as a quadratic form on  $\mathbb{R}$  (as a vector space); we generalize that concept by introducing a  $n$  dimensional positive definite symmetric matrix  $A$  (i.e. it has all positive eigenvalues) that naturally induces a quadratic form  $\mathbb{A}(\vec{x})$  on  $\mathbb{R}^n$

$$(1.2) \quad \mathbb{A}(\vec{x}) = \sum_{i,j=1}^n x_i A_{i,j} x_j = \vec{x}^T A \vec{x}$$

Embedding this in an exponential, for convenience with a prefactor  $1/2$ , yields a Gaussian weight  $\mathcal{G}(\vec{x}) = \exp[-\mathbb{A}(\vec{x})/2]$ . An example of such weight for a two-dimensional vector  $\vec{x} = (x_1, x_2)$  and

$$A = \begin{bmatrix} 3 & -1 \\ -1 & 3 \end{bmatrix}$$

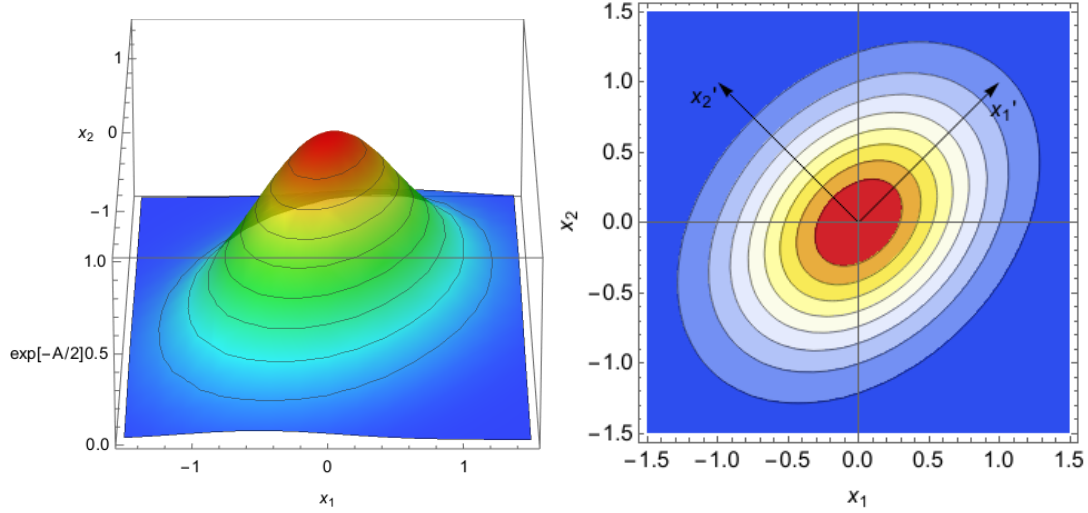
is shown in Fig. 1.  $A$  has eigenvalues  $\lambda_1 = 2$  and  $\lambda_2 = 4$ , which are inversely proportion to the decay of the function  $\mathcal{G}$  along the two orthogonal directions  $x'_1$  and  $x'_2$ . In the following we adopt  $\mathcal{G}$  as a weight in the distribution of  $\vec{x}$ . In this case, the off-diagonal terms  $A_{12} = A_{21}$  introduce a correlation between  $x_1$  and  $x_2$ , i.e. their covariance is not zero.

Now consider the Gaussian integral

$$(1.3) \quad Z[A] = \int_{\mathbb{R}^n} d^n x e^{-\frac{1}{2} \mathbb{A}(\vec{x})} = \int_{\mathbb{R}^n} d^n x e^{-\frac{1}{2} \sum_{i,j=1}^n x_i A_{i,j} x_j}$$

The variables are in general coupled by  $A_{ij} \neq 0$  and the integral is solved by diagonalizing the matrix  $A$  (this can be done thanks to the spectral theorem) via an orthogonal matrix  $O : OO^T = \mathbb{I}_n$  and changing the variables:  $x' = Ox$ . The Jacobian of this transformation is 1. Hence, by calling  $a_i, i = 1 \dots n$  the eigenvalues of  $A$ , we have

$$(1.4) \quad Z[A] = \prod_{i=1}^n \int_{-\infty}^{\infty} dx_i e^{-\frac{a_i}{2} x_i^2} = \frac{(2\pi)^{n/2}}{\sqrt{\det A}}$$



**Figure 1.** Three-dimensional plot (left) and contour plot (right) of the Gaussian weight discussed in the text. By expressing such weight in the orthonormal basis  $(x'_1, x'_2)$ , one would obtain uncorrelated Gauss weights.

since  $\prod_{i=1}^n a_i = \det A$ .

The last result that we need is a further generalization of  $Z[A]$ ; it is done by adding a linear term to the argument of the exponential, i.e.  $\sum_{i=1}^n b_i x_i = \vec{b}^T \vec{x} = \vec{b} \cdot \vec{x}$  where  $b \in \mathbb{R}^n$ .

$$(1.5) \quad Z[A, \vec{b}] = \int_{\mathbb{R}^n} d^n x e^{-\frac{1}{2} \mathbb{A}(\vec{x}) + \vec{b} \cdot \vec{x}} = Z[A, 0] e^{\frac{1}{2} \vec{b}^T A^{-1} \vec{b}}$$

(we have defined  $Z[A, 0] = Z[A]$ ). This result can be derived by either completing the square or by changing the variables to  $\vec{y} = \vec{x} - \vec{x}^*$  where  $\vec{x}^* = A^{-1} \vec{b}$  is the extremum of the exponential's argument. From now on we call  $Z[A, \vec{b}]$  a *generating function*.

**1.1.2. Correlations Functions.** Since we calculated  $Z[A, 0]$  we can now define a Gaussian probability density over  $x \in \mathbb{R}^N$  (namely a multivariate normal distribution with zero mean and covariance matrix  $A^{-1}$ ),

$$(1.6) \quad p(\vec{x}) = \frac{1}{Z[A, 0]} e^{-\frac{1}{2} \mathbb{A}(\vec{x})}$$

From this distribution we can calculate expected values of products (also called correlation functions) of  $l$  of the variables  $x_i$ .

$$(1.7) \quad \langle x_{k_1} \dots x_{k_l} \rangle = \frac{1}{Z[A, 0]} \int_{\mathbb{R}^n} x_{k_1} \dots x_{k_l} e^{-\frac{1}{2} \mathbb{A}(\vec{x})}$$

where  $k_j = 1 \dots N$ . To do so we exploit the generating function property of  $Z[A, b]$ , i.e.:

$$(1.8) \quad \begin{aligned} \langle x_{k_1} \dots x_{k_l} \rangle &= \frac{1}{Z[A, 0]} \int_{\mathbb{R}^n} x_{k_1} \dots x_{k_l} e^{-\frac{1}{2} \mathbb{A}(\vec{x})} = \\ &= \frac{1}{Z[A, 0]} \frac{\partial}{\partial b_{k_1}} \dots \frac{\partial}{\partial b_{k_l}} \int_{\mathbb{R}^n} d^n x e^{-\frac{1}{2} \mathbb{A}(\vec{x}) + \vec{b} \cdot \vec{x}} \Big|_{b=0} \\ &= \frac{1}{Z[A, 0]} \frac{\partial}{\partial b_{k_1}} \dots \frac{\partial}{\partial b_{k_l}} Z[A, b] \Big|_{b=0} \\ &= \frac{\partial}{\partial b_{k_1}} \dots \frac{\partial}{\partial b_{k_l}} e^{\frac{1}{2} \vec{b}^T A^{-1} \vec{b}} \end{aligned}$$

Hence, for symmetry, any correlation function that has an odd number of variables vanishes identically (at least one  $x_i$  remains with an odd power while this Gaussian is an even function centered around the origin). Instead any even correlation function can be calculated using Wick's Theorem, as discussed below.

**1.1.3. Wick's Theorem.** We discovered that correlation functions can be computed using derivatives of  $Z[A, b]$ . Wick's theorem states that any even-number correlation function can be written as the sum of products of two points correlation functions. For instance, by defining  $C_{i,j} = A_{i,j}^{-1}$ , we have

$$(1.9) \quad \langle x_a x_b x_c x_d \rangle = C_{ab} C_{cd} + C_{ac} C_{bd} + C_{ad} C_{bc}$$

where indices could also be equal (e.g.  $a = b$  is allowed but one still needs to compute all terms as if they were distinct). In the right-hand side one notes that there are all possible pairs of indices  $(a, b, c, d)$ , obtained from their permutations. This is also the structure in general of Wick's Theorem. By defining a permutation  $\mathcal{P}$  of indices  $(k_1, k_2, \dots, k_l)$  for even  $l$  as  $(k_1^{\mathcal{P}}, k_2^{\mathcal{P}}, \dots, k_l^{\mathcal{P}})$ , one has

$$(1.10) \quad \langle x_{k_1} x_{k_2} \dots x_{k_l} \rangle = \sum_{\text{"all"} \mathcal{P}} C_{k_1^{\mathcal{P}} k_2^{\mathcal{P}}} \dots C_{k_{l-1}^{\mathcal{P}} k_l^{\mathcal{P}}}$$

Here we thus summed products of  $C_{ab}$  taking into account all possible permutations of the indices. The number of terms in this expression, in the case of  $l = 2m$  variables, is  $(2m - 1)!!$  (double factorial).

## 1.2. Steepest descent method

We recall the method of steepest descent to approximate integrals with Gaussian integrals in some suitable limit. Here we deal with real variables and thus we are discussing Laplace's method. More in general, such integrals would be available also for complex variables within a saddle point scheme.

We deal with integrals of the form  $\int d^n x e^{-F(\vec{x})/\lambda}$  for  $\lambda \rightarrow 0$ . We have

$$(1.11) \quad I(\lambda) = \int d^n x e^{-F(\vec{x})/\lambda} \approx \lambda^{n/2} e^{-F(\vec{x}_c)/\lambda} \frac{(2\pi)^{n/2}}{\det(\partial^2 F(\vec{x}_c))^{1/2}}$$

where  $\vec{x}_c$  is the maximum of  $F(\vec{x})$  and  $\partial^2 F(\vec{x}_c)$  is a shorthand notation for the matrix with second derivatives of  $F$ , which plays the role of  $A$  in the previous section:  $\partial_{x_i, x_j}^2 F(\vec{x}_c) = A_{ij}$ . To derive this result we just change the variable  $\vec{x} = \vec{x}_c + \sqrt{\lambda} \vec{y}$ , expand the exponent argument in  $\lambda$  and ignore all factors  $O(\lambda^{1/2})$ .

Sometimes it is more natural to think of a parameter  $s \rightarrow \infty$  (e.g. the systems size in a thermodynamic limit). Trivially, one may set  $s = 1/\lambda$  in the previous treatment. In more general contexts the integral could contain also another function  $g(x)$  as a prefactor of the exponential. Moreover, the range  $C$  of integration needs not to be the full real line. In the one-dimensional case, such integral becomes

$$(1.12) \quad I(s) = \int_C g(x) e^{sf(x)} dx \approx \frac{(2\pi)^{1/2} g(x_c) e^{sf(x_c)}}{|sf''(x_c)|^{1/2}}$$

where  $x_c$  is the maximum of  $f(x)$  within the interval  $C$ . This formula holds if the maximum  $x_c$  stays far from the boundary of  $C$ . See the exercises for an example in which it is better to not apply directly this formula (because  $x_c$  tends to the boundary for increasing  $s$ ).

## 1.3. Fourier Transform (FT)

The FT of a function  $f(x)$  is here defined as

$$\mathcal{F}(f) = \tilde{f}(k) = \int_{-\infty}^{\infty} e^{-ikx} f(x) dx$$

and its inverse consequently is defined as

$$\mathcal{F}^{-1}(\tilde{f}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} \tilde{f}(k) dk$$



Note that other definitions with different splitting of the  $2\pi$  factor and with opposite signs in the exponential are also used in other contexts. We stick to this one in most of our lessons.

**1.3.1. FT of the Dirac's Delta  $\delta(x)$ .** One finds immediately that

$$\mathcal{F}(\delta) = \int_{-\infty}^{\infty} e^{-ikx} \delta(x) dx = 1$$

and consequently that there is a representation of the  $\delta$  function in terms of the inverse Fourier transform,  $\delta = \mathcal{F}^{-1}(1)$ , which becomes

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk$$

This is a form used often to perform useful mathematical tricks.

**1.3.2. FT of the Heavyside function  $\theta(x)$ .** The step function, or Heavyside function, is defined as

$$\theta(x) = \begin{cases} 1 & \text{if } x > 0 \\ 1/2 & \text{if } x = 0 \\ 0 & \text{if } x < 0 \end{cases}$$

The  $1/2$  value at  $x = 0$  derives from the definition of the step function as a shift of the rescaled “sign” function,  $\theta(x) = 1/2 + \text{sgn}(x)/2$ , where

$$\text{sgn}(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x = 0 \\ -1 & \text{if } x < 0 \end{cases}$$

By noting that

$$\delta(x) = \frac{d}{dx} \theta(x) = \frac{1}{2} \frac{d}{dx} \text{sgn}(x)$$

and by recalling (exercise: use partial integration) that the FT of a derivative of  $f(x)$  is

$$\mathcal{F}\left(\frac{d}{dx} \theta(x)\right) = ik \tilde{f}(k)$$

we arrive at

$$\begin{aligned} \tilde{\theta}(k) &= \frac{1}{ik} \mathcal{F}\left(\frac{d}{dx} \theta(x)\right) + \mathcal{F}\left(\frac{1}{2}\right) \\ &= \frac{1}{ik} \mathcal{F}(\delta(x)) + \frac{1}{2} \mathcal{F}(1) \\ (1.13) \quad &= \frac{1}{ik} + \pi \delta(k) \end{aligned}$$

where we used  $\mathcal{F}(1) = 2\pi \delta(k)$  in the last step.

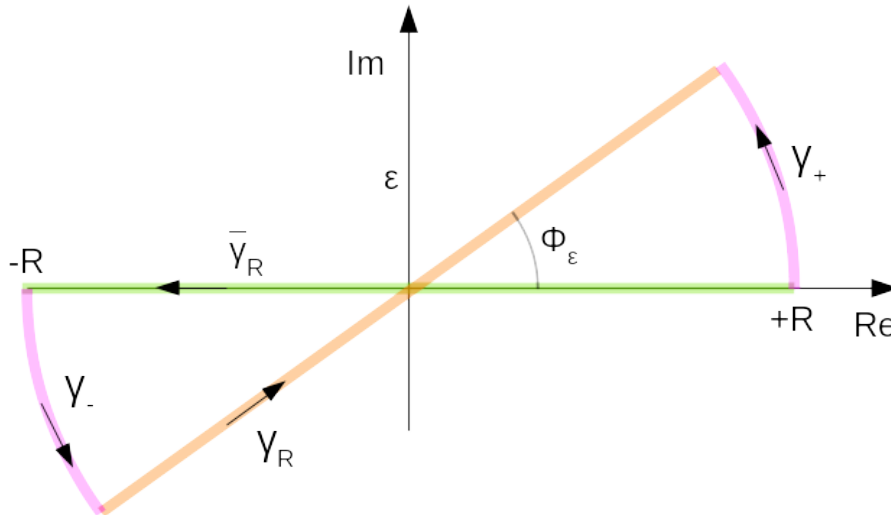
## 1.4. Gaussian with imaginary mean

We want to give a sense to the Gaussian integral

$$(1.14) \quad \int_{\mathbb{R}} e^{-a(x-ib)^2} dx$$

where  $b \in \mathbb{R}$ . Since the integrand is analytic, we can continue it to a complex variable  $z$  and consider a contour  $\Gamma_R = \gamma_1 \cup \gamma_2 \cup \gamma_+ \cup \gamma_-$  where  $\gamma_1$  is the interval  $[-R, R]$ ,  $-\gamma_2$  is  $[-R+ib, R+ib]$ ,  $\gamma_+$  is  $[R, R+ib]$  and  $\gamma_-$  is  $[-R+ib, -R]$ . The contribution for  $R \rightarrow \infty$  is zero on  $\Gamma_R$  and on  $\gamma_{\pm}$ ; instead  $\gamma_{1,2}$  give opposite results, hence:

$$(1.15) \quad \int_{\mathbb{R}} e^{-a(x-ib)^2} dx = \sqrt{\frac{\pi}{a}}$$



**Figure 2.** Contour used to compute the Fresnel integral.

This implies that

$$(1.16) \quad \int_{\mathbb{R}} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}$$

for all  $b \in \mathbb{C}$  and  $a > 0$ .

**1.4.1. Fresnel integral.** The Fresnel integral

$$(1.17) \quad \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-iak^2-ibk} = (4\pi ai)^{-1/2} e^{\frac{ib^2}{4a}}$$

has a structure for example found in the FT of the Schrödinger equation (see below). It looks like a normal Gaussian integral where complex variables are used for its variance and mean. However, to prove its convergence, we follow an explicit procedure. We thus prove its formula by showing that  $I(a, b) \equiv \lim_{\epsilon \rightarrow 0} I_\epsilon(a, b)$ , where

$$(1.18) \quad I_\epsilon(a, b) = \lim_{R \rightarrow \infty} \int_{-R}^R \frac{dk}{2\pi} e^{-ak^2 e^{i(\pi/2-\epsilon)} - ibk}$$

is a deformed and regularized version of  $I(a, b)$ .

We consider  $a, b \in \mathbb{R}$  and we start with the case  $a > 0$ . By looking at the exponent in  $I_\epsilon$  we find it useful to introduce the variable  $z = ke^{i(\pi/4-\epsilon/2)} = ke^{i\phi_\epsilon}$  with angle  $\phi_\epsilon = \pi/4 - \epsilon/2 < \pi/4$  for small  $\epsilon > 0$ . This variable moves along a line  $\gamma$  in the complex plane that is tilted of  $\phi_\epsilon$  with respect to the real axis. We then construct a contour  $\Gamma_R = \gamma_R \cup \gamma_+ \cup \bar{\gamma}_R \cup \gamma_-$  (see Figure 2) composed of

- $\gamma_+ = \{z = Re^{i\theta} : \theta \in [0, \phi_\epsilon]\}$
- $\gamma_- = \{z = Re^{i\theta} : \theta \in [\pi, \pi + \phi_\epsilon]\}$
- $\gamma_R = \{|z| \leq R, \arg z = \phi_\epsilon\}$
- $\bar{\gamma}_R = [-R, R]$  (with orientation reversed)

In  $\Gamma$  a portion  $\gamma_R$  is tilted as  $\gamma$  and will tend to it for  $R \rightarrow \infty$ .

The closed contour in the complex plane allows us to use Cauchy's Theorem. In this case the contour encloses no pole and the full integral along  $\Gamma$  of an analytic function is zero. The strategy is to show that the contributions on  $\gamma_+$  and  $\gamma_-$  become negligible for  $R \rightarrow \infty$  and that the integral on  $\bar{\gamma}_R$  (after reversing its orientation) matches that on  $\gamma_R$ .

Consider the integrand calculated on  $\gamma_+$  with parametrization  $z = Re^{i\theta}$  for  $0 \leq \theta \leq \phi_\epsilon$ . To show that it becomes negligible we use an inequality for its modulus. Thus,

$$\begin{aligned} R \left| \frac{e^{-i\phi_\epsilon}}{2\pi} \int_{\gamma_+} e^{-az^2 - izb} dz \right| &\leq R \int_0^{\phi_\epsilon} d\theta \left| e^{i\theta - aR^2 e^{2i\theta} - iRbe^{i(\theta - \phi_\epsilon)}} \right| \\ &= R \int_0^{\phi_\epsilon} d\theta e^{-aR^2 \cos(2\theta) + Rb \sin(\theta - \phi_\epsilon)} \xrightarrow{R \rightarrow 0} 0 \end{aligned}$$

because  $\phi_\epsilon < \pi/4$  and the term with  $\cos(2\theta) > 0$  in the exponent guarantees the decay with  $R$ . The same holds on  $\gamma_-$ .

By calling  $b' = be^{-i\phi_\epsilon}$ , on  $\bar{\gamma}_R$  we have

$$\lim_{R \rightarrow \infty} \frac{e^{-i(\phi_\epsilon)}}{2\pi} \int_{-R}^R e^{-az^2 - ib'z} = \left(\frac{\pi}{a}\right)^{1/2} \frac{e^{-\frac{b'^2}{4a}}}{2\pi} \xrightarrow{\epsilon \rightarrow 0} (4\pi ai)^{-1/2} e^{\frac{ib^2}{4a}}$$

(to show how a Gaussian integral with imaginary  $b$  is computed, see the exercises). Since the integral over  $\Gamma_R$  is zero by Cauchy we conclude that

$$I(a, b) \equiv \lim_{\epsilon \rightarrow 0} I_\epsilon(a, b) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-iak^2 - ibk} = (4\pi ai)^{-1/2} e^{\frac{ib^2}{4a}}$$

for  $a > 0$ .

For the case  $a < 0$  use  $I(a, b) = I^*(-a, -b)$ ,  $(-ia) = (ia)^*$ , and  $b^2 = (b^2)^*$  to show that the same formula holds.

**1.4.2. Example: Schrödinger Equation.** Consider the free Schrödinger equation:

$$(1.19) \quad i\hbar \partial_t \psi(x, t) = -\frac{\hbar^2}{2m} \partial_x^2 \psi(x, t)$$

Set  $\hbar = 1$  and move to Fourier space:

$$(1.20) \quad \psi(x, t) = \int \frac{dp}{2\pi} \tilde{\psi}(p, t) e^{ipx}$$

$$(1.21) \quad i\partial_t \tilde{\psi}(p, t) = \frac{p^2}{2m} \tilde{\psi}(p, t)$$

$$(1.22) \quad \tilde{\psi}(p, t) = \tilde{\psi}(p, 0) e^{-i\frac{p^2 t}{2m}}$$

Since we use  $\psi(x, 0) = \delta(x)$  we have  $\tilde{\psi}(p, 0) = e^{-i\frac{p^2 t}{2m}}$ . To find  $\psi(x, t)$  we make use of Fresnel integrals ( $a = \frac{t}{2m}$  and  $b = -ix$ ):

$$(1.23) \quad \psi(x, t) = \frac{1}{2\pi} \int dp e^{-i\frac{p^2 t}{2m} + ipx} = \left(4\pi \frac{t}{2m} i\right)^{-1/2} e^{\frac{i(-ix)^2}{4\frac{t}{2m}}} = \left(\frac{m}{2\pi i t}\right)^{1/2} e^{-\frac{mx^2}{2it}}$$

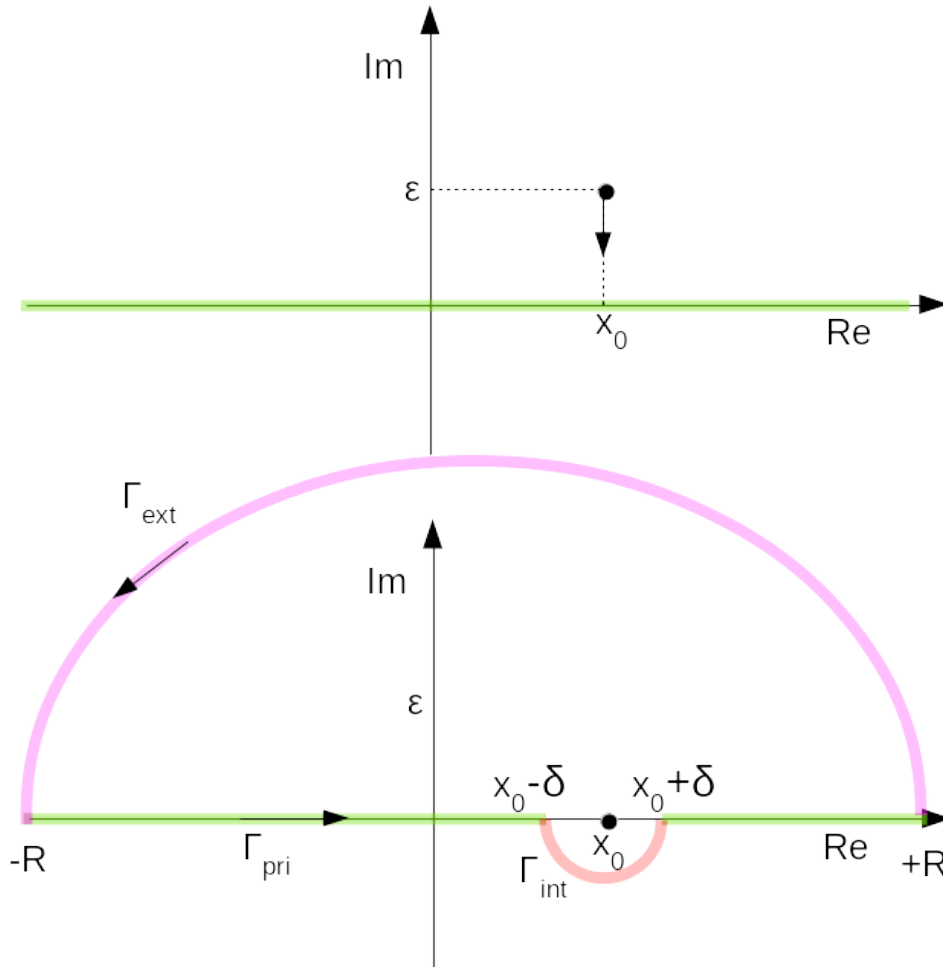
Putting back  $\hbar$ :

$$(1.24) \quad \psi(x, t) = \left(\frac{m}{2\pi \hbar i t}\right)^{1/2} e^{-\frac{mx^2}{2\hbar i t}}$$

This is called the propagator for the free Schrödinger equation.

## 1.5. Indented Integrals and $\epsilon$ prescription

In some integrals of complex variables one finds poles tending to the real axis for say  $\epsilon \rightarrow 0$ , which are dealt with a limiting procedure as follows. We show that these integrals, pictorially represented by the green path in the upper panel of Figure. 3, are equivalent to another limiting procedure in which the pole already lays on the real axis and is progressively encircled by a contour (lower panel of Figure. 3). In the depicted scenario, the pole is approaching  $x_0$  from above and the contour is encircling the pole. The other case with contour not encircling a pole that is approaching  $x_0$  from below is found in the exercises.



**Figure 3.** Contour used to compute the indented integral discussed in the text. The green portion is the path  $\Gamma_{pri}$  where the principal value of the integral emerges.

The equation we want to prove is, for any analytic function in the upper complex plane  $\text{Im}(z) \geq 0$  that tends to zero sufficiently fast for  $|z| \rightarrow \infty$ ,

$$(1.25) \quad \lim_{\epsilon \rightarrow 0^+} \int_{\mathbb{R}} \frac{f(x)}{x - x_0 - i\epsilon} dx = \mathbb{P} \int_{\mathbb{R}} \frac{f(x)}{x - x_0} dx + i\pi f(x_0)$$

The validity for a quite generic  $f$  leads physicists to crudely summarize the equation with the notation

$$\lim_{\epsilon \rightarrow 0} \frac{1}{x - x_0 - i\epsilon} = \mathbb{P} \frac{1}{x - x_0} + i\pi\delta(x - x_0)$$

The notation  $\mathbb{P} \int \dots$  denotes the principal value of an integral:

$$\mathbb{P} \int_{\mathbb{R}} \frac{f(x)}{x - x_0} dx = \lim_{\delta \rightarrow 0} \left[ \int_{-\infty}^{x_0 - \delta} \frac{f(x)}{x - x_0} dx + \int_{x_0 + \delta}^{\infty} \frac{f(x)}{x - x_0} dx \right]$$

For instance, for  $f = 1/x^2$  and  $x_0 = 0$ , for symmetry we have

$$\mathbb{P} \int_{\mathbb{R}} \frac{1}{x^3} dx = \lim_{\delta \rightarrow 0} \left[ \int_{-\infty}^{-\delta} \frac{1}{x^3} + \int_{\delta}^{\infty} \frac{1}{x^3} \right] = \lim_{\delta \rightarrow 0} 0 = 0$$

Without principal value extraction, the integral of  $1/x^3$  in  $\mathbb{R}$  would not be well defined.

To prove (1.25), we use Cauchy Theorem for closed contours once more, and again we need that the contribution of the integral in the outer semicircle  $\Gamma_{ext}$  (Figure 3) vanishes for  $R \rightarrow \infty$ . In this case it is granted by the selection of functions  $f(z)$  that tend to zero quickly enough for  $R \rightarrow \infty$ .

The two remaining contributions to the integral for  $\delta \rightarrow 0$  become, respectively, the principal value (integral on  $\Gamma_{pri}$  in the Figure) and half of the residue in  $x_0$  (integral on the semicircle  $\Gamma_{int}$ ), which is indeed  $i\pi f(x_0)$

## 1.6. Characteristic Functions

Here we define the characteristic function for a random variable and then prove the central limit theorem for the sum of independent and identically distributed (i.i.d.) random variables. Let be  $x$  a random variable with probability density  $p(x)$ . Its mean or first moment  $\mu$  is defined as

$$(1.26) \quad \mu = \langle x \rangle = \int dx x p(x)$$

and its variance, also known as second cumulant or central second moment,  $\sigma^2$  is

$$(1.27) \quad \sigma^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

In general for a function  $f(x)$  it holds that

$$(1.28) \quad \langle f \rangle = \int dx f(x) p(x)$$

$$(1.29) \quad p(f) = \langle \delta(f - f(x)) \rangle = \int dx p(x) \delta(f - f(x))$$

$$(1.30) \quad \langle f^k \rangle = \int dx f^k(x) p(x)$$

If  $f(x) = x$  the expected values  $\langle x^k \rangle$  for  $k \geq 1 \in \mathbb{N}$  are called moments of the random variable  $x$ . The moments are easily computed using the Fourier transform of the distribution of  $x$  (here defined with plus sign in the exponent  $e^{ikx}$ , the inverse thus gets a minus in the exponent, see the Dirac  $\delta(x) = \mathcal{F}^{-1}(1)$  below), also known as the *characteristic function* of  $x$ , which we denote by  $\varphi(k)$ :

$$(1.31) \quad \varphi(k) = \langle e^{ikx} \rangle = \int dx e^{ikx} p(x)$$

Indeed, since  $e^{ikx} = 1 + ikx - \frac{1}{2}k^2x^2 + \dots = \sum_{n=0}^{\infty} \frac{i^n k^n x^n}{n!}$ , the series representation for  $\varphi(k)$  is

$$(1.32) \quad \varphi(k) = \langle e^{ikx} \rangle = \sum_{n=0}^{\infty} \frac{i^n k^n}{n!} \langle x^n \rangle$$

from which

$$(1.33) \quad \langle x^n \rangle = (-i)^n \left. \frac{\partial}{\partial k^n} \varphi(k) \right|_{k=0}$$

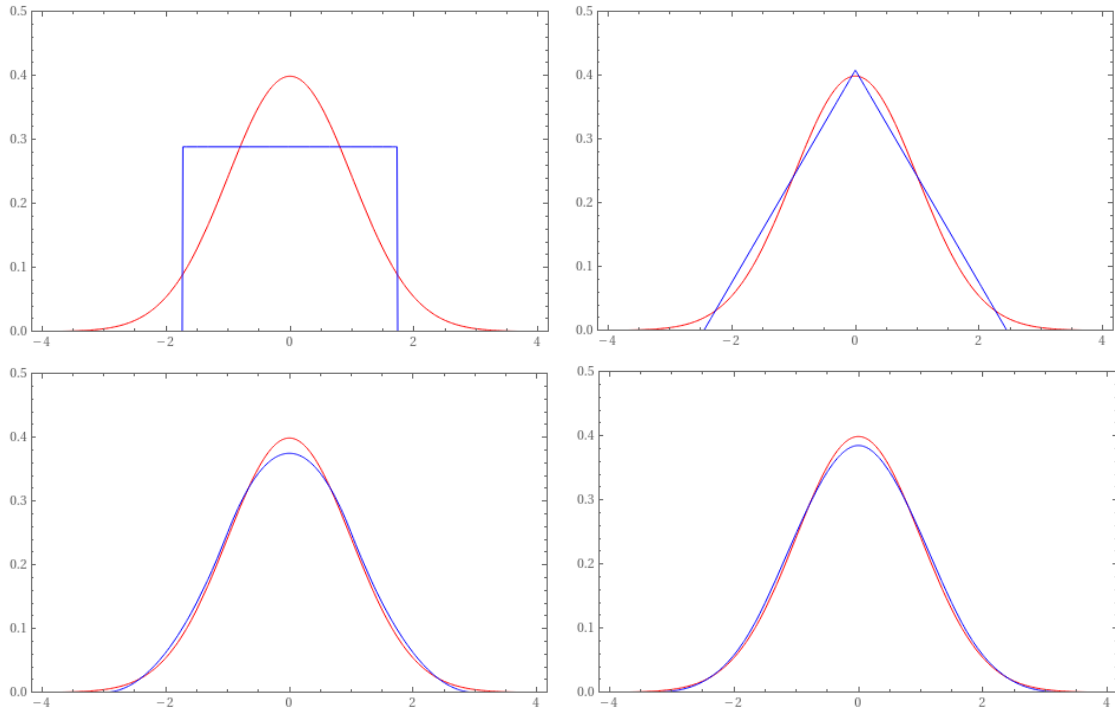
A nice property is that a probability density arising from the convolution of two other probability densities,

$$p(x) = \int dx' p_1(x') p_2(x - x') = \int dx' \int dx'' \delta(x - x' - x'') p_1(x') p_2(x'')$$

has a characteristic function that is the product of the other two

$$\varphi(k) = \varphi_1(k) \varphi_2(k)$$

Such property is useful when considering the sum  $x = x' + x''$  of two i.i.d. variables  $x'$  and  $x'' = x - x'$ .



**Figure 4.** Convergence to a normal distribution (red curve) for the rescaled sum of i.i.d. variables, each one following a flat distribution as in the first panel. The panels are for  $n = 1, 2, 3, 4$  and blue curves are the probability densities of rescaled sums  $Y_n$ .

## 1.7. Central Limit Theorem

Consider a set  $x = \{x_1, \dots, x_n\}$  of  $n$  i.i.d. random variables with mean  $\mu$  and variance  $\sigma^2$  and call  $S_n = \sum_{i=1}^n x_i$  their sum. We want to prove that this sum follows to a better and better degree a Gaussian distribution in the limit of large  $n$ , that is, we aim at proving the

**Central Limit Theorem:** *a properly normalized sum of i.i.d. random variables tends toward a normal distribution even if original variables are not normally distributed. It is required that their distribution has a finite variance  $\sigma^2 < \infty$ .*

A pictorial example of this convergence is shown in Figure 4.

With the sum  $S_n$  we define the random variable

$$(1.34) \quad Y_n(x) \equiv \frac{S_n - n\mu}{\sqrt{n}\sigma}$$

It is easy to find that  $\langle Y_n \rangle = 0$  and  $\text{Var}(Y_n) = 1$ . Thus, this variable is rescaled to remain with a constant variance and zero mean for all  $n$ 's.

We want to find the distribution for  $Y_n$  in the limit  $n \rightarrow \infty$ :

$$\begin{aligned}
 p(Y_n(x) = y) &= \langle \delta(y - Y_n(x)) \rangle \\
 &= \left\langle \frac{1}{2\pi} \int_{\mathbb{R}} d\alpha e^{-i\alpha[y - Y_n(x)]} \right\rangle \\
 &= \left\langle \frac{1}{2\pi} \int_{\mathbb{R}} d\alpha e^{-i\alpha y + i\alpha[\sum_i x_i - n\mu]/(\sqrt{n}\sigma)} \right\rangle \\
 &= \frac{1}{2\pi} \int_{\mathbb{R}} d\alpha e^{-i\alpha y - i\alpha \frac{n\mu}{\sqrt{n}\sigma}} \int \prod_{i=1}^n dx_i p(x_i) e^{\frac{i\alpha}{\sqrt{n}\sigma} x_i} = \\
 (1.35) \quad &= \frac{1}{2\pi} \int_{\mathbb{R}} d\alpha e^{-i\alpha \left( y + \frac{n\mu}{\sqrt{n}\sigma} \right)} \left( \int dx p(x) e^{\frac{i\alpha}{\sqrt{n}\sigma} x} \right)^n
 \end{aligned}$$

The quantity in the parenthesis is the characteristic function for  $k = \frac{\alpha}{\sqrt{n}\sigma}$ , hence for  $n \rightarrow \infty$

$$(1.36) \quad \varphi\left(k = \frac{\alpha}{\sqrt{n}\sigma}\right) = 1 + i\mu \frac{\alpha}{\sqrt{n}\sigma} - \frac{\alpha^2}{2n\sigma^2} (\sigma^2 + \mu^2) + o(n^{-3/2}) =$$

$$(1.37) \quad = e^{\frac{i\alpha\mu}{\sqrt{n}\sigma} - \frac{\alpha^2}{2n} + o(n^{-3/2})}$$

Please spend a second to appreciate that in the last step there remains only  $-\frac{\alpha^2}{2n}$  in the second order in  $\alpha$  of the exponent. One can check that the Taylor expansion of the last function gives the previous one in (1.36).

In the end,

$$(1.38) \quad p(Y_n(x) = y) = \frac{1}{2\pi} \int_{\mathbb{R}} d\alpha e^{-i\alpha y - i\alpha \frac{n\mu}{\sqrt{n}\sigma}} \left( e^{\frac{i\alpha\mu n}{\sqrt{n}\sigma} - \frac{\alpha^2}{2} + o(n^{-1/2})} \right)$$

$$(1.39) \quad = \frac{1}{2\pi} \int_{\mathbb{R}} d\alpha e^{-i\alpha y - \frac{\alpha^2}{2} + o(n^{-1/2})}$$

$$(1.40) \quad \rightarrow \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} \quad \text{for } n \rightarrow \infty$$

Since we have  $\lim_{n \rightarrow \infty} Y_n(x) \sim \mathcal{N}(0, 1)$  from the normal distribution properties we find  $S_n \rightarrow \mathcal{N}(n\mu, n\sigma^2)$  and  $\frac{1}{n}S_n \rightarrow \mathcal{N}(\mu, \frac{\sigma^2}{n})$ . In Figure 4 there is an example of flat  $p(x)$  and distributions of rescaled sums of up to  $n = 4$  i.i.d. variables  $x$ .

## Problems

**Exercise 1.1.** Given  $\vec{x} = (x_1, x_2)$ ,

$$A = \begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix}$$

and  $\vec{b} = (1, 0)$ , compute the Gaussian integrals

$$Z(A) = \int d^2x \exp\left[-\frac{1}{2} \vec{x}^T A \vec{x}\right]$$

and

$$Z(A, \vec{b}) = \int d^2x \exp\left[-\frac{1}{2} \vec{x}^T A \vec{x} + \vec{b} \cdot \vec{x}\right]$$

**Exercise 1.2.** With the saddle-point strategy, compute the approximation for large  $s$  of

$$I(s) = \int_{-\infty}^{\infty} e^{sx - \cosh x} dx$$

**Exercise 1.3.** With the saddle-point strategy, compute the approximation for large  $N$  of

$$I(N) = \int_0^{\infty} \cos(x) e^{-N[(x-\pi/3)^2 + (x-\pi/3)^4]} dx$$

**Exercise 1.4.** Show that the following formula holds for the Fourier transform ( $\mathcal{F}(f) = \tilde{f}(k)$ ) of a derivative of the function  $f(x)$  (under the usual mathematical assumptions for having a Fourier transform and its derivative):

$$\mathcal{F}\left(\frac{d}{dx}\theta(x)\right) = ik\tilde{f}(k)$$

**Exercise 1.5.** Show that  $\mathcal{F}(1) = 2\pi\delta(k)$ .

**Exercise 1.6.** To complete the case discussed during the lecture, compute

$$\lim_{\epsilon \rightarrow 0} \frac{1}{x - x_0 + i\epsilon} = P\left[\frac{1}{x - x_0}\right] - i\pi\delta(x - x_0)$$

Note that this limit and that discussed in the lecture are a physicists' crude shorthand notation for the full equation

$$\lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0 \mp i\epsilon} dx = P \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0} dx \pm i\pi f(x_0)$$

and  $f(z) \rightarrow 0$  for  $|z| \rightarrow \infty$  and analytic in the  $\text{Im}(z) \geq 0$  portion of the complex plane.

**Exercise 1.7.** Compute the Gaussian integral

$$I = \int_{-\infty}^{\infty} dx e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}} e^{b^2/(4a)}$$

for  $a \in \mathbb{R}$ ,  $a > 0$  and complex  $b = \beta + i\nu$  (with  $\beta, \nu \in \mathbb{R}$ ). For the solution, one may shift to a new variable  $z$  with  $x = z + iq$ , so that the exponent in the integral does not contain a term  $\sim iz$  and the new path of integration can be mapped back to the real axis by using Cauchy's theorem.





# Stochastic Processes and Path Integrals

## 2.1. Diffusion Equation

Suppose we have a particle in a bath composed of another kind of particles, e.g. a fluid as air or water. Moreover, the inertia of this particle is low enough to make the collision between that particle and the bath particles produce movement. This process could be described in principle using Newton's law of motion (we stay for now in the classical framework) but in practice this is impossible: we would have to deal with a number of order  $10^{23}$  of equations of motion; the solution to this problem is found treating the bath as a random noise applied to the particle (this is possible if we are interested to time scales much larger than the time between successive collisions of the particles of the bath). To begin, we introduce the particle density  $\rho$  at position  $x \in \mathbb{R}^d$  and at time  $t$  such that the integral over a region  $A \subseteq \mathbb{R}^d$  of  $\rho$  gives the fraction of particles inside that region:

$$(2.1) \quad \int_A d^d x \rho(x, t)$$

We are now considering an ensemble of independent particles, rather than just one, moving in the fluid. Since the particles leave or enter the region  $A$  through the boundary,  $\partial A$ , we need to introduce the current vector  $\mathbf{j}(x, t)$  whose surface integral  $\int_S \hat{n}(x) \cdot \mathbf{j}(x, t) dS$  is the net number of particles crossing  $S$  per unit time.  $\hat{n}(x)$  represents the unit normal vector at the position  $x$  on the surface  $S$ .

$$(2.2) \quad \partial_t \int_A d^d x \rho(x, t) = - \int_{\partial A} \mathbf{j}(x, t) \cdot \hat{n}(x) dS = - \int_A d^d x \nabla \cdot \mathbf{j}(x, t)$$

In the previous equation  $\hat{n}$  is oriented outward the region  $A$ : the minus sign is due to the fact that when  $\mathbf{j}(x, t) \cdot \hat{n}(x) > 0 (< 0)$  particles are leaving (entering in)  $A$ . Since the region  $A$  is arbitrary we get:

$$(2.3) \quad \partial_t \rho(x, t) = -\nabla \cdot \mathbf{j}(x, t)$$

At this moment we don't have any external field so the only way to construct the current  $\mathbf{j}(x, t)$  is from  $\rho$  and its derivatives; assuming  $\rho$  is small (along with its derivatives) we choose:

$$(2.4) \quad \mathbf{j}(x, t) = -D(x, t) \nabla \rho(x, t)$$

(the minus sign is due to a similar argument as before); we arrive at:

$$(2.5) \quad \partial_t \rho(x, t) = \nabla \cdot (D(x, t) \nabla \rho(x, t))$$

For constant  $D$  we derive Fick's Law (diffusion equation):

$$(2.6) \quad \partial_t \rho(x, t) = D \nabla^2 \rho(x, t)$$

Side note: we can always choose  $\rho$  normalized to 1 and interpret it as a probability distribution, thing that we'll do later on.

Let us consider for simplicity the 1-dimensional case and evaluate the average and the variance of the position of our particle(s). In general the average of a function  $f(x)$  at time  $t$  is defined as

$$(2.7) \quad \langle f(x) \rangle_t \equiv \int_{-\infty}^{\infty} \rho(x, t) f(x) dx$$

Using eq. (2.6) and the boundary conditions  $\lim_{x \rightarrow \pm\infty} \rho(x, t) = 0$  and  $\lim_{x \rightarrow \pm\infty} \partial \rho(x, t) / \partial x = 0$  one finds that

$$(2.8) \quad \frac{d}{dt} \langle f(x) \rangle_t = \dots = D \int_{-\infty}^{\infty} \rho(x, t) \frac{d^2 f(x)}{dx^2} dx$$

from which we derive that  $d\langle x \rangle_t / dt = 0$  and  $d\langle x^2 \rangle_t / dt = 2D$ . If the initial condition is  $\rho(x, 0) = \delta(x)$ , i.e. initially the particle is at the origin,  $\langle x \rangle_t = 0$  and  $\langle x^2 \rangle_t = 2Dt$  implying that  $\text{Var}_t x \equiv \langle x^2 \rangle_t - \langle x \rangle_t^2 = 2Dt$ . The last result is due to Einstein (1905)

## 2.2. Random walk and diffusion equation

We can derive diffusion equation using a more "microscopic" (not in the strict sense) approach, by means of Discrete Markov Process. Consider a particle moving on a one dimensional lattice of spacing  $l$  and take a discrete time with unit  $\epsilon$ . We call the transition matrix of jumping in a time step  $\epsilon$  from site  $j$  to site  $i$   $W_{ij}$  whereas the probability of being at site  $i$  at time  $t_n = n\epsilon$  is denoted  $w_i(t_n)$ . By the definition of the transition matrix we have the following evolution equation, known as Master Equation (ME):

$$(2.9) \quad w_i(t_n) = \sum_j W_{ij} w_j(t_{n-1})$$

In vector form:

$$w(t_n) = W w(t_{n-1}) = W^n w(0)$$

Notice that since probability must be conserved, i.e.  $\sum_i w_i(t_n) = 1 \forall t_n$ , and this is guaranteed if we require that  $\sum_j W_{ij} = 1 \forall i$ . Suppose that the only possible jumps are the ones from nearest neighbour sites, i.e.:

$$(2.10) \quad W_{ij} = p_+ \delta_{i,j+1} + p_- \delta_{i,j-1}$$

where  $p_+$  is the probability of a right jump, while  $p_- = 1 - p_+$  of a left one. We now derive  $w_i(t_n)$ ; in  $n$  time steps  $n_+$  steps on the right are done and  $n_-$  on the left such that  $n_+ + n_- = n$ ; the position  $i$  is  $i = n_+ - n_-$ , i.e.:

$$(2.11) \quad n_+ \equiv \frac{n+i}{2} \in \{0, 1, \dots, n-1, n\}$$

$$(2.12) \quad n_- \equiv \frac{n-i}{2} \in \{0, 1, \dots, n-1, n\}$$

If  $n \pm i$  is odd or  $|i| > n$  the probability is zero (why?) otherwise the solution of the ME eq. (2.9) is the binomial  $n_+ \sim \mathcal{B}(p_+, n)$ :

$$(2.13) \quad w_i(n) = \binom{n}{n_+} p_+^{n_+} p_-^{n-n_+} = \binom{n}{n_+} p_+^{n_+} p_-^{n-n_+} = \binom{n}{n_+} p_+^{\frac{n+i}{2}} p_-^{\frac{n-i}{2}}$$

Notice that the above solution satisfies the initial condition  $w_i(0) = \delta_{i,0}$ . To calculate moments we use the generating function method. For our case we define the following function

$$(2.14) \quad \hat{w}(z, n) = \sum_{n_+=0}^n z^{n_+} \binom{n}{n_+} p_+^{n_+} p_-^{n-n_+} = (p_+ z + p_-)^n$$

Why is  $\hat{w}(z=1, n) = 1$  ?

The moments of  $w_i(t_n)$  can be easily calculated as derivative of the generating function:

$$(2.15) \quad \langle n_+ \rangle = z \frac{\partial}{\partial z} \hat{w}|_{z=1} = np_+$$

$$(2.16) \quad \langle n_+^2 \rangle = \left( z \frac{\partial}{\partial z} \right)^2 \hat{w}|_{z=1} = np_+(1 + (n-1)p_+)$$

Since  $x_i = il(n_+ - n_-) = l(2n_+ - n)$  we obtain:

$$(2.17) \quad \langle x \rangle_{t_n} = nl(p_+ - p_-)$$

$$(2.18) \quad \text{Var}_{t_n}(x) = 4l^2 p_+ p_- n$$

**2.2.1. The continuum limit.** We consider now the continuum limit in space and time. We start with the simplest case  $p_+ = p_- = 1/2$  and  $n = t/\epsilon$ . Then  $\langle x \rangle_{t_n} = 0$  and

$$\text{Var}_t(x) = \frac{l^2}{\epsilon} t$$

A meaningful continuum limit with fixed  $t$ ,  $l \rightarrow 0$  and  $\epsilon \rightarrow 0$  and thus  $n \rightarrow \infty$  is obtained keeping  $\frac{l^2}{\epsilon} \equiv 2D$  constant:

$$(2.19) \quad \text{Var}_t(x) = 2Dt$$

This is the same result obtained in previous section.

We want now to see where the exact solution of the ME, eq. (2.13) converges in the large  $n$  limit for given  $t = n\epsilon$  and  $x = li$ . We use the Stirling's approximation

$$(2.20) \quad \ln n! = n \ln n - n + \frac{1}{2} \ln(2\pi n) + O(1/n)$$

in order to evaluate  $\ln w_i(t_n)$ . After some elementary steps one gets:

$$(2.21) \quad w_i(t_n) = \sqrt{\frac{2}{\pi n}} e^{-\frac{i^2}{2n} + O(i^2/n^2)}$$

Consider now a  $\Delta x = 2kl$  such that  $l \ll \Delta x \ll Dt$  with  $k$  and define the probability distribution in the continuum limit as

$$(2.22) \quad w(x, t)\Delta x = \sum_{j=i-k}^{i+k} w_j(t_n) \approx kw_i(t_n)$$

where  $t_n = t$  and  $x = il$  and we have taken into account that only half of the terms appearing in the summation is different from zero. The final result is:

$$(2.23) \quad w(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

For further insights let's take the continuum limit of the discrete ME itself, eqs. (2.9) and (2.10):

$$(2.24) \quad w_i(t_{n+1}) = \frac{1}{2} (w_{i-1}(t_n) + w_{i+1}(t_n))$$

Since we are looking for a continuum distribution we substitute  $il$  with  $x$   $t_n = n\epsilon$  and  $lw_i(t_n) = w(x, t)$  the previous eq. can be re-written as:

$$(2.25) \quad w(x, t + \epsilon) = \frac{1}{2} (w(x-l, t) + w(x+l, t))$$

$$(2.26) \quad w(x, t + \epsilon) - w(x, t) = \frac{1}{2} (w(x-l, t) + w(x+l, t) - w(x, t))$$

Expanding according to Taylor  $w(x, t + \epsilon) = w(x, t) + \epsilon \partial_t w(x, t) + \dots$  and  $w(x \pm l, t) = w(x, t) \pm l \partial_x w(x, t) + 1/2 l^2 \partial_x^2 w(x, t) + \dots$  and taking  $\epsilon \rightarrow 0$ ,  $l \rightarrow 0$  and  $n \rightarrow \infty$  keeping  $\frac{l^2}{\epsilon} \equiv 2D$  fixed, we obtain:

$$(2.27) \quad \partial_t w(x, t) = D \partial_x^2 w(x, t)$$

i.e. we arrived at the diffusion equation (2.6). Find out what the dots in the above Taylor expansions are and show that in the continuum limit the neglected terms converges to zero.

**2.2.2. Solution of the diffusion equation in  $\mathbb{R}$ .** We assume that the diffusion occurs in  $\mathbb{R}$  since  $\mathbb{R}^d$  is just a trivial extension of the formulas we will derive. Thus  $\nabla^2$  is simply  $\partial_x^2$  whose eigenfunctions are:

$$(2.28) \quad \partial_x^2 \varphi_k(x) = -k^2 \varphi_k(x)$$

$$(2.29) \quad \varphi_k(x) = e^{ikx}$$

for  $k \in \mathbb{R}$ . We will use the measure  $dk/2\pi$  in  $k$ -space and the normalization of the eigenfunction is such that

$$(2.30) \quad \int_{\mathbb{R}} \varphi_k(x) \varphi_{k'}^*(x) dx = \int_{\mathbb{R}} e^{i(k-k')x} dx = 2\pi \delta(k - k')$$

whereas

$$(2.31) \quad \int_{\mathbb{R}} \varphi_k(x) \varphi_{k'}^*(x') \frac{dk}{2\pi} = \int_{\mathbb{R}} e^{i(x-x')k} \frac{dk}{2\pi} = \delta(x - x')$$

Expanding  $w(x, t)$  in terms of eigenfunctions  $\varphi_k$  (it is a complete basis in  $L^2$  and it leads to the well known Fourier's transform):

$$(2.32) \quad w(x, t) = \int_{\mathbb{R}} c_k(t) \varphi_k(x) \frac{dk}{2\pi}$$

and using eq. (2.27) one obtains:

$$(2.33) \quad \begin{aligned} \frac{dc_k(t)}{dt} &= -Dk^2 c_k(t) \\ c_k(t) &= c_k(t_0) e^{-Dk^2(t-t_0)} \\ w(x, t) &= \int_{\mathbb{R}} c_k(t_0) e^{-Dk^2(t-t_0)} e^{ikx} \frac{dk}{2\pi} \end{aligned}$$

The initial condition leads to:

$$w(x, t_0) = \int_{\mathbb{R}} c_k(t_0) e^{ikx} \frac{dk}{2\pi}$$

and inverting the Fourier's transform

$$c_k(t_0) = \int_{\mathbb{R}} w(x', t_0) e^{-ikx'} dx'$$

If the particle is at  $x_0$  at time  $t = t_0$  then  $w(x, t_0) = \delta(x - x_0)$  we obtain  $c_k(t_0) = e^{-ikx_0}$  and:

$$(2.34) \quad w(x, t) \equiv W(x, t|x_0, t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} e^{-\frac{(x-x_0)^2}{4D(t-t_0)}} \quad t > t_0,$$

which is the same as eq. (2.23) as obtained in the continuum limit of the discrete ME. In the previous equation we have introduced the the so called propagator for the Brownian motion,  $W(x, t|x_0, t_0)$ , which is the solution of the diffusion eq. (2.27) satisfying the initial condition  $W(x, t_0|x_0, t_0) = \delta(x - x_0)$ . It satisfies:

$$W(x, t|x_0, t_0) = W(x - x_0, t - t_0|0, 0)$$

Show that the general solution of eq. (2.27) with arbitrary initial condition  $w(x, t_0)$  is given by

$$(2.35) \quad w(x, t) = \int dx_0 W(x, t|x_0, t_0) w(x_0, t_0)$$

Considering now  $t_0 < t' < t$ :

$$\begin{aligned} w(x', t') &= \int dx_0 W(x', t'|x_0, t_0) w(x_0, t_0) \\ w(x, t) &= \int dx' W(x, t|x', t') w(x', t') \end{aligned}$$

we obtain by combining these two equations:

$$w(x, t) = \int dx' W(x, t|x', t') \int dx_0 W(x', t'|x_0, t_0) w(x_0, t_0)$$

by comparison with the previous result (2.35), given the generic  $w(x, t_0)$ , we get:

$$(2.36) \quad W(x, t|x_0, t_0) = \int dx' W(x, t|x', t') W(x', t'|x_0, t_0)$$

i.e. the propagator satisfies the Einstein-Smoluchowski-Kolmogorov-Chapman relation.

**2.2.3. Scale invariance of the diffusion.** If we set  $x_0 = 0 = t_0$  we notice that eq. (2.34) obeys the following homogeneity equation

$$(2.37) \quad W(x, t|0, 0) = \lambda W(\lambda x, \lambda^2 t|0, 0)$$

This could have been deduced directly from the diffusion eq. (2.27). Indeed it is immediate to prove that if  $W(x, t|0, 0)$  satisfies the diffusion equation then also  $W(\lambda x, \lambda^2 t|0, 0)$  satisfies it. The extra factor  $\lambda$  in the r.h.s. of eq. (2.37) is a consequence of the fact that the l.h.s. is normalized to 1.

## 2.3. Wiener Path Integral

**2.3.1. Correlation functions.** The joint probability distribution to find the Brownian particle at positions in the intervals  $(x_1, dx_1)$  at time  $t_1$ ,  $(x_2, x_2 + dx_2)$  at time  $t_2$ , ...,  $(x_n, x_n + dx_n)$  at time  $t_n$  with  $t_0 < \dots < t_n$  is given by

$$(2.38) \quad \begin{aligned} d\mathbb{P}_{t_1, \dots, t_n}(x_1, \dots, x_n|x_0, t_0) &= W(x_n, t_n|x_{n-1}, t_{n-1}) W(x_{n-1}, t_{n-1}|x_{n-2}, t_{n-2}) \\ &\dots W(x_1, t_1|x_0, t_0) dx_1 dx_2 \dots dx_n = \\ &= \exp\left\{-\sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{4\Delta t_i D}\right\} \prod_{i=1}^n \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \end{aligned}$$

where initially, at time  $t_0$ , the particle is at  $x_0$ . The average of a generic function,  $f(x(t_1), \dots, x(t_n))$ , of the positions of the particle at times  $t_1, \dots, t_n$  is then defined as

$$(2.39) \quad \langle f(x(t_1), \dots, x(t_n)) \rangle_w = \int_{\mathbb{R}^n} f(x_1, \dots, x_n) d\mathbb{P}_{t_1, \dots, t_n}(x_1, \dots, x_n|x_0, t_0)$$

Let  $T$  be a finite subset of  $\mathbb{R}$  or an interval, e.g.:  $T = \{t_1, \dots, t_n\}$  or  $T = [0, \infty)$  and  $\mathbb{R}^T$  as the set of all functions having as domain  $T$ : in our example if  $T = [0, \infty)$ ,  $\mathbb{R}^T$  is the set of all functions  $x : [0, \infty) \rightarrow \mathbb{R}$  or if  $T = \{t_1, \dots, t_n\}$ ,  $\mathbb{R}^T$  is the set of all sequences  $\{x_1, \dots, x_n\} = \{x(t_1) \dots x(t_n)\}$  for some  $x_i$ 's. In the following we will be interested in  $T = [0, t)$  where  $0 < t \leq \infty$ .

Using  $T$  and  $\mathbb{R}^T$ , we want to construct a Brownian motion measure  $P_w$  for *appropriate* sets  $A \subset \mathbb{R}^T$ , i.e. associate a probability to this set.

We begin with a special case: consider  $n \in \mathbb{N}$  and a finite set of time instants  $\{t_1, \dots, t_n\}$  (where  $t_i < t_{i+1}$  and  $t_i \in \mathbb{R}$ ). Define  $\Delta t_i = t_i - t_{i-1}$  and  $H_i = [a_i, b_i] \forall i = 1 \dots n$  with  $a_i < b_i \in \mathbb{R}$ . We now define the cylindrical sets of  $\mathbb{R}^T$  as subsets of the form  $A = \{x(t) : x(t_1) \in H_1, \dots, x(t_n) \in H_n\}$ . We can now use the probability distribution (2.38) to define the measure of  $A$ -like sets as:

$$(2.40) \quad P_w(A) \equiv \mathbb{P}_{t_1, \dots, t_n}(A) = \int_{H_1} dx_1 \dots \int_{H_n} dx_n \prod_{i=1}^n \frac{1}{(4\pi D \Delta t_i)^{1/2}} \exp\left\{-\frac{(x_i - x_{i-1})^2}{4D \Delta t_i}\right\},$$

which is nothing else than the probability of a Brownian particle, starting at  $x_0$  at time  $t_0$ , is found, at later times  $t_i$ , in the interval  $H_i$  with  $i = 1, \dots, n$ . Notice that this relation is valid for any  $n \in \mathbb{N}$  and by the use of Kolmogorov extension theorem we are free to extend this result to any subset of the  $\sigma$ -algebra of  $\mathbb{R}^T$ ,  $\mathcal{F}$ , generated by the cylindrical subsets. This way we

constructed a probability space  $(\mathbb{R}^T, \mathcal{F}, P_w)$  where  $\mathcal{F}$  is the set of measurable subsets of  $\mathbb{R}^T$  to which  $A$  belongs.<sup>1</sup> The measure so obtained will be written as

$$(2.41) \quad P_w(A) = \int_A dx_w(\tau),$$

Practically for any computation we rely on discretization; for example, if we have to find the expected value of a functional of the trajectory  $x(\tau)$  such as  $F(x(\tau)) = \int_0^\infty a(\tau)x(\tau)d\tau$  we should use  $\sum_{i=0}^n \Delta t_i a(t_i)x(t_i)$ , use the finite dimensional probability distribution (2.38) and at the end of the calculation take the limit  $n \rightarrow \infty$  (in the following  $n$  we will denote by  $N$  with the tacit assumption that at the end  $N \rightarrow \infty$ ). This is what we will be illustrating in the next section for some typical examples where the calculations can be analytically performed.

## 2.4. Some Calculations

Before continuing we define  $\mathcal{C} = [0, 0; t]$  as the ensemble of trajectories of  $\mathbb{R}^T$  starting from 0 at time 0 and lasting a time span  $t$ ;  $\mathcal{C} = [0, 0; x, t]$  as the ensemble of trajectories of  $\mathbb{R}^T$  obtained by fixing the endpoints: the particle starts at time 0 from position 0 ending up, after a time  $t$ , at position  $x$ .

**2.4.1. Identity.** Using normalization of Wiener measure:

$$(2.42) \quad \langle 1 \rangle_w = \int_{\mathcal{C}=[0,0;t]} 1 dx_w(\tau) = 1$$

**2.4.2. Probability of returning at the origin after a time  $t$ .** We already know the answer since this is nothing else  $W(x=0, t|0, 0) = (4\pi Dt)^{-1/2}$  as given by eq. (2.34). We want to re-derive it using the path integral.

$$(2.43) \quad W(x, t|0, 0) = \langle \delta(x - x(t)) \rangle_w = \lim_{N \rightarrow \infty} W_N(x, t|0, 0)$$

where

$$(2.44) \quad W_N(x, t|0, 0) = \int \prod_{i=1}^{N+1} \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} e^{-\sum_{i=0}^N \frac{(x_{i+1} - x_i)^2}{4D \Delta t_i}} \delta(x - x_{N+1})$$

The delta sets  $x_{N+1} \equiv x(t)$  to  $x$ . For simplicity we illustrate the procedure for  $x=0$  and we will use a uniform time mesh, i.e.  $\Delta t_i = t/(N+1) = \epsilon$ , even though the calculation can be done without any difficulty for a generic mesh (a more practical method will be developed in a successive chapter). Since the argument of the exponential in the integrand is quadratic in the  $x$ 's we can introduce a matrix  $A$  such that

$$(2.45) \quad W_N(x=0, t|0, 0) = \frac{1}{(4\pi D \epsilon)^{\frac{N+1}{2}}} \int d^N x e^{-\frac{1}{4D\epsilon} x^T A_N x} = (4\pi D \epsilon \det A_N)^{-1/2}$$

with

$$A_N(i, i) = 2 \\ A_N(i, j) = -\delta_{i, j+1} - \delta_{i, j-1}$$

Notice that in the above equations we have used the fact that  $x_0 = x_{N+1} = 0$  and we are integrating over  $x_i$  with  $i = 1, \dots, N$ . We need to compute the determinant of  $A_N$ : using Laplace expansion in the last column we obtain:

$$\det A_N = 2 \det A_{N-1} - \det A_{N-2}$$

with initial conditions  $A_1 = 2$  and  $A_2 = 3$  we obtain:

$$\det A_N = N + 1$$

<sup>1</sup>For a very nice and rigorous account of the above procedure see chapter 7 of Billingsley, P. (2013) *Probability and measure*, John Wiley & Sons.

leading to  $W_N(x=0, t|0, 0) = [4\pi D\epsilon(N+1)]^{-1/2}$ . Since  $(N+1)\epsilon = t$  we have that  $W_N(x=0, t|0, 0)$  is independent of  $N$  and so the limit is trivial and we get

$$(2.46) \quad \langle \delta(x(t)) \rangle_w = \frac{1}{(4\pi Dt)^{1/2}},$$

which is the expected result.

**2.4.3. Two point correlation.** To compute the two point correlation function it's straightforward to use eqs. (2.38) and (2.39):

$$(2.47) \quad \langle x(t_1)x(t_2) \rangle_w = \int \frac{dx_1}{\sqrt{4\pi D\Delta t_1}} \frac{dx_2}{\sqrt{4\pi D\Delta t_2}} e^{-\frac{x_1^2}{4D\Delta t_1}} e^{-\frac{(x_2-x_1)^2}{4D\Delta t_2}} x_1 x_2$$

Using  $x = x_1$  and  $y = x_2 - x_1$  one immediately gets:

$$\langle x(t_1)x(t_2) \rangle_w = 2Dt_1$$

If the initial condition is  $x(t_0) = x_0$  the above equation becomes (see exercises)

$$(2.48) \quad \langle x(t_1)x(t_2) \rangle_w = x_0^2 + 2D \min\{t_1 - t_0, t_2 - t_0\}$$

**2.4.4. Averaging a functional of the full trajectory.** We want to compute the expected value for the functional  $F(\int_0^t a(\tau)x(\tau)d\tau)$ . First introduce  $A(\tau) = \int_\tau^t a(s)ds$ , i.e.  $\dot{A}(\tau) = -a(\tau)$ ; then integration by parts and using that  $x(0) = 0$ :

$$(2.49) \quad \int_0^t a(\tau)x(\tau)d\tau = \int_0^t A(x(\tau))\dot{x}(\tau)d\tau = \int_0^{x(t)} A(x)dx$$

Discretizing:

$$\sum_{i=1}^N A(x_i)(x_i - x_{i-1}) = \sum_{i=1}^N A_i(x_i - x_{i-1})$$

Then the average of the functional  $F$  is the limit  $N \rightarrow \infty$  of (we set  $D = 1/4$  in the following ... the  $D$  can be recovered in the final formulas by replacing  $t$  with  $4Dt$ ):

$$(2.50) \quad I_N = \int \prod_{i=1}^N \frac{dx_i}{(\pi\Delta t_i)^{1/2}} F\left(\sum_{i=1}^N A_i(x_i - x_{i-1})\right) e^{-\sum_{i=1}^N \frac{(x_i - x_{i-1})^2}{\Delta t_i}}$$

and by the change of variables  $x_i - x_{i-1} = y_i$  (show that the Jacobian of the transformation is 1) we get

$$(2.51) \quad I_N = \int \prod_{i=1}^N \frac{dy_i}{(\pi\Delta t_i)^{1/2}} F\left(\sum_{i=1}^N A_i y_i\right) e^{-\sum_{i=1}^N \frac{y_i^2}{\Delta t_i}}$$

We introduce the identity  $\int \delta(z - \sum_{i=1}^N A_i y_i) dz = 1$  and interchange the integrals so that the last to be done is the one over  $z$  and then use the Fourier representation of the delta<sup>2</sup>:

$$\begin{aligned} & \int \frac{d\alpha}{2\pi} \int dz e^{i\alpha z} F(z) \int \prod_{i=1}^N \frac{dy_i}{(\pi\Delta t_i)^{1/2}} e^{-\sum_{i=1}^N (\frac{y_i^2}{\Delta t_i} + i\alpha A_i y_i)} \\ &= \int dz F(z) \int \frac{d\alpha}{2\pi} \exp\left\{-\frac{\alpha^2}{4} \sum_{i=1}^N A_i^2 \Delta t_i + i\alpha z\right\} = \\ &= \sqrt{\frac{1}{\pi \sum_{i=1}^N A_i^2 \Delta t_i}} \int dz F(z) \exp\left\{-z^2 / \sum_{i=1}^N A_i^2 \Delta t_i\right\} \end{aligned}$$

<sup>2</sup> $2\pi\delta(x) = \int_{\mathbb{R}} e^{i\alpha x} d\alpha$



As  $N \rightarrow \infty$ :

$$(2.52) \quad \lim_{N \rightarrow \infty} \sum_{i=1}^N A_i^2 \Delta t_i = \int_0^t A^2(\tau) d\tau = \int_0^t \left[ \int_{\tau}^t a(s) ds \right]^2 d\tau \equiv R$$

$$(2.53) \quad \langle F \left( \int_0^t a(\tau) x(\tau) d\tau \right) \rangle_w = \sqrt{\frac{1}{\pi R}} \int dz F(z) e^{-z^2/R}$$

For  $D \neq 1/4$  send  $R \rightarrow 4DR$ .

As an example use  $F(z) = e^{hz}$ . We obtain the moment generating function for  $\int_0^t a(\tau) x(\tau) d\tau$ :

$$(2.54) \quad \langle e^{h \int_0^t a(\tau) x(\tau) d\tau} \rangle_w = e^{h^2 R/4}$$

$$(2.55) \quad \left\langle \left( \int_0^t a(\tau) x(\tau) d\tau \right)^{2k+1} \right\rangle_w = 0$$

$$(2.56) \quad \left\langle \left( \int_0^t a(\tau) x(\tau) d\tau \right)^{2k} \right\rangle = \left( \frac{R}{2} \right)^2 \frac{(2k)!}{2^k k!}$$

**2.4.5. The Gelfand-Yaglom method.** In this section we want to compute the expected value for the functional:

$$(2.57) \quad e^{-\int_0^t p(\tau) x^2(\tau) d\tau}$$

Start by discretizing:

$$(2.58) \quad I_4^{(N)} = \int \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{\pi \epsilon}} \right) e^{-\sum_{i=1}^N \left[ \frac{(x_i - x_{i-1})^2}{\epsilon} + p_i x_i^2 \epsilon \right]}$$

We can re-written the argument of exponential as a bilinear form using the matrix  $a$ : this matrix, calling  $a_i = p_i \epsilon + \frac{2}{\epsilon}$  for  $i = 1 \dots N-1$  and  $a_N = p_N \epsilon + \frac{1}{\epsilon}$ , is a three-diagonal matrix having as diagonal elements  $a_i$ 's and  $-\frac{1}{\epsilon}$  as the other two off-diagonals elements.

$$(2.59) \quad a = \begin{bmatrix} a_1 & -\frac{1}{\epsilon} & 0 & \dots & \dots & 0 \\ -\frac{1}{\epsilon} & a_2 & -\frac{1}{\epsilon} & \dots & \dots & 0 \\ 0 & -\frac{1}{\epsilon} & a_3 & -\frac{1}{\epsilon} & \dots & 0 \\ \vdots & \dots & -\frac{1}{\epsilon} & \dots & \dots & \vdots \\ \vdots & & & & & -\frac{1}{\epsilon} \\ 0 & \dots & \dots & 0 & -\frac{1}{\epsilon} & a_N \end{bmatrix}$$

So, in terms of  $\det a$ , we have that:

$$I_4^{(N)} = (\epsilon^N \det a)^{-1/2} = (\det(\epsilon a))^{-1/2}$$

We denote the determinant of the matrix  $\epsilon a$  by  $D_1^N$  and define  $D_k^N$  as the determinant of the matrix obtained by removing the first  $k-1$  rows and columns from  $\epsilon a$ .

$$(2.60) \quad D_k^N = \begin{bmatrix} \epsilon a_k & -1 & 0 & \dots & \dots & 0 \\ -1 & \epsilon a_{k+1} & -1 & 0 & \dots & 0 \\ 0 & -1 & \ddots & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & -1 & 0 \\ \vdots & \vdots & \ddots & -1 & \epsilon a_{N-1} & -1 \\ 0 & 0 & \dots & 0 & -1 & \epsilon a_N \end{bmatrix}$$

By Laplace expansion on the first row of  $D_k^N$ :

$$(2.61) \quad D_k^N = \epsilon a_k D_{k+1}^N - D_{k+2}^N = (\epsilon^2 p_k + 2) D_{k+1}^N - D_{k+2}^N$$

$$(2.62) \quad \frac{D_k^N - 2D_{k+1}^N + D_{k+2}^N}{\epsilon^2} = p_k D_{k+1}^N$$

Calling  $\tau = (k-1)/N$ ,  $D_{k-1}^N = D(\tau)$  in the  $\epsilon \rightarrow 0$  and  $N \rightarrow \infty$  at fixed  $\tau$  we arrive at:

$$(2.63) \quad \partial_\tau^2 D(\tau) = p(\tau) D(\tau)$$

From this we find that  $D_1^N \rightarrow D(0)$ .

Since  $D_N^{(N)} = p_N \epsilon^2 + 1$  we find that  $D(t) = 1$ .

Since  $D_{N-1}^{(N)} = p_N p_{N-1} \epsilon^4 + 2p_N \epsilon^2 + p_{N-1} \epsilon^2 + 1$  we have that:

$$\dot{D}(t) = \lim_{\epsilon \rightarrow 0} \frac{D_N^{(N)} - D_{N-1}^{(N)}}{\epsilon} = 0$$

Going back to our integral:

$$I_4 = \frac{1}{\sqrt{D(0)}}$$

For  $p(\tau) = k^2$ :

$$(2.64) \quad D(\tau) = A e^{k\tau} + B e^{-k\tau}$$

$$(2.65) \quad \dot{D}(\tau) = k (A e^{k\tau} - B e^{-k\tau})$$

Using the previous stated final conditions,  $D(t) = 1$  and  $\dot{D}(t) = 0$ :

$$(2.66) \quad D(\tau) = \frac{1}{2} e^{(t-\tau)k} + \frac{1}{2} e^{-(t-\tau)k} = \cosh[(t-\tau)k]$$

$$(2.67) \quad D(0) = \cosh(kt)$$

From which:

$$(2.68) \quad \lim_{N \rightarrow \infty} I_4^{(N)} = I_4 = \frac{1}{\sqrt{\cosh(kt)}}$$

A generalization of the previous computation is:

$$(2.69) \quad \langle e^{-\int_0^t p(\tau) x^2(\tau) d\tau} \delta(x(t) - x) \rangle_w$$

i.e. the previous expected value but with fixed endpoint. Start by rewriting the delta function in its Fourier representation we get:

$$(2.70) \quad \langle e^{-\int_0^t p(\tau) x^2(\tau) d\tau} \delta(x - x(t)) \rangle_w = \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} e^{i\alpha x} \langle e^{-\int_0^t p(\tau) x^2(\tau) d\tau} e^{-i\alpha x(t)} \rangle_w$$

As usual we discretize the expected value ( $a$  is the matrix above) and obtain that the above expectation is the  $N \rightarrow \infty$  limit of:

$$(2.71) \quad \hat{I}_4^{(N)}(x) = \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} e^{i\alpha x} \int \left( \prod_{i=1}^N \frac{dx_i}{\sqrt{\pi\epsilon}} \right) e^{-\sum_{i=1}^N \left[ \frac{(x_i - x_{i-1})^2}{\epsilon} + p_i x_i^2 \epsilon - i\alpha x_N \right]} =$$

$$(2.72) \quad = \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} e^{i\alpha x} \int \frac{d^N x}{(\pi\epsilon)^{N/2}} e^{-x^T a x - i\alpha x_N} = (\pi a_{N,N}^{-1} D_1^{(N)})^{-1/2} e^{-\frac{x^2}{a_{N,N}^{-1}}}$$

where  $a^{-1}$  is the inverse matrix of  $a$ . The value of  $a_{N,N}^{-1}$  can be determined from the form of the matrix  $a$ :

$$(2.73) \quad a_{N,N}^{-1} = \frac{|a'|}{|a|} = \frac{\epsilon^N |a'|}{D_1^{(N)}} = \frac{\tilde{D}_1^{(N-1)}}{D_1^{(N)}}$$

we introduced  $a'$  as the matrix obtained from removing the last row and column from  $a$ . Introduce now  $\tilde{D}_k^{(N-1)}$  as the determinant of the matrix obtained from  $D_1^{(N-1)} \equiv \epsilon^N |a'|$  by eliminating the first  $k-1$  rows and columns:

$$(2.74) \quad \tilde{D}_k^{(N-1)} = \epsilon \begin{bmatrix} \epsilon a_k & -1 & 0 & \cdots & \cdots & 0 \\ -1 & \epsilon a_{k+1} & -1 & 0 & \cdots & 0 \\ 0 & -1 & \ddots & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & -1 & 0 \\ \vdots & \vdots & \ddots & -1 & \epsilon a_{N-2} & -1 \\ 0 & 0 & \cdots & 0 & -1 & \epsilon a_{N-1} \end{bmatrix}$$

As  $N \rightarrow \infty$  we get for  $\tilde{D}$  the same differential equation as the one of  $D$ :

$$(2.75) \quad \partial_\tau^2 \tilde{D}(\tau) = p(\tau) \tilde{D}(\tau)$$

but with different initial conditions (remember that  $\epsilon = t/N$  with fixed  $t$ ):

$$(2.76) \quad \tilde{D}_{N-1}^{(N-1)} = \epsilon^2 a_{N-1} = p_{N-1} \epsilon^3 + 2\epsilon \rightarrow 0$$

$$(2.77) \quad \tilde{D}_{N-2}^{(N-1)} = \epsilon (\epsilon^2 a_{N-2} a_{N-1} - 1) =$$

$$(2.78) \quad = \epsilon (p_{N-1} p_{N-2} \epsilon^4 + 2(p_{N-1} + p_{N-2}) \epsilon^2 + 3)$$

$$(2.79) \quad \frac{\tilde{D}_{N-1}^{(N-1)} - \tilde{D}_{N-2}^{(N-1)}}{\epsilon} = \frac{2\epsilon - 3\epsilon + o(\epsilon)^2}{\epsilon} \rightarrow -1$$

leading to the final conditions  $\tilde{D}(t) = 0$  and  $\dot{\tilde{D}}(t) = -1$ . So given  $D(\tau)$  and  $\tilde{D}(\tau)$ :

$$(2.80) \quad \hat{I}_4^{(N)}(x) = \frac{1}{\sqrt{\pi \tilde{D}_1^{(N-1)}}} e^{-x^2 \frac{D_1^{(N)}}{\tilde{D}_1^{(N-1)}}} \rightarrow \hat{I}_4(x) = \frac{1}{\sqrt{\pi \tilde{D}(0)}} e^{-x^2 \frac{D(0)}{\tilde{D}(0)}}$$

**2.4.6. A special solvable case.** For the special case  $p(\tau) = k^2$  we have to solve the following differential equations:

$$(2.81) \quad \partial_\tau^2 D(\tau) = k^2 D(\tau), \quad 0 \leq \tau \leq t, \quad D(t) = 1, \quad \partial_\tau D(\tau)|_{\tau=t} = 0$$

$$(2.82) \quad \partial_\tau^2 \tilde{D}(\tau) = k^2 \tilde{D}(\tau), \quad 0 \leq \tau \leq t, \quad \tilde{D}(t) = 0, \quad \partial_\tau \tilde{D}(\tau)|_{\tau=t} = -1$$

The two independent solutions for both differential equations are  $\exp\{\pm k\tau\}$  (see also eqs. (2.64) - (2.66)). Thus

$$(2.83) \quad D(\tau) = A e^{k\tau} + B e^{-k\tau}, \quad \tilde{D}(\tau) = \tilde{A} e^{k\tau} + \tilde{B} e^{-k\tau}$$

where the constants  $A, B, \tilde{A}, \tilde{B}$  have to be chosen in order to satisfy the final conditions. This immediately gives

$$(2.84) \quad D(\tau) = \cosh[k(t-\tau)], \quad \tilde{D}(\tau) = \sinh[k(t-\tau)]$$

and, using (2.80),

$$(2.85) \quad \hat{I}_4(x) = \sqrt{\frac{k}{\pi \sinh(kt)}} e^{-x^2 k \coth(kt)}$$

Integrating the above equation over  $x$  we get

$$(2.86) \quad \int_{-\infty}^{\infty} dx \hat{I}_4(x) = \int_{-\infty}^{\infty} dx \langle e^{-\int_0^t p(\tau) x^2(\tau)} \delta(x - x(t)) \rangle_w = I_4$$

where  $I_4$  is given by eq. (2.68).

## 2.5. Heuristics

**2.5.1. Formal expression of the Wiener measure.** Eqs. (2.38) and (2.41) can be written in the suggestive form

$$(2.87) \quad dx_w(\tau) = \mathcal{N} \prod_{\tau=0^+}^t dx(\tau) e^{-\frac{1}{4D} \int_0^t \dot{x}(\tau)^2 d\tau},$$

where the normalization constant  $\mathcal{N}$  is given by:

$$(2.88) \quad \mathcal{N} = \left[ \int \prod_{\tau=0^+}^t dx(\tau) e^{-\frac{1}{4D} \int_0^t \dot{x}(\tau)^2 d\tau} \right]^{-1}$$

and it is infinite! Of course this formula is purely formal and we have seen several instances how one should interpret it: discretize it together the functional of which we wish to calculate the Wiener expectation value and, only at the end of the calculation, take the continuum limit of the chosen discretization.<sup>3</sup> The fact that the above expression is formal derives also by the fact that the Brownian trajectories,  $\{x(\tau) : 0 \leq \tau \leq t\}$ , are never differentiable, as explained in the subsection 2.5.3. However the formal expression (2.87) will be very useful for the calculation of averages of functionals that are exponentials of quadratic expressions of the trajectory,  $\{x(\tau) : 0 \leq \tau \leq t\}$ , or for powerful approximations based on a generalization of the saddle point method. We will see applications to the former case later on.

**2.5.2. Continuity of the Brownian trajectories.** The rigorous proof that Brownian trajectories,  $\{x(\tau) : 0 \leq \tau \leq t\}$ , are continuous it is not easy. One has to go through: i) the definition of a suitable  $\sigma$ -algebra in  $\mathbb{R}^T$ , i.e. the ensembles of trajectories that are measurable; ii) the definition of a suitable probability measure, i.e. the Wiener measure; iii) then show that the ensemble of trajectories that are continuous belongs to the  $\sigma$ -algebra; iv) and finally show that the ensemble of trajectories that are not continuous has measure zero. For a very nice and rigorous account of the above procedure see chapter 7 of Billingsley, P. (2013) *Probability and measure, John Wiley & Sons*.<sup>4</sup> An heuristic account of the continuity of Brownian trajectories can be derived estimating how probable would be to observe a jump  $\Delta x < \varepsilon$  at some generic time  $\tau$  when the discretized form of the Wiener measure with a mesh size  $\Delta t \rightarrow 0^+$ . This entails to evaluate the following integral:

$$(2.89) \quad P(|\Delta x| < \varepsilon) = \lim_{\Delta t \rightarrow 0^+} \int_{|\Delta x| < \varepsilon} \frac{d\Delta x}{\sqrt{4\pi D \Delta t}} e^{-\frac{(\Delta x)^2}{4D \Delta t}},$$

which can be easily shown to be 1 independently of  $\varepsilon > 0$  (see exercise 2.15), i.e. the probability to observe a discontinuity less than an arbitrary small amount is equal to 1.

**2.5.3. Differentiability of the Brownian trajectories.** Similar comments as above can be done concerning the differentiability of Brownian trajectories. Using an heuristic approach and from the following result (see exercise 2.16):

$$(2.90) \quad P(|\Delta x / \Delta t| > k) = \lim_{\Delta t \rightarrow 0^+} \int_{|\Delta x| > k \Delta t} \frac{d\Delta x}{\sqrt{4\pi D \Delta t}} e^{-\frac{(\Delta x)^2}{4D \Delta t}} = 1 \quad \forall k > 0,$$

one argue that the Brownian trajectories are never differentiable.

## Problems

**Exercise 2.1.** Use  $\int_0^\infty x^{n-1} e^{-x} dx \equiv \Gamma(n)$ ,  $n > 0$  and that  $\Gamma(n+1) = n!$  together to the saddle point approximation to derive the result used in chapter 2 of the Lecture Notes (LN in the following)  $\ln n! = n \ln n - n + (1/2) \ln(2\pi n) + O(1/n)$ , eq. (2.20).

<sup>3</sup>Notice that besides the naive discretization we have used, there are other methods: for example there is one described in your textbook in sec. 1.2.7.

<sup>4</sup>The proof presented in your textbook in sec. 1.1.2, besides not being rigorous, is not correct.

**Exercise 2.2.** Implement a numerical simulation to explicitly show how the solution of the ME for the 1-dimensional random walk with  $p_{\pm} = 1/2$  tends to the Gaussian.

**Exercise 2.3.** Write the analogous of eq. (2.25) in the LN for the case with  $p_+ = 1 - p_- \neq p_-$  and determine: i) how they depend on  $l$  and  $\epsilon$  in order to have a meaningful continuum limit; ii) the resulting continuum equation and how to map it in the diffusion eq. (2.27).

**Exercise 2.4.** Write the analogous of eq. (2.25) for the case where the probability to make a step of length  $sl \in \{\pm nl : n \text{ positive integer}\}$  is  $p(s) = (1/Z) \exp\{-|s|\alpha\}$  where  $\alpha$  is some fixed constant. Determine: i) the normalization constant  $Z$ ; ii) what is the condition to have a meaningful continuum limit, discussing why the neglected terms do not contribute to such limit; iii) which equation you get in the continuum limit.

**Exercise 2.5** Use eq. (2.34) to determine  $\langle x \rangle_t$ ,  $\langle x^2 \rangle_t$  and  $\text{Var}_t(x)$ .

**Exercise 2.6** Consider the diffusion eq. (2.27) in the domain  $[0, \infty)$  instead of  $(-\infty, \infty)$  like in the sec. 2.2 of the LN. To do that one needs the boundary condition (bc) that  $w(x, t)$  has to satisfy at 0. Determine the bc for the following two cases and for each of them solve the diffusion equation with the initial condition  $w(x, t=0) = \delta(x - x_0)$  with  $x_0 > 0$ .

1) *Case of reflecting bc* : when the particle arrives at the origin it bounces back and remains in the domain. How is the flux of particles at 0?

2) *Case of absorbing bc* : when the particle arrives at the origin it is removed from the system (captured by a trap acting like a filter!) What is  $w(x=0, t)$  at all time  $t$ ? Notice that in this case we do not expect that the probability is conserved, i.e. Survival probability  $\mathcal{P}(t) \equiv \int_0^{\infty} w(x, t) dx$  decreases with  $t$ . Calculate it and determine its behavior in the two regimes  $t \ll x_0^2/D$  and  $t \gg x_0^2/D$ . Why  $x_0^2/D$  is a relevant time scale? <sup>5</sup>

(Hint: use the fact that  $e^{\pm ikx}$  are eigenfunctions of  $\partial_x^2$  corresponding to the same eigenvalue and choose an appropriate linear combination of them so to satisfy the bc for the two cases. Be aware to ensure that the eigenfunctions so determined are orthonormal. Use the fact that  $\int_{\mathbb{R}} e^{iqx} dx = \delta(q)$ )

**Exercise 2.5.** For a Brownian motion  $X(s)$ ,  $0 \leq s \leq t$ , with diffusion coefficient  $D$  and initial condition  $X(0) = 0$  show that

$$(2.91) \quad \text{Prob} \left( \sup_{0 \leq s \leq t} X(s) \geq a \right) = \frac{2}{\sqrt{4\pi Dt}} \int_a^{\infty} e^{-\frac{z^2}{4Dt}} dz = \text{erfc} \left( \frac{a}{\sqrt{4Dt}} \right)$$

(Hint: some of the results of previous exercise are useful to derive the above result.)

**Exercise 2.6.** Solve the diffusion eq.  $\partial w(\mathbf{x}, t)/\partial t = D\nabla^2 w(\mathbf{x}, t)$  in  $\mathbb{R}^d$ . 1) Determine the propagator  $w(\mathbf{x}, t|\mathbf{x}_0, t_0)$ ; 2) the averages  $\langle \mathbf{x} \rangle$  and  $\langle \mathbf{x}^2 \rangle$ ; 3) the general solution for a generic initial condition  $w(\mathbf{x}_0, t_0)$ .

**Exercise 2.7.** Deduce the analogous of eq. (2.37) in the Lecture Notes for the d-dimensional case of the previous exercise.

**Exercise 2.8.** Prove by a direct calculation that the propagator in eq. (2.34) satisfies eq. (2.36) (ESCK relation).

**Exercise 2.9.** If in eqs. (2.49-53) we use  $a(\tau) = \delta(\tau - t')$  with  $0 < t' < t$  and  $F(z) = \delta(z - x)$  what do we get? Is this a known result?

<sup>5</sup>This case has some relevance for the determination of the extinction time distribution of species with initial population equal to  $x_0$ . Indeed one might consider that the population of a species undergoes a 1-dimensional random walk and an extinction occurs when the population reaches zero for the first time.

**Exercise 2.10.** Using the Wiener measure explain what the following average means

$$(2.92) \quad \langle \delta(x_1 - x(t_1))\delta(x_2 - x(t_2)) \cdots \delta(x_n - x(t_n)) \rangle_w$$

where  $0 < t_1 < t_2 < \cdots < t_n < t$ .

**Exercise 2.11.** Determine the following average  $J(x) = \langle e^{-ik^2 \int_0^t x^2(\tau) d\tau} \delta(x - x(t)) \rangle_w$  using the Wiener measure as done in sec. 2.4.5 with the initial condition  $x(0) = 0$ . Determine also  $\int_{\mathbb{R}} J(x) dx$ .

**Exercise 2.12.** Determine  $K(a, k) = \langle e^{-\int_0^t [a(\dot{x}(\tau))^2 + ik\dot{x}(\tau)] d\tau} \rangle_w$ , where  $a$  and  $k$  are arbitrary (real) constants. How this result can be used to determine  $\langle \delta(x - x(t)) \rangle_w$ ?

**Exercise 2.13.** Show that  $P(|\Delta x| < \varepsilon) = \lim_{\Delta t \rightarrow 0^+} \int_{|\Delta x| < \varepsilon} \frac{d\Delta x}{\sqrt{4\pi D \Delta t}} e^{-\frac{(\Delta x)^2}{4D \Delta t}} = 1$  for  $\forall \varepsilon > 0$ . We have used this result to argue that Brownian trajectories are continuous with probability 1.

**Exercise 2.14.** Show that  $P(|\Delta x / \Delta t| > k) = \lim_{\Delta t \rightarrow 0^+} \int_{|\Delta x| > k \Delta t} \frac{d\Delta x}{\sqrt{4\pi D \Delta t}} e^{-\frac{(\Delta x)^2}{4D \Delta t}} = 1$  for  $\forall k > 0$ . We have used this result to argue that Brownian trajectories are never differentiable with probability 1.



# Fokker-Planck Equation and Stochastic Processes

*In this chapter we will define more general stochastic processes starting from discrete time and discrete state space and then considering both the continuum time and state space version. This will naturally lead to the so called Fokker-Planck equation describing the time evolution of the probability distribution function of a generic state variable. An corresponding description in terms of single trajectories of the state variable will lead to the Langevin equation, the analogous of the Newton equation with a stochastic noise. We will show that the Langevin equation can be formulated in terms of path integrals using what we have learn in chapter 2. The introduction of the stochastic noise necessitates of new rules for the differential calculus, which we will illustrate using practical examples.*

## 3.1. Master Equation

We want to describe a process where a *particle* evolves in time via a discrete Markov Process: this particle would jump from state/position  $j$  to a state/position  $i$  in a time step  $\epsilon > 0$  according to a transition matrix  $W_{ij}$ . The probability  $w_j(t_{n+1})$  at time  $t_{n+1}$  would then be given by:

$$(3.1) \quad w_i(t_{n+1}) = \sum_j W_{ij}(t_n) w_j(t_n),$$

where the following condition has to be satisfied by the transition matrix:

$$(3.2) \quad 1 = \sum_i W_{ij}(t_n),$$

which guarantees that eq. (3.1) preserves normalization (see exercise 3.1). The time instants are  $t_n = n\epsilon$ ,  $n \in \mathbb{N}$ , while the position is taken to lie in a one dimensional lattice of spacing  $\ell$ . We want define a continuous version of this equation. Let us introduce the probability density  $w(x_i, t_n)$  such that the probability to find the particle in an interval of size  $\ell$  around position  $x_i \equiv i\ell$ , is  $w(x_i, t_n)\ell = w_i(t_n)$ . Instead of using the previous equation we prefer the more general integral formulation

$$(3.3) \quad w(x, t_{n+1}) = \int dz W(z|x-z, t_n) w(x-z, t_n)$$

where  $W(z|x-z, t)$  describes the probability of moving by an amount  $z$  starting from  $x-z$  with the analogous of (3.2) being

$$(3.4) \quad 1 = \int dz W(z|x, t_n) .$$



Using (3.4) we can re-write eq.(3.3) as:

$$(3.5) \quad w(x, t_{n+1}) - w(x, t_n) = \int dz [W(z|x-z, t_n)w(x-z, t_n) - W(z|x, t_n)w(x, t_n)] .$$

The goal is now to find a suitable  $W$  depending on the temporal step,  $\epsilon$ , so that in the small  $\epsilon$  limit we get a meaningful continuum time limit. The l.h.s. of eq. (3.5) can be expanded as  $w(x, t_{n+1}) - w(x, t_n) = \partial_t w(x, t_n)\epsilon + \mathcal{O}(\epsilon^2)$ , whereas in the r.h.s. we can expand  $W(z|x-z, t_n)w(x-z, t_n)$  in the argument  $x-z$  for  $z \approx 0$ . Indeed we expect that in the very short time interval  $t_{n+1} - t_n = \epsilon$  the probability to make large jumps is negligible. We thus obtain

$$(3.6) \quad \partial_t w(x, t_n) = - \lim_{\epsilon \rightarrow 0} \int dz \left\{ z \partial_x [W(z|x, t_n)w(x, t_n)] + \right.$$

$$(3.7) \quad \left. - \frac{z^2}{2} \partial_x^2 [W(z|x, t_n)w(x, t_n)] + \dots \right\} / \epsilon$$

Exchanging the derivatives with the integral and writing  $t_n = t$  we get:

$$(3.8) \quad \partial_t w(x, t) = \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \partial_x^k \left[ w(x, t) \lim_{\epsilon \rightarrow 0} \int dz z^k W(z|x, t) / \epsilon \right]$$

If the jump is the one of a Brownian motion we expect that  $\int dz z^2 W(z|x, t) \approx \epsilon$  since it represents the mean square average of a jump during the time interval  $\epsilon$ . On the other hand if there is a bias due to some external force (analogous to the  $p_{\pm}$  in sec. 2.2) we expect that that also  $\int dz z W(z|x, t) \approx \epsilon$ . This is consistent with the Newton equation of a particle moving in a viscous fluid in presence of an external force  $F_{ext}(x)$ ,  $m\ddot{x}(t) = -\gamma\dot{x}(t) + F_{ext}(x(t))$ , where  $1/\gamma$  is the mobility ( $\gamma$  is the friction coefficient ... see more later on). If  $m/\gamma$ , which has the dimension of a time scale, is much smaller of the time scale of observation, the dynamics becomes simply  $\dot{x}(t) = F_{ext}(x(t))/\gamma$  and for a small time increment  $x(t+\epsilon) - x(t) = \epsilon F_{ext}(x(t))/\gamma + \mathcal{O}(\epsilon^2)$ . These observations on the mean and variance jump size being both of order of the time interval  $\epsilon$ , lead to the following ansatz for the transition matrix:

$$(3.9) \quad W(z|x, t) = F \left( \frac{z - f(x, t)\epsilon}{\sqrt{\epsilon \hat{D}(x, t)}} \right) \frac{1}{\sqrt{\epsilon \hat{D}(x, t)}}$$

for some functions  $f$ ,  $\hat{D}$  and  $F$  satisfying the following conditions:

$$(3.10) \quad \int dy F(y) = 1$$

$$(3.11) \quad \int dy F(y) y = 0 .$$

The first condition on  $F$  imply the normalization, eq. (3.4) (see exercise), whereas the second condition guarantees that

$$(3.12) \quad \int dz z W(z|x, t) = f(x, t)\epsilon$$

Furthermore (see exercises)

$$(3.13) \quad \int dz z^2 W(z|x, t) = \epsilon \hat{D}(x, t) \int dy F(y) y^2 + \mathcal{O}(\epsilon^2)$$

and

$$(3.14) \quad \int dz z^k W(z|x, t) = \mathcal{O}(\epsilon^{k/2}), \quad k \geq 3 ,$$

that is all other integer moments of  $F$  are negligible in the small  $\epsilon$  limit. Thus taking the the  $\epsilon \rightarrow 0$  limit and setting  $D = \frac{1}{2} \hat{D} \int dy F(y) y^2$  we finally get:

$$(3.15) \quad \partial_t w(x, t) = \partial_x [-f(x, t)w(x, t) + \partial_x [D(x, t)w(x, t)]]$$

This is the Fokker-Planck equation and it is a particular case of continuity equation

$$(3.16) \quad \partial_t w(x, t) = -\partial_x J(x, t)$$

where  $J(x, t) = f(x, t)w(x, t) - \partial_x [D(x, t)w(x, t)]$  is the probability current. The form eq.(3.16) guarantees probability conservation during the time evolution. Notice that in the particular case  $f = 0$  and  $D(x, t) = D$  independent of  $x$  and  $t$  we recover the diffusion equation of chapter 2, eq.(2.27).

### 3.2. Langevin Equation

We will now introduce a more intuitive and physical approach based on the Brownian motion described in chapter 2 and on Newton equation. Let's go back to the Wiener path integral and in particular to the probability density of a jump of size  $x_{i+1} - x_i = z$  at a generic time instant  $t_i$  during the time interval  $\Delta t_i$ :

$$(3.17) \quad d\mathbb{P}(x_{i+1} - x_i = z_i) = \frac{dz_i}{\sqrt{4\pi D \Delta t_i}} e^{-\frac{z_i^2}{4D \Delta t_i}},$$

which is equivalent to the following (discrete) time evolution:

$$(3.18) \quad x_{i+1} = x_i + z_i$$

where  $x_i \equiv x(t_i)$  and  $z_i$  is a random *noise* drawn from a normal distribution, i.e.

$$(3.19) \quad z_i \sim \mathcal{N}(0, \sqrt{2D \Delta t_i}).$$

We can re-write the above equations in terms of a rescaled random variable  $\Delta B_i$  such that  $z_i = \sqrt{2D} \Delta B_i$  (i.e.:  $\Delta B_i \sim \mathcal{N}(0, \Delta t_i)$ ) as:

$$(3.20) \quad \Delta x(t) = x(t + \Delta t) - x(t) = \sqrt{2D} \Delta B(t) \quad \text{with} \quad \Delta B(t) \sim \mathcal{N}(0, \Delta t),$$

or in the infinitesimal form:

$$(3.21) \quad dX(t) = \sqrt{2D} dB(t),$$

where  $B(t)$  is a Brownian motion. We recall eq.(2.38) for the joint probability distribution of a Brownian trajectory to visit positions in the intervals  $(B_1, dB_1)$  at time  $t_1$ ,  $(B_2, B_2 + dB_2)$  at time  $t_2$ , ...,  $(B_N, B_N + dB_N)$  at time  $t_N$  with  $t_0 < \dots < t_N$

$$(3.22) \quad d\mathbb{P}_{t_1, \dots, t_N}(B_1, \dots, B_N | B_0, t_0) = e^{-\sum_{i=1}^N \frac{(B_i - B_{i-1})^2}{2\Delta t_i}} \prod_{i=1}^N \frac{dB_i}{\sqrt{2\pi \Delta t_i}}$$

In the following we will assume that the initial condition  $B_0 = 0$ . Very often in the physics literature one finds that eq.(3.21) is written in the formal way:

$$(3.23) \quad \frac{dX}{dt}(t) = \sqrt{2D} \xi(t) \quad \frac{dB}{dt}(t) \equiv \xi(t),$$

One can show that the statistical properties of  $B(t)$  imply that  $\xi(t)$  is a gaussian variable (and as such its statistical properties are determined only by its mean and covariance) with (see exercise)

$$(3.24) \quad \langle \xi(t) \rangle = 0 \quad \text{and} \quad \langle \xi(t_1) \xi(t_2) \rangle = \delta(t_2 - t_1).$$

However as seen in sec.2.5.3 Brownian trajectories are never differentiable and thus the above equation has no rigorous meaning and Van Kampen refers to it as a *quasi equation*. Eq.(3.21) is the rigorous way to write it and  $\Delta B(t)$  as appearing in eq.(3.20) is given by

$$(3.25) \quad \Delta B(t) = \int_t^{t+\Delta t} dB(t),$$

where the r.h.s. represents the first (trivial) case of stochastic integral (see next sections for a simplified introduction).

If the motion occurs in 3-d space the generalization of the above equations is

$$(3.26) \quad \Delta x_\mu(t) = x_\mu(t + \Delta t) - x_\mu(t) = \sqrt{2D} \Delta B_\mu(t) \quad \mu = 1, 2, \dots, d,$$

In the infinitesimal form:

$$(3.27) \quad dX_\mu(t) = \sqrt{2D}dB_\mu(t) ,$$

and  $\Delta B_\mu(t) = \int_t^{t+\Delta t} dB_\mu(t)$  in eq.(3.26). where  $\Delta B_\mu(t)$  are random variable with normal distribution  $\mathcal{N}(0, \Delta t)$ <sup>1</sup>. In the infinitesimal form:

$$(3.29) \quad dX_\mu(t) = \sqrt{2D}dB_\mu(t) ,$$

and  $\Delta B_\mu(t) = \int_t^{t+\Delta t} dB_\mu(t)$  in eq.(3.26). In order to make progress we now consider a particle of mass  $m$  whose size is much larger than the particles composing the fluid where it is moving, referred as Brownian particle in the following. The fluid particles could be of the order of 1nm in diameter whereas the Brownian particles could be as small as a dust particle, i.e. of order 10–1000 nm in diameter (see exercise). In general the Brownian particle, besides to the friction, is also subjected to force composed by a deterministic external force,  $F_{ext}$ , and the one,  $F_{noise}$ , due to the collisions with fluid particles of the thermal bath. Thus the Newton equation becomes (we consider again the 1-D case for simplicity but the generalization to general case is obvious):

$$(3.30) \quad m\ddot{x}(t) = -\gamma\dot{x}(t) + F_{ext}(x(t), t) + F_{noise}(t),$$

where  $\gamma = 6\pi\eta R$  is the friction coefficient,  $\eta$  is the fluid viscosity and  $R$  is the radius of the spherical particle we are considering<sup>2</sup>. If we are interested at time scales  $t \gg m/\gamma$  ( $m/\gamma$  is the time scale after which a particle of mass  $m$  relaxes to an almost uniform velocity, i.e. acceleration becomes almost zero), the previous equation simplifies and can be re-written as:

$$(3.31) \quad \dot{x}(t) = \frac{1}{\gamma}F_{ext}(x(t), t) + \frac{1}{\gamma}F_{noise}(t)$$

or in its differential form:

$$(3.32) \quad dx(t) = \frac{1}{\gamma}F_{ext}(x(t), t)dt + \frac{1}{\gamma}F_{noise}(t)dt ,$$

or its corresponding discretized form:

$$(3.33) \quad x_{i+1} = x_i + \frac{1}{\gamma}F_{ext,i}\Delta t_i + \frac{1}{\gamma}F_{noise,i}\Delta t_i ,$$

where  $F_{ext,i} \equiv F_{ext}(x_i, t_i)$ . When  $F_{ext} = 0$  we expect to recover the equations eqs.(3.20) and (3.21). We thus ought to identify:

$$(3.34) \quad \frac{1}{\gamma}F_{noise}(t)dt = \sqrt{2D}dB(t) \quad \text{or equivalently} \quad \frac{1}{\gamma}F_{noise}(t)\Delta t = \sqrt{2D}\Delta B(t)$$

Setting  $f = F_{ext}/\gamma$  we get the Langevin equation, known as *over-damped Langevin equation*:

$$(3.35) \quad dx(t) = f(x(t), t)dt + \sqrt{2D}dB(t) \quad f(x(t), t) \equiv F_{ext}(x(t), t)/\gamma ,$$

or the corresponding *quasi equation* expression:

$$(3.36) \quad \dot{x}(t) = f(x(t), t) + \sqrt{2D}\xi(t) ,$$

which generalizes eq.(3.23). The discretized form of eq.(3.35) takes the form (remember that  $B$  is not differentiable):

$$(3.37) \quad x_{i+1} = x_i + f(x_i, t_i)\Delta t_i + \sqrt{2D}\Delta B_i .$$

<sup>1</sup>In this case eq.(3.22) becomes simply

$$(3.28) \quad d\mathbb{P}_{t_1, \dots, t_N}(\mathbf{B}_1, \dots, \mathbf{B}_N | \mathbf{B}_0, t_0) = e^{-\sum_{i=1}^N \sum_{\mu=1}^d \frac{(B_i^\mu - B_{i-1}^\mu)^2}{2\Delta t_i}} \prod_{i=1}^N \frac{d^d \mathbf{B}_i}{(2\pi\Delta t_i)^{d/2}}$$

<sup>2</sup>In the textbook  $\gamma$  has been denoted  $\eta$ , not typically done in the physics literature.

### 3.3. Stochastic Calculus

**3.3.1. Introduction.** In the previous section we have introduced the quantity  $\Delta B_i$  and its infinitesimal version  $dB(t)$ . Thus one faces the problem to define a new kind of integrals such as:

$$(3.38) \quad S = \int_{t_0}^t G(s)dB(s)$$

for some class of function  $G$ . Since  $B(t)$  is never differentiable we cannot use directly Riemann or Stieltjes-Riemann integral<sup>3</sup>. This integral must be understood in a mean squared sense:

$$(3.39) \quad S = ms \lim_{\max\{\Delta t_i: i=1,2,\dots,n\} \rightarrow 0} \sum_{i=1}^n G(\tau_i)(B(t_i) - B(t_{i-1}))$$

where  $\tau_i$  is a point lying in the interval  $[t_{i-1}, t_i]$ :  $\tau_i = \lambda t_i + (1 - \lambda)t_{i-1}$  for  $0 \leq \lambda \leq 1$  and  $t_n = t$ . The mean squared limit means, calling  $S_n = \sum_{i=1}^n G(\tau_i)(B(t_i) - B(t_{i-1}))$ :

$$(3.40) \quad \lim_{n \rightarrow \infty} \langle (S - S_n)^2 \rangle = 0 ,$$

where the simplified notation

$$(3.41) \quad \lim_{n \rightarrow \infty} \text{ means } ms \lim_{\max\{\Delta t_i: i=1,2,\dots,n\} \rightarrow 0}$$

and

$$(3.42) \quad S_n \equiv \sum_{i=1}^n G(\tau_i)\Delta B_i \quad \text{with} \quad \Delta B_i \equiv B(t_i) - B(t_{i-1}) .$$

In the following we will use the simplified notation

$$(3.43) \quad \max_1^n \{\Delta t_i\} \equiv \max\{\Delta t_i : i = 1, 2, \dots, n\} .$$

Since  $|\langle S \rangle - \langle S_n \rangle| \leq \langle (S - S_n)^2 \rangle^{1/2}$  (why?) we have that eq.(3.40), i.e. ms-convergence, implies also that

$$(3.44) \quad \lim_{n \rightarrow \infty} \langle S_n \rangle = \langle S \rangle .$$

$\lambda = 0$  is known as the Ito prescription and corresponds to the choice  $\tau_i = t_{i-1}$  (it preserves causality: the noise acts before the jump occurs) whereas  $\lambda = 1/2$  is known as the Stratonovich or mid-point prescription and corresponds to  $\tau_i = (t_i + t_{i-1})/2$  (it is symmetric with respect to the two interval extrema and has the advantage to be invariant with respect to time inversion). When one of these two prescriptions is used the integral eq.(3.38) is denoted as

$$(3.45) \quad S_{Ito} = \int_{t_0}^t G(s)dB(s) \quad \lambda = 0 \quad \text{Ito}$$

$$(3.46) \quad S_{Strat} = \int_{t_0}^t G(s) \circ dB(s) \quad \lambda = 1/2 \quad \text{Stratonovich}$$

As a warm up, let's calculate the expected value of  $S_n$  when  $G = B$  in eq.(3.38). In this case:

$$(3.47) \quad S_n \equiv \sum_{i=1}^n B(\tau_i)\Delta B_i \quad \text{with} \quad \Delta B_i \equiv B(t_i) - B(t_{i-1}) .$$

We now use the properties of the Brownian trajectories and in particular eq.(2.48) (where we were using  $x(t)$  instead of  $B(t)$  with  $D = 1/2$  since in the above equations we are taking into account

<sup>3</sup>The rest of this chapter is adapted from the textbook by Gardiner, Crispin W. Handbook of stochastic methods, III ed., Springer, 2004, sec. 4.1- 4.3

$D$  explicitly) with the initial condition  $B(t = t_0) = 0$ . Thus  $\langle B(t)B(t') \rangle = \min\{t - t_0, t' - t_0\}$ . We thus obtain

$$(3.48) \quad \langle S_n \rangle = \sum_{i=1}^n [\tau_i - t_0 - t_{i-1} + t_0] = (t - t_0)\lambda .$$

Thus stochastic integrals will depend on the discretization, i.e. on the free parameter  $\lambda$ ): by fixing it we choose a particular set of rules for stochastic integrals containing Brownian trajectories. We now continue our calculation with  $G(s) = B(s)$  and use Ito prescription (for generic  $\lambda$  see exercises). From eq.(3.47) we have now:

$$(3.49) \quad S_n = \sum_{i=1}^n B_{i-1} (B_i - B_{i-1}) = \frac{1}{2} \sum_{i=1}^n [(B_{i-1} + \Delta B_i)^2 - B_{i-1}^2 - (\Delta B_i)^2] .$$

The first part is:

$$(3.50) \quad \sum_{i=1}^n [(B_{i-1} + \Delta B_i)^2 - B_{i-1}^2] = \sum_{i=1}^n (B_i^2 - B_{i-1}^2) = B_n^2 - B_0^2 ,$$

which leads to:

$$(3.51) \quad S_n = \frac{B_n^2 - B_0^2}{2} - \frac{1}{2} \sum_{i=1}^n (\Delta B_i)^2$$

For the second term we have to make a guess. Since  $\langle (\Delta B_i)^2 \rangle = \Delta t_i$ , due to eq.(3.22), it follows that  $\langle \sum_{i=1}^n (\Delta B_i)^2 \rangle = t - t_0$ . Thus our guess is that the ms-limit of  $\sum_{i=1}^n (\Delta B_i)^2$  is  $t - t_0$ . We want to show that indeed

$$(3.52) \quad \lim_{n \rightarrow \infty} \left\langle \left( \sum_{i=1}^n (\Delta B_i)^2 - (t - t_0) \right)^2 \right\rangle = 0$$

Notice that the previous equation is equivalent to

$$(3.53) \quad \lim_{n \rightarrow \infty} \left\langle \left( \sum_{i=1}^n [(\Delta B_i)^2 - \Delta t_i] \right)^2 \right\rangle = 0$$

since the  $\Delta B_i$ 's are independent gaussian random variable with zero mean and variance  $\Delta t_i = t_i - t_{i-1}$ . Thus  $\langle \sum_i (\Delta B_i)^2 \rangle = \sum_i \Delta t_i = t - t_0$ . The average appearing in eq.(3.53) can be re-written as

$$(3.54) \quad \begin{aligned} \left\langle \left( \sum_{i=1}^n [(\Delta B_i)^2 - \Delta t_i] \right)^2 \right\rangle &= \left\langle \sum_{i=1}^n [(\Delta B_i)^2 - \Delta t_i]^2 \right\rangle + \\ &+ \left\langle \sum_{i \neq j} [(\Delta B_i)^2 - \Delta t_i][(\Delta B_j)^2 - \Delta t_j] \right\rangle = 2 \sum_{i=1}^n (\Delta t_i)^2 \end{aligned}$$

(see exercise). Notice that  $\sum_{i=1}^n (\Delta t_i)^2 \leq \max_1^n \{\Delta t_i\} \sum_{i=1}^n \Delta t_i = (t - t_0) \max_1^n \{\Delta t_i\}$ . Thus

$$(3.55) \quad \lim_{n \rightarrow \infty} \left\langle \left( \sum_{i=1}^n (\Delta B_i)^2 - (t - t_0) \right)^2 \right\rangle \leq \lim_{n \rightarrow \infty} 2(t - t_0) \max_1^n \{\Delta t_i\} = 0 .$$

This conclude the proof that:

$$(3.56) \quad S_{Ito} = \int_0^t B(\tau) dB(\tau) = \frac{B^2(t) - B^2(0)}{2} - \frac{t - t_0}{2} \quad (\lambda = 0).$$

This is the result using the Ito prescription, the one we will be using through the notes. The Stratonovich prescription consists in finding the mean square limit of:

$$(3.57) \quad S_n = \sum_{i=1}^n B \left( \frac{t_i + t_{i-1}}{2} \right) (B(t_i) - B(t_{i-1}))$$

i.e. taking  $\tau_i = (t_i + t_{i-1})/2$ , i.e. the midpoint of  $[t_{i-1}, t_i]$ . The full calculation gives:

$$(3.58) \quad S_{Strat} = \int_0^t B(\tau) \circ dB(\tau) = \frac{B^2(t) - B^2(0)}{2} \quad (\lambda = 1/2).$$

An heuristic proof of this result is easily obtained by substituting  $B((t_i + t_{i-1})/2)$  in eq.(3.58) with  $(B(t_i) + B(t_{i-1}))/2$ . One gets  $S_n = (B^2(t) - B^2(0))/2$  independently of  $n$  and so the ms-convergence to eq.(3.58) is trivial. See exercise for a rigorous proof of the more general result

$$(3.59) \quad \int_0^t B(\tau) dB(\tau)|_\lambda = (B^2(t) - B^2(0))/2 + (t - t_0)(2\lambda - 1)/2$$

where  $|_\lambda$  means *using  $\lambda$ -prescription*. The result (3.59) contains both eq.(3.56) and eq.(3.58) as particular cases.

**3.3.2. Ito Integrals.** In general a stochastic integral  $\int_{t_0}^t G(\tau) dB(\tau)$ , understood according to Ito prescription, is well defined if the integrand is a non anticipating function, i.e.  $G(t)$  independent of  $B(s) - B(t)$  for  $\forall s > t$ . In other words  $G(t)$  does not depend on the Wiener process  $B$  in the future of  $t$  (causality). We will be interested in the general Langevin eq.(3.35)

$$(3.60) \quad dx(t) = f(x(t), t)dt + \sqrt{2D(x(t), t)}dB(t) ,$$

whose integral form is

$$(3.61) \quad x(t) = x(t_0) + \int_{t_0}^t f(x(\tau), \tau)d\tau + \int_{t_0}^t \sqrt{2D(x(\tau), \tau)}dB(\tau) ,$$

and so  $D$  should be non-anticipating (so not necessarily constant like in eq.(3.35)). Examples of non anticipating functions are:

- (1)  $B(t)$
- (2)  $G(t) = \int_{t_0}^t d\tau g(\tau)dB(\tau)$  for  $g$  non anticipating
- (3)  $G(t) = \int_{t_0}^t g(\tau)d\tau$  for  $g$  non anticipating
- (4)  $G(t) = \int_{t_0}^t F(B(\tau))dB(\tau)$

In the case 4 we have

$$(3.62) \quad G(t) = \lim_{n \rightarrow \infty} \sum_{i=1}^n F(B(t_{i-1})) (B(t_i) - B(t_{i-1})) ,$$

with  $t_n = t$ , which obviously does not depend on  $B(s) - B(t)$ ,  $\forall s > t$  (see the joint  $B$ - distribution eq.(3.22) where  $N > n$  and  $s = t_k$ ,  $n < k \leq N$ ). As a consequence we have that

$$(3.63) \quad \left\langle \int_{t_0}^t F(B(\tau))dB(\tau) \right\rangle = \int_{t_0}^t \langle F(B(\tau)) \rangle \langle dB(\tau) \rangle = 0$$

since  $F(B(\tau))$  is independent of  $dB(\tau)$  (see the discretized form eq.(3.61)) and  $\langle dB(\tau) \rangle = 0$ . Now we want to prove a very powerful differential relation:

$$(3.64) \quad (dB(\tau))^2 = d\tau .$$

Indeed given a non-anticipating function  $G$  we want prove that:

$$(3.65) \quad \int_{t_0}^t G(\tau)(dB(\tau))^2 = \int_{t_0}^t G(\tau)d\tau .$$

Since we have to prove the ms-convergence, the previous equation is equivalent to prove:

$$(3.66) \quad \lim_{n \rightarrow \infty} I_n = 0 \quad \text{where}$$

$$(3.67) \quad I_n \equiv \left\langle \left( \sum_{i=1}^n G_{i-1}(\Delta B_i^2 - \Delta t_i) \right)^2 \right\rangle$$

(remember the notation in eq.(3.41)) where we have used the fact that

$$(3.68) \quad \int_{t_0}^t G(\tau)d\tau = \lim_{\max_1^n \{\Delta t_i\} \rightarrow 0} \sum_{i=1}^n G_{i-1} \Delta t_i$$

In order to prove eq.(3.66) we re-write eq.(3.67) as follows

$$(3.69) \quad I_n = \sum_{i,j} \langle G_{i-1} G_{j-1} (\Delta B_i^2 - \Delta t_i) (\Delta B_j^2 - \Delta t_j) \rangle =$$

$$(3.70) \quad = \sum_{i=1}^n \langle G_{i-1}^2 ((\Delta B_i)^2 - \Delta t_i)^2 \rangle + 2 \sum_{i>j} \langle G_{i-1} G_{j-1} (\Delta B_i - \Delta t_i) (\Delta B_j - \Delta t_j) \rangle$$

Consider the first term in the previous expression; since  $G_{i-1}$  is non anticipating it is independent of  $\Delta B_i$ :

$$(3.71) \quad \langle G_{i-1}^2 ((\Delta B_i)^2 - \Delta t_i)^2 \rangle = \langle G_{i-1}^2 \rangle \underbrace{\langle (\Delta B_i^4) \rangle}_{3\Delta t_i^2} - 2\Delta t_i \underbrace{\langle \Delta B_i^2 \rangle}_{\Delta t_i} + (\Delta t_i)^2 =$$

$$(3.72) \quad = 2(\Delta t_i)^2 \langle G_{i-1}^2 \rangle$$

where we have used eq.(3.22) to calculate the averages terms involving  $B$ . Consider now a generic addendum in the second term in eq.(3.69):

$$(3.73) \quad \langle G_{i-1} G_{j-1} (\Delta B_i^2 - \Delta t_i) (\Delta B_j^2 - \Delta t_j) \rangle$$

where  $i > j$ . The fact that  $i > j$  implies that  $(G_{i-1} G_{j-1}) (\Delta B_j^2 - \Delta t_j)$  is independent of  $\Delta B_i^2 - \Delta t_i$  and the previous equation factorizes and becomes:

$$(3.74) \quad \langle G_{i-1} G_{j-1} (\Delta B_j^2 - \Delta t_j) \rangle \underbrace{\langle (\Delta B_i^2 - \Delta t_i) \rangle}_{=0}$$

(the second factor is zero since  $\langle \Delta B_i^2 \rangle = \Delta t_i$ ). Thus eq.(3.69) simplifies and becomes:

$$(3.75) \quad I_n = 2 \sum_{i=1}^n (\Delta t_i)^2 \langle G_{i-1}^2 \rangle \leq 2 \max_1^n \{\Delta t_i\} \sum_{i=1}^n \Delta t_i \langle G_{i-1}^2 \rangle.$$

If  $\sum_i \langle G_{i-1}^2 \rangle \Delta t_i < \infty$  or  $\sup_{t_0 < \tau < t} \langle G^2(\tau) \rangle < \infty$ :

$$(3.76) \quad \lim_{n \rightarrow \infty} I_n \leq \text{const} \lim_{n \rightarrow \infty} \max_1^n \{\Delta t_i\} \rightarrow 0$$

We have proved eq.(3.64), that is  $(dB(\tau))^2 = d\tau$ . Along the same arguments the following generalization can be proved (see exercise):

$$(3.77) \quad (dB(\tau))^{k+2} = 0 \quad \forall k > 0 \quad \text{and} \quad dB(\tau)dt = 0$$

The idea behind the above rules is simply due to the distribution eq.(3.22) according to which  $\Delta B(\tau) \sim \Delta\tau$  and thus the only non-trivial integrals are  $\int dB(\tau)$  and  $\int (dB(\tau))^2$ . all the other  $\int (dB(\tau))^{2+k}$ . being of order  $(\max_1^n \{\Delta t_i\})^{k+1}$ , at least (see exercise).

**3.3.3. Differentiation rules.** Consider now a function  $h(x(t), t)$  which is differentiable as many times we need. We have the following Taylor expansion (up to second order):

$$\begin{aligned} \Delta h(x, t) &\equiv h(x + \Delta x, t + \Delta t) - h(x, t) = \partial_t h(x, t) \Delta t + \partial_x h(x, t) \Delta x + \\ &+ \frac{1}{2} \partial_t^2 h(x, t) (\Delta t)^2 + \frac{1}{2} \partial_x^2 h(x, t) (\Delta x)^2 + \dots \end{aligned}$$

If  $x(t)$  was  $B(t)$ , i.e. a pure Brownian motion, we would have:

$$(3.78) \quad \Delta h = \partial_t h(B, t) \Delta t + \partial_B h(B, t) \Delta B + \frac{1}{2} \partial_t^2 h(B, t) (\Delta t)^2 + \frac{1}{2} \partial_B^2 h(B, t) (\Delta B)^2 + \dots$$

Considering the differentials (one formally makes the substitution  $\Delta t \rightarrow dt$  and terms of higher order than  $dt$  are ignored) and remembering that  $(dB(t))^2 = dt$  (see eq.(3.64)) we get the so called *Ito formula*:

$$(3.79) \quad dh(B, t) = \left[ \partial_t h(B, t) + \frac{1}{2} \partial_B^2 h(B, t) \right] dt + \partial_B h(B, t) dB(t)$$

i.e. the terms of order  $dt$  are coming from the first derivative w.r.t. time and the second derivative w.r.t Brownian motion.

**Example** Compute the differential of  $B^n(t)$ , i.e.  $h(B, t) = B^n$  in the above equations:

$$d(B^n(t)) \equiv (B(t) + dB(t))^n - B^n(t) = \left( \sum_{k=0}^n \binom{n}{k} B^{n-k}(t) (dB)^k(t) \right) - B^n(t)$$

Ignoring all terms  $(dB(\tau))^{m+2}$  for  $m > 0$  (they are zero!):

$$(3.80) \quad d(B^n(t)) = \binom{n}{0} B^n(t) + \binom{n}{1} B^{n-1}(t) dB(t) + \binom{n}{2} B^{n-2}(t) (dB(t))^2(t) - B^n(t)$$

$$d(B^n(t)) = nB^{n-1}(t)dB(t) + \frac{n(n-1)}{2}B^{n-2}(t)dt$$

The differential is made up of the regular part ( $nx^{n-1}$ ) coming from standard calculus and the Ito part related to second derivative! ( $\frac{n(n-1)}{2}x^{n-2}$ ). Now take  $n = m + 1$ :

$$d(B^{m+1}(t)) = (m+1)B^m dB(t) + \frac{m(m+1)}{2}B^{m-1}dt$$

Divide by  $m+1$ , integrate and rearrange:

$$(3.81) \quad \int_{t_0}^t B^m(\tau) dB(\tau) = \frac{B^{m+1}(t) - B^{m+1}(t_0)}{m+1} - \frac{m}{2} \int_{t_0}^t B^{m-1}(\tau) d\tau.$$

Notice that for  $m = 1$  we get again the result eq.(3.56) (remember that we are always using Ito-prescription).

**3.3.4. Correlations.** Let  $G$  and  $H$  non anticipating functions. We want to prove that:

$$(3.82) \quad \left\langle \int_{t_0}^t G(\tau_1) dB(\tau_1) \int_{t_0}^t H(\tau_2) dB(\tau_2) \right\rangle = \int_{t_0}^t \langle G(\tau) H(\tau) \rangle d\tau$$

As usual we proceed with the discretization with the Ito-prescription:

$$(3.83) \quad \left\langle \sum_{i=1}^n \sum_{j=1}^n G_{i-1} H_{j-1} \Delta B_i \Delta B_j \right\rangle =$$

$$= \sum_{i=1}^n \langle G_{i-1} H_{i-1} (\Delta B_i)^2 \rangle + \sum_{i>j} \langle (G_{i-1} H_{j-1} + G_{j-1} H_{i-1}) \Delta B_j \Delta B_i \rangle$$

Since  $\Delta B_i$  is independent of  $(G_{i-1} H_{j-1} + G_{j-1} H_{i-1}) \Delta B_j$ , the second term factorizes leading to:

$$(3.84) \quad \sum_{i>j} \langle (G_{i-1} H_{j-1} + G_{j-1} H_{i-1}) \Delta B_j \Delta B_i \rangle = \sum_{i>j} \langle (G_{i-1} H_{j-1} + G_{j-1} H_{i-1}) \Delta B_j \rangle \underbrace{\langle \Delta B_i \rangle}_{=0}$$

The remaining term, the first one in eq.(3.83), is (again due to independence):

$$(3.85) \quad \sum_{i=1}^n \langle G_{i-1} H_{i-1} \rangle \underbrace{\langle (\Delta B_i)^2 \rangle}_{=\Delta t_i} \rightarrow \int_{t_0}^t \langle G(\tau) H(\tau) \rangle d\tau.$$

In the last eq. we are dealing with standard numerical series and not with random variables. Thus the limit is the standard one (no ms-convergence is involved!).



**3.3.5. Change of Variables.** Here we want to generalize the Ito formula eq.(3.79) for the general Langevin equation (3.60).

$$(3.86) \quad dx(t) = f(x(t), t)dt + g(x(t), t)dB(t) \quad \text{with} \quad g(x, t) \equiv \sqrt{2D(x, t)}.$$

We want to determine the change of a function  $h(x)$ ,  $dh(x) = h(x+dx) - h(x)$ , due to eq. (3.86):

$$(3.87) \quad \begin{aligned} dh(x(t)) &= dx(t) \frac{\partial h}{\partial x} + \frac{(dx(t))^2}{2} \frac{\partial^2 h}{\partial x^2} + \dots \\ &= h'(x(t)) [f(x(t), t)dt + g(x(t), t)dB(t)] + \\ &+ \frac{h''(x(t))}{2} [f(x(t), t)dt + g(x(t), t)dB(t)]^2 + \dots \end{aligned}$$

Using the results eqs.(3.64) and (3.77) we get (omitting the arguments for simplicity):

$$(3.88) \quad dh = \left[ h'f + \frac{h''}{2}g^2 \right] dt + h'g dB$$

where the neglected terms are of higher order in  $dt$ . Ito formula eq.(3.79) is recovered when  $D = 1/2$ , i.e.  $g(x, t) = 1$ . From the previous equation we obtain the very important integration formula for the Ito stochastic integrals in terms of ordinary integrals

$$(3.89) \quad \begin{aligned} \int_{t_0}^t h'(x(\tau))g(x(\tau), \tau)dB(\tau) &= h(x(t)) - h(x(t_0)) + \\ - \int_{t_0}^t \left[ h'(x(\tau))f(x(\tau), \tau) + \frac{h''(x(\tau))}{2}g^2(x(\tau), \tau) \right] d\tau. \end{aligned}$$

In the case of a non-anticipating  $G(x(\tau))$  the stochastic integral  $\int_{t_0}^t G(x(\tau))dB(\tau)$  can be calculated using eq.(3.89) by defining  $h(x) = \int_{x_0}^x G(x')/g(x')dx'$  (see exercise 3.11)

**3.3.6. Derivation of the Fokker-Planck from Langevin equation.** Our goal is to determine the probability distribution of  $x(t)$  for trajectories satisfying the Langevin equation (3.86) or (3.60). This is given by  $w(x, t) = \langle \delta(x - x(t)) \rangle_B$  (the average is done over a Brownian motion as explained in chapter 2). Take an arbitrary function  $h \in C_c^2(\mathbb{R})$  (set of functions with continuous second derivative with compact support, i.e. the function is zero outside a closed and bounded subset of  $\mathbb{R}$ ). From the change of variable formula (3.88) we have (now we make the slight generalization with  $h$  having also an explicit time dependence):

$$(3.90) \quad \begin{aligned} \langle dh(x(t)) \rangle_B &= dt \langle h'(x(t))f(x(t), t) + \frac{h''(x(t))g^2(x(t), t)}{2} \rangle_B + \\ &+ \underbrace{\langle h'(x(t))g(x(t), t)dB(t) \rangle_B}_{=0}. \end{aligned}$$

The last term is zero due to the non-anticipating character of both  $h$  and  $g$  (i.e.  $D$ ) so that  $h'(x(t))g(x(t), t)$  is independent of  $dB(t) \equiv B(t+dt) - B(t)$  (see definition just before eq.(3.60)) and the fact that  $\langle dB(t) \rangle = 0$  (see eq.(3.22)). Going from differentials to derivatives the previous equation becomes:

$$(3.91) \quad \left\langle \frac{dh}{dt} \right\rangle_B = \left\langle h'(x(t))f(x(t), t) + \frac{h''(x(t))g^2(x(t), t)}{2} \right\rangle_B.$$

As we have learnt for a generic function  $a(x)$  we have the following identity:

$$(3.92) \quad \begin{aligned} \langle a(x(t)) \rangle_B &= \left\langle \int_{\mathbb{R}} dx \delta(x - x(t)) a(x) \right\rangle_B = \\ &= \int_{\mathbb{R}} dx \langle \delta(x - x(t)) \rangle_B a(x) = \int_{\mathbb{R}} dx w(x, t) a(x). \end{aligned}$$

In terms of  $w$  eq.(3.91) becomes:

$$\frac{d}{dt} \int_{\mathbb{R}} dx w(x, t) h(x) dx = \int_{\mathbb{R}} dx w(x, t) \left[ h'(x)f(x, t) + \frac{h''(x)g^2(x, t)}{2} \right].$$

Since  $h$  and its derivatives are zero at infinity (remember that  $h \in C_c^2(\mathbb{R})$ ) we can integrate by parts the r.h.s. of the previous equation (why?) and get:

$$(3.93) \quad \int_{\mathbb{R}} dx \frac{\partial w}{\partial t}(x, t) h(x) dx = \int_{\mathbb{R}} dx h(x) \partial_x \left[ -f(x, t) w(x, t) + \frac{1}{2} \partial_x (g^2(x, t) w(x, t)) \right].$$

Since  $h$  is arbitrary we can choose its support smaller and smaller around a generic point  $x$  and in the limit we get

$$(3.94) \quad \partial_t w(x, t) = \partial_x \left[ -f(x, t) w(x, t) + \frac{1}{2} \partial_x (g^2(x, t) w(x, t)) \right]$$

i.e. the Fokker Planck (FP) equation eq.(3.15) (since  $g = \sqrt{2D}$ ).

**Remark:** Notice that the FP equation (3.94) is concerned *only* with the time evolution of the probability distribution of the *final point* of the stochastic trajectories  $x(t)$  obeying the Langevin eq.(3.60).

## Problems

**Exercise 3.1.** Show that the master equations Eqs. (3.1) and (3.2) in the lecture notes preserve the normalization, i.e. if  $\sum_i w_i(t_n) = 1$  when  $n = 0$  then it holds for all  $n > 0$ . Idem for  $\int dx w(x, t_n)$ .

**Exercise 3.2.** Show that eqs. (3.9) and (3.10) in the Lecture notes imply the normalization condition eq.(3.4).

**Exercise 3.3.** Show that the ansatz eq. (3.9) together with eqs. (3.10) and (3.11) in the Lecture notes imply  $\int dz z W(z|x, t) = \epsilon f(x, t)$ ,  $\int dz z^2 W(z|x, t) = \epsilon \hat{D}(x, t) \int dy y^2 F(y) + \mathcal{O}(\epsilon^2)$  and  $\int dz z^k W(z|x, t) = \mathcal{O}(\epsilon^{k/2})$  for  $k \geq 3$ .

**Exercise 3.4.** Consider a spherical particle of radius  $r$  subjected to the collisions of an ideal gas of  $N$  particles in a volume  $V$  at equilibrium at temperature  $T$ . If the number of collisions during a time interval  $\Delta t$  satisfies the central limit theorem, determine the average number of collisions and its variance in a time interval  $\Delta t$ .

**Exercise 3.5.** Show that the statistical properties of the Brownian motion,  $B(t)$ , implies that  $\langle \xi(t) \rangle = 0$  and  $\langle \xi(t_1) \xi(t_2) \rangle = \delta(t_2 - t_1)$ . We have defined in a purely formal way  $\xi(t) = dB(t)/dt$  in eq. (3.23) (remember that the Brownian trajectories are not differentiable) (Hint:  $\langle \Delta B_i \rangle = 0$  and  $\langle \Delta B_i \Delta B_j \rangle = \delta_{i,j}$ ). This result is also consistent with the following formal expression for the  $\xi$  trajectories  $d\mathbb{P}(\{\xi(\tau)\}) \propto \prod_{\tau} d\xi(\tau) e^{-\frac{1}{2} \int d\tau \xi^2(\tau)}$ , which can be deduced from the analogous expression for the  $d\mathbb{P}(\{B(\tau)\})$  (see eqs.(2.38), (2.87) and (3.22)).

**Exercise 3.6.** Use the probability distribution for a Brownian trajectory,

$$d\mathbb{P}_{t_1, \dots, t_n}(B_1, \dots, B_n | B_0, t_0) = e^{-\sum_{i=1}^n \frac{(B_i - B_{i-1})^2}{2\Delta t_i}} \prod_{i=1}^n \frac{dB_i}{\sqrt{2\pi\Delta t_i}},$$

to show that

$$\langle (\Delta B_i)^2 (\Delta B_j)^2 \rangle = 3\delta_{i,j} \Delta t_i^2 + (1 - \delta_{i,j}) \Delta t_i^2 \Delta t_j^2$$

.

**Exercise 3.7.** Show that  $\left\langle \left[ \sum_{i=1}^n \left( (\Delta B_i)^2 - \Delta t_i \right) \right]^2 \right\rangle = 2 \sum_{i=1}^n (\Delta t_i)^2$ , as in eq. (3.52) in the lecture notes.

**Exercise 3.8.** Show that for the generic  $\lambda$ -prescription

$$\int_0^t B(\tau) dB(\tau) = \frac{B^2(t) - B^2(t_0)}{2} + \frac{2\lambda - 1}{2} (t - t_0),$$

where we have considered a generic initial condition,  $B(t_0)$ , at  $\tau = t_0$ .

**Exercise 3.9.** Show that  $\int_0^t B(\tau)dB(\tau)|_\lambda = (B^2(t) - B^2(0))/2 + (t - t_0)(2\lambda - 1)/2$  (using the  $\lambda$  prescription). (Hint: Consider the time mesh  $t_i, i = 0, \dots, 2n$  with  $t_{2n} = t, t_{2i-1} = \lambda t_{2i} + (1 - \lambda)t_{2i-2}$  and  $S_n = \sum_{i=1}^{2n} B_{2i-1}(B_{2i} - B_{2i-2})$ ).

**Exercise 3.10.** Show that  $(dB(\tau))^{k+2} = 0 \forall k > 0$ . This is done in a similar way as in the proof of  $(dB(\tau))^2 = d\tau$ . You have to show that  $\int_{t_0}^t G(\tau)(dB(\tau))^{2+k} = 0$  using ms-convergence. Assume for simplicity that  $G$  is bounded. On the same token derive also that  $\int_{t_0}^t G(\tau)dB(\tau)d\tau = 0$ .

**Exercise 3.11.** . Use the following Ito formula (see eq.(3.90)),

$$(3.95) \quad \int_{t_0}^t h'(x(\tau))g(x(\tau), \tau)dB(\tau) = h(x(t)) - h(x(t_0)) + \\ - \left[ h'(x(\tau))f(x(\tau), \tau) + \frac{h''(x(\tau))}{2}g^2(x(\tau), \tau) \right] d\tau.$$

to give an expression in terms of ordinary integrals of  $\int_{t_0}^t G(x(\tau))dB(\tau)$  where  $G$  is a non-anticipating function. The trajectory  $x(\tau)$  satisfies the Langevin eq.  $dx(t) = f(x(t), t)dt + g(x(t), t)dB(t)$ . Explain the meaning of the obtained result... has it to be considered an equality valid for any trajectory  $x(\tau)$ ?

**Exercise 3.12.** Generalize the results for the change of variable of section 3.3.5 to the case of a generic  $\lambda$ -prescription and re-derive the result of problem 3.9.

# Particle in a Thermal Bath

The goal of the present chapter is to apply the theory developed in chapter 3 to the paradigmatic case of the harmonic oscillator, a particle in a thermal bath at temperature  $T$  and subjected to an harmonic external force. This example will also allow to identify the noise amplitude  $D$  in the Langevin equation so that the particle reaches equilibrium at large times. The result is known as Einstein relation. A generalization of the approach to the case of an arbitrary external potential will be presented. Then we will consider the further generalization to the case when, besides to the spatial coordinates, we want to keep track also of the particle velocity/momentum. This will lead to the underdamped Langevin equation and to the corresponding Fokker-Planck equation that, for this case, is known as Kramers' equation. We will also deal with the formal solution of the Fokker-Planck equation that will allow to derive the backward Fokker-Planck equation.

## 4.1. Over-damped Langevin equation

We will consider the motion of a particle in a fluid at temperature  $T$  and subjected to an external force  $F_{ext}(x, t)$  as described by eq.(3.30). For large enough time scale this, as explained in sec.3.2 lead to the over-damped Langevin equation:

$$(4.1) \quad dx(t) = f(x(t), t)dt + \sqrt{2D}dB(t) \quad f(x(t), t) \equiv F_{ext}(x(t), t)/\gamma ,$$

where  $D$  is considered constant. If the external force is harmonic with elastic constant  $m\omega^2$ , i.e.  $F_{ext}(x) = -m\omega^2x$ , the previous equation becomes:

$$(4.2) \quad dx(t) = kx(t)dt + \sqrt{2D}dB(t) \quad k \equiv m\omega^2/\gamma ,$$

and its discretized version, as given by eq.(3.37), reads

$$(4.3) \quad x_i = x_{i-1} - kx_{i-1}\Delta t_i + \sqrt{2D}\Delta B_i \quad k \equiv m\omega^2/\gamma .$$

where  $\Delta B_i \equiv B_i - B_{i-1}$  and  $B_i \equiv B(t_i)$  as usually done. The discretized Wiener measure for  $B_i$  is given by eq.(3.22). The Jacobian matrix,  $J$ , for the change of variables from  $B$  to  $x$ , has its  $(i, j)$  entry given by:

$$(4.4) \quad J_{ij} \equiv \frac{\partial x_i}{\partial B_j} = \begin{cases} 0 & j > i \\ \sqrt{2D} & i = j \\ \frac{\partial x_i}{\partial B_j} & \text{otherwise} \end{cases}$$

$J_{ij}$  is a lower diagonal matrix so the Jacobian is  $|J| = (2D)^{N/2}$ . From eq.(4.3) we obtain that  $\Delta B_i = (\Delta x_i + kx_{i-1}\Delta t_i)/\sqrt{2D}$  and thus the measure eq.(3.22) transforms as:

$$(4.5) \quad d\mathbb{P}(x_1, \dots, x_N | x_0, 0) = |J|^{-1} d\mathbb{P}(B_1, \dots, B_N | B_0, 0) =$$

$$(4.6) \quad = \prod_{i=1}^N \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\sum_{i=1}^N \frac{(\Delta x_i + kx_{i-1}\Delta t_i)^2}{4D\Delta t_i}\right) =$$

Expanding the square in the exponential argument we get:

$$(4.7) \quad \prod_{i=1}^N \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\sum_{i=1}^N \frac{\Delta x_i^2}{4D\Delta t_i}\right) \exp\left(-\sum_{i=1}^N \frac{kx_{i-1}\Delta x_i}{2D} - \sum_{i=1}^N \Delta t_i \frac{k^2 x_{i-1}^2}{4D}\right)$$

Taking the formal  $N \rightarrow \infty$  limit (in the mean squared sense):

$$(4.8) \quad d\mathbb{P}(\{x(\tau)\} | x_0, 0) = \mathcal{N} \underbrace{\prod_{\tau=0^+}^t dx(\tau) e^{-\frac{1}{4D} \int_0^t d\tau \dot{x}^2(\tau)}}_{dx_w(\tau) \text{ eq.(2.87)}} e^{-\frac{k}{2D} \int_0^t x(\tau) dx(\tau) - \frac{k^2}{4D} \int_0^t x^2(\tau) d\tau}$$

Some remarks follow:

- (1) The normalization constant,  $\mathcal{N}$ , is the same as in eq.(2.87) (see discussion there), i.e.

$$(4.9) \quad \mathcal{N} = \left[ \int \prod_{\tau=0^+}^t dx(\tau) e^{-\frac{1}{4D} \int_0^t \dot{x}(\tau)^2 d\tau} \right]^{-1};$$

- (2) The stochastic integral  $\int_0^t x(\tau) dx(\tau)$  is the ms-limit, as defined in chapter 3, of its discrete version  $\sum_{i=1}^N kx_{i-1}\Delta x_i$  using the Ito-prescription.

Due to the Wiener measure factor,  $dx_w(\tau)$ , in eq.(4.8), corresponding to the Langevin eq.  $dx(\tau) = \sqrt{2D} dB(\tau)$ , using the results of sec.3.3.5 and in particular eq.(3.89) with  $g = \sqrt{2D}$ ,  $f = 0$ ,  $h'(x) = x$  with  $dx = \sqrt{g} dB$ , we get the following result for the Ito stochastic integral:

$$(4.10) \quad \int_0^t x(\tau) dx(\tau) = \frac{x^2(t) - x^2(0)}{2} - Dt,$$

(compare to eq.(3.56)) which inserted in eq.(4.8) leads to:

$$(4.11) \quad d\mathbb{P}(\{x(\tau)\} | x_0, 0) = \mathcal{N} \prod_{\tau=0^+}^t dx(\tau) e^{-\frac{1}{4D} \int_0^t d\tau \dot{x}^2(\tau)} e^{-k \frac{x^2(t) - x^2(0)}{4D} + \frac{kt}{2} - \frac{k^2}{4D} \int_0^t x^2(\tau) d\tau}$$

Now we are ready to compute the propagator, the analogous of eq.(2.34):

$$(4.12) \quad W(x, t | x_0, 0) = \langle \delta(x(t) - x) \rangle = \int d\mathbb{P}(\{x(\tau)\}) \delta(x(t) - x) =$$

$$(4.13) \quad = \exp\left\{-k \frac{x^2 - x_0^2}{4D} + \frac{kt}{2}\right\} \left\langle e^{-\frac{k^2}{4D} \int_0^t x^2(\tau) d\tau} \delta(x(t) - x) \right\rangle_w$$

where, we have used the usual notation for the Wiener average of a generic functional the trajectory,  $F(\{x(\tau)\})$ ,

$$(4.14) \quad \langle F(\{x(\tau)\}) \rangle_w \equiv \frac{\int \prod_{\tau=0^+}^t dx(\tau) e^{-\frac{1}{4D} \int_0^t d\tau \dot{x}^2(\tau)} F(\{x(\tau)\})}{\int \prod_{\tau=0^+}^t dx(\tau) e^{-\frac{1}{4D} \int_0^t d\tau \dot{x}^2(\tau)}}$$

No need to do anything else, since we have already computed the last term for  $D = 1/4$  in sub-sections 2.4.5 and 2.4.6; we just need to send  $t \rightarrow 4Dt$  and  $k \rightarrow k/4D$ :

$$(4.15) \quad \langle e^{-\frac{k^2}{4D} \int_0^t x^2(\tau) d\tau} \delta(x(t) - x) \rangle_w = \sqrt{\frac{k}{4\pi D \sinh(kt)}} e^{-\frac{kx^2}{4D} \coth(kt)}$$

Assembling everything together and, for simplicity setting  $x_0 = 0$ :

$$(4.16) \quad \begin{aligned} W(x, t|0, 0) &= \sqrt{\frac{k}{4\pi D \sinh(kt)}} e^{-k \frac{x^2}{4D} + \frac{kt}{2} - \frac{kx^2}{4D} \coth(kt)} = \\ &= \sqrt{\frac{k}{2\pi D(1 - e^{-2kt})}} e^{-\frac{k}{2D} \frac{x^2}{1 - e^{-2kt}}}. \end{aligned}$$

Notice that in the limit  $k \rightarrow 0^+$  we get the propagator of the Brownian particle eq.(2.34). In the large time limit,  $t \rightarrow \infty$  we get that the propagator relax to the stationary solution

$$(4.17) \quad W^*(x) = \sqrt{\frac{k}{2\pi D}} e^{-\frac{kx^2}{2D}}$$

Since the particle is immersed in a thermal bath at temperature  $T$  and it is subjected to an harmonic potential  $V(x) = m\omega^2 x^2/2$ , we must have that  $W^*(x) = Z^{-1} \exp\{-V(x)/\kappa_B T\}$ , the Boltzmann weight ( $Z$  being the partition function/normalization) corresponding to thermal equilibrium. In order for the two distributions to coincide one must have that

$$(4.18) \quad \frac{k}{D} = \frac{m\omega^2}{\kappa_B T}$$

$$(4.19) \quad D = \frac{\kappa_B T}{\gamma} = \frac{\kappa_B T}{6\pi\eta R}$$

Eq.(4.19) is the famous Einstein relation relating the amplitude of the fluctuation,  $\sqrt{D}$ , to the temperature and to the dissipation term  $\gamma$  (see eq.(3.30) and its over-damped version eq.(4.2)). This is a particular case of the *fluctuation dissipation theorems*. Notice that in this relation there is no trace of the external force, suggesting it is valid beyond the particular case considered here (see next section).

An alternative way to derive the expression of the propagator is by using the Fokker-Planck equation (3.94) associated to the Langevin equation (4.2):

$$(4.20) \quad \partial_t W(x, t|x_0, 0) = \partial_x [kxW(x, t|x_0, 0) + D\partial_x W(x, t|x_0, 0)]$$

The stationary state is easily obtained as solution of:

$$(4.21) \quad 0 = \partial_x [kxW^*(x) + D\partial_x W^*(x)]$$

and it coincides with eq.(4.17). To derive the full time dependent solution we lean on the Fourier transform that poses the Fokker-Planck equation in "momentum" space. In order to do this we need to know how to transform a function like  $xf(x)$ :

$$\mathcal{F}(xf(x))(p) = \int dx xf(x)e^{-ipx} = \int dx f(x)(i\partial_p e^{-ipx}) = i\partial_p \tilde{f}(p)$$

The expression of the FP equation for the Fourier transform is:

$$(4.22) \quad \partial_t \tilde{W}(p, t) = -kp\partial_p \tilde{W}(p, t) - Dp^2 \tilde{W}(p, t)$$

To solve this equation one uses the method of characteristics (see exercise 5.3) and derive result (4.16).

## 4.2. Multidimensional Wiener Path Integral

The generalization of the Wiener path integral to more than one dimension is quite straightforward: each dimension is independent so we just consider a collection of  $d$  independent Brownian motions  $B^\alpha$   $\alpha = 1, \dots, d$ ; i.e.:

$$(4.23) \quad d\mathbb{P}_{t_1, \dots, t_N}(B_1, \dots, B_N | B_0, t_0) = \prod_{\alpha=1}^d d\mathbb{P}_{t_1, \dots, t_N}(B_1^\alpha, \dots, B_N^\alpha | B_0^\alpha, t_0)$$

where  $B$  is a  $d$ -dimensional vector  $B = (B^1, \dots, B^d)^T$  and (see eq.(3.22):

$$(4.24) \quad d\mathbb{P}_{t_1, \dots, t_N}(B_1^\alpha, \dots, B_N^\alpha | B_0^\alpha, t_0) = e^{-\sum_{i=1}^N \frac{(B_i^\alpha - B_{i-1}^\alpha)^2}{2\Delta t_i}} \prod_{i=1}^N \frac{dB_i^\alpha}{\sqrt{2\pi\Delta t_i}}$$

The properties of the measure are easy to derive. For example:

$$(4.25) \quad \langle dB^\alpha(\tau) \rangle = 0$$

$$(4.26) \quad \langle dB^\alpha(\tau)dB^\beta(\tau) \rangle = \delta^{\alpha\beta}d\tau,$$

and the analogous of eqs.(3.64) and (3.77) for the ms-convergence:

$$(4.27) \quad dB^\alpha(\tau)dB^\beta(\tau) = \delta^{\alpha\beta}d\tau$$

$$(4.28) \quad dB^\alpha(\tau)d\tau = 0$$

$$(4.29) \quad dB^{\alpha_1} \dots dB^{\alpha_k} = 0 \quad \forall k > 2.$$

can be re-derived without much effort.

The multidimensional Langevin equation reads:

$$(4.30) \quad dx^\alpha(t) = f^\alpha(\mathbf{x}(t), t)dt + \sqrt{2D^\alpha(\mathbf{x}(t), t)}dB^\alpha(t)$$

along with the change of variables formula, analogous to (3.88):

$$(4.31)$$

$$dh(\mathbf{x}(t), t) = dt\partial_t h(\mathbf{x}, t) \Big|_{\mathbf{x}=\mathbf{x}(t)} + \sum_{\alpha=1}^d \partial_\alpha h(\mathbf{x}, t)dx^\alpha \Big|_{\mathbf{x}=\mathbf{x}(t)} + \frac{1}{2} \sum_{\alpha, \beta=1}^d \partial_\alpha \partial_\beta h(\mathbf{x}, t)dx^\alpha dx^\beta \Big|_{\mathbf{x}=\mathbf{x}(t)}$$

$$(4.32)$$

$$= dt \left[ \partial_t h + \sum_{\alpha=1}^d (\partial_\alpha h f^\alpha + D^\alpha \partial_\alpha^2 h) \right] + \sum_{\alpha=1}^d \sqrt{2D^\alpha} \partial_\alpha h dB^\alpha(t)$$

For  $h$  not explicitly dependent on time and  $D^\alpha = D \quad \forall \alpha$ :

$$(4.33) \quad dh(\mathbf{x}(t)) = dt[\mathbf{f} \cdot \nabla h + D\nabla^2 h] + \sqrt{2D}\nabla h \cdot d\mathbf{B}$$

The Fokker-Planck counterpart is (see exercise 5.4):

$$(4.34) \quad \partial_t w(\mathbf{x}, t | \mathbf{x}_0, t_0) = \sum_{\alpha=1}^d \partial_\alpha [-f^\alpha w + \partial_\alpha (D^\alpha w)]$$

The last thing we need derive is the multidimensional Wiener measure for  $\mathbf{x}(t)$ . We start from the discretized version of eq.(4.30)

$$(4.35) \quad \Delta x_i^\alpha \equiv x^\alpha(t_i) - x^\alpha(t_{i-1}) = f_{i-1}^\alpha \Delta t_i + \sqrt{2D_{i-1}^\alpha} \Delta B_i^\alpha$$

with  $f_i^\alpha \equiv f^\alpha(\mathbf{x}_i, t_i)$ ,  $D_i^\alpha \equiv D^\alpha(\mathbf{x}_i, t_i)$ ,  $\Delta B_i^\alpha \equiv B_i^\alpha - B_{i-1}^\alpha$ . The Jacobian is:

$$(4.36) \quad J = \left| \frac{\partial(x_1^1, \dots, x_N^d)}{\partial(B_1^1, \dots, B_N^d)} \right| = \prod_{i=1}^N \prod_{\alpha=1}^d (2D_{i-1}^\alpha)$$

and the discretize measure:

$$(4.37) \quad d\mathbb{P}_{t_1, \dots, t_N}(\mathbf{x}_1, \dots, \mathbf{x}_N | \mathbf{x}_0, t_0) = \prod_{i=1}^N \prod_{\alpha=1}^d \frac{dx_i^\alpha}{\sqrt{4\pi D_{i-1}^\alpha \Delta t_i}} \exp\left(-\sum_{i=1}^N \sum_{\alpha=1}^d \frac{(\Delta x_i^\alpha - f_{i-1}^\alpha \Delta t_i)^2}{4D_{i-1}^\alpha \Delta t_i}\right)$$

which we can write in a formal form as  $N \rightarrow \infty$ :

$$(4.38) \quad d\mathbb{P}(\{\mathbf{x}(\tau)\} | \mathbf{x}_0, 0) = \prod_{\tau=0^+}^t \prod_{\alpha=1}^d \frac{dx^\alpha(\tau)}{\sqrt{4\pi D^\alpha(\mathbf{x}(\tau), \tau)} d\tau} e^{-\frac{1}{4} \int_0^t d\tau \sum_{\alpha=1}^d [\dot{x}^\alpha(\tau) - f^\alpha(\mathbf{x}(\tau), \tau)]^2 / D^\alpha(\mathbf{x}(\tau), \tau)}$$

which generalize eq.(4.8).

**4.2.1. Observation.** A further generalization of the Langevin equation (4.30) is

$$(4.39) \quad dx^\omega(t) = f^\omega(x, t) + \sum_{\alpha=1}^d g_\alpha^\omega(x, t) dB^\alpha(t) \quad \omega = 1, \dots, k$$

where  $\mathbf{B}$  is the  $d$ -dimensional Brownian motion eqs.(4.23) and (4.24) and quite generally  $k \neq d$ . The corresponding FP is (see exercise):

$$(4.40) \quad \partial_t w(x, t) = \sum_{\omega=1}^k \partial_\omega (-f^\omega(x, t)w(x, t) + \sum_{\nu=1}^k \partial_\nu (D^{\omega\nu}(x, t)w(x, t))),$$

where  $D^{\omega\nu} = \sum_{\alpha=1}^d g_\alpha^\omega g_\alpha^\nu$  is a semi-positive definite matrix (why?). The case considered above corresponds to  $k = d$  and  $g_\alpha^\nu(x, t) = \delta_\alpha^\nu \sqrt{2D^\alpha(x, t)}$ . There exists also a path integral formulation similar to the one given above for the case when  $k = d$  and  $g$  is invertible (see exercise).

### 4.3. The Fokker-Planck Equation with Velocity

As an application of multidimensional Wiener path integral of the previous section consider the so called under-damped Langevin equation for a particle in a thermal bath (we have already seen the corresponding 1-d case, eq.(3.30)):

$$(4.41) \quad m\dot{\mathbf{v}}(t) = -\gamma\mathbf{v} + \mathbf{F}(\mathbf{r}) + \gamma\sqrt{2D}\xi$$

where we use the notation  $\mathbf{F}$  instead of  $\mathbf{F}_{ext}$ , for simplicity. The previous second order differential equation can be re-written in the form of two first order differential equations, as known from the course of analytical mechanics:

$$(4.42) \quad \begin{cases} d\mathbf{v}(t) = \left(-\frac{\gamma\mathbf{v}}{m} + \frac{\mathbf{F}(\mathbf{r})}{m}\right) dt + \frac{\gamma\sqrt{2D}}{m} d\mathbf{B} \\ d\mathbf{r}(t) = \mathbf{v}dt \end{cases}$$

This system is a six dimensional system of Brownian particles in the variables  $\mathbf{x} = (v_x, v_y, v_z, x, y, z)^T$  and with diffusion constants:

$$(4.43) \quad D^\alpha = \begin{cases} \frac{\gamma^2 D}{m^2} & \alpha = 1, 2, 3 \\ 0 & \alpha = 4, 5, 6 \end{cases}$$

Since the diffusion constants for the position variables  $(x, y, z)$  are (going to) zero the Gaussian-like measures involving  $(x, y, z)$  collapse into delta functions (the zero variance limit of the gaussian distribution is a delta function). The formal Wiener measure in the continuum limit, is:

$$(4.44) \quad d\mathbb{P}(\{\mathbf{x}(\tau), \mathbf{v}(\tau)\} | \mathbf{x}_0, \mathbf{v}_0, 0) = \prod_{\tau=0^+}^t \left( \frac{d^3v}{(4\pi D d\tau)^{3/2}} \frac{\delta^3(\dot{\mathbf{r}}(\tau) - \mathbf{v}(\tau))}{(d\tau)^3} \right) \exp\left(-\frac{1}{4D} \int_0^t d\tau \left[ \dot{\mathbf{v}} + \frac{\gamma\mathbf{v}}{m} - \frac{\mathbf{F}(\mathbf{r})}{m} \right]^2\right).$$

The Fokker-Planck equation can be derived using eq.(4.34) and (4.43):

$$(4.45) \quad \partial_t w(\mathbf{v}, \mathbf{r}, t | \mathbf{v}_0, \mathbf{x}_0) = \nabla_{\mathbf{v}} \cdot \left[ \left( \frac{\gamma\mathbf{v}}{m} - \frac{\mathbf{F}(\mathbf{r})}{m} \right) w + \frac{\gamma^2 D}{m^2} \nabla_{\mathbf{v}} w \right] - \nabla_{\mathbf{r}}(\mathbf{v}w)$$

The stationary version of this equation is called Kramers' equation. If the force is conservative, i.e.  $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$  with  $V$  being the potential, the stationary solution is the Maxwell-Boltzmann distribution, as one would have expected:

$$(4.46) \quad W^* = \frac{1}{Z^*} e^{-\beta\left(\frac{m\mathbf{v}^2}{2} + V(\mathbf{r})\right)}, \quad Z^* = \int_{\mathbb{R}} d^3v \int_{\mathcal{V}} d^3r e^{-\beta\left(\frac{m\mathbf{v}^2}{2} + V(\mathbf{r})\right)}$$

with  $\mathcal{V}$  being the volume of the system and  $1/\beta = \kappa_B T$  if  $D$  satisfies the Einstein relation eq.(4.19) (see exercise).



#### 4.4. Stationary Solution of the Fokker-Planck Equation

<sup>1</sup> The FP eq.(4.34) with the force derived from a potential  $V$ , i.e.  $f^\alpha(\mathbf{x}) = \partial_\alpha V(\mathbf{x})$ , and  $D^\alpha = D = \text{constant}$  becomes:

$$(4.47) \quad \partial_t W(\mathbf{x}, t) = \sum_{\alpha=1}^d [-\partial_\alpha V W + D\partial_\alpha W].$$

If we define  $\hat{W}(\mathbf{x}, t) = e^{V(\mathbf{x})/(2D)}W(\mathbf{x}, t)$  and using the rule

$$(4.48) \quad e^{-f}\partial(e^f g) = (\partial f + \partial)g$$

eq.(4.47) can be re-written as

$$(4.49) \quad \partial_t \hat{W} = D \sum_{\alpha=1}^d (\partial_\alpha - \partial_\alpha \hat{V})(\partial_\alpha + \partial_\alpha \hat{V})\hat{W} = -D \sum_{\alpha=1}^d A_\alpha^\dagger A_\alpha$$

where  $\hat{V} = V/(2D)$ ,  $A_\alpha(\mathbf{x}, \partial_\alpha) = \partial_\alpha + \partial_\alpha \hat{V}$  is a differential operator and  $A_\alpha^\dagger(\mathbf{x}, \partial_\alpha) = -\partial_\alpha + \partial_\alpha \hat{V}$  its adjoint. Notice that

$$(4.50) \quad \int_{\mathbb{R}^d} d^d x \phi(\mathbf{x}) \sum_{\alpha=1}^d A_\alpha^\dagger A_\alpha \phi(\mathbf{x}) = \sum_{\alpha=1}^d \int_{\mathbb{R}^d} d^d x A_\alpha \phi(\mathbf{x}) A_\alpha \phi(\mathbf{x}) = \sum_{\alpha=1}^d \int_{\mathbb{R}^d} d^d x (A_\alpha \phi(\mathbf{x}))^2 \geq 0,$$

where the equality holds if and only if  $0 = A_\alpha \phi(\mathbf{x}) \forall \alpha$ , that is  $\hat{W} = \hat{W}^* \propto e^{-\hat{V}}$ . Thus  $\hat{W}^*$  is the stationary solution of eq.(4.49) and  $W^* = \exp\{-V/D\}/Z$  ( $Z = \int_{\mathbb{R}^d} d^d x \exp\{-V/D\}$ ) is the stationary solution of eq.(4.47). The operator  $D \sum_{\alpha=1}^d A_\alpha^\dagger A_\alpha$  is self-adjoint and due to eq.(4.50) it has positive eigenvalues except for the zero eigenvalue associated to the eigenfunction  $\hat{W}^*$ . Let us call  $\psi_i$  the eigenfunctions and  $E_i$  the corresponding eigenvalues with  $\psi_0 = \exp\{-V/(2D)\}/\sqrt{Z} \propto \hat{W}^{*2}$ ,  $E_0 = 0$  and  $E_i > 0$ . The general solution of (4.49) satisfying the initial condition  $\hat{W}_0 = \exp\{V/(2D)\}W_0$  is

$$(4.51) \quad \hat{W}(\mathbf{x}, t) = \sum_{i \geq 0} c_i \psi_i(\mathbf{x}) e^{-DE_i t}$$

where  $c_i = \int_{\mathbb{R}^d} d^d x \psi_i^* \hat{W}_0$ ,  $\psi_i^*$  being the complex conjugate of  $\psi_i$  and  $\int_{\mathbb{R}^d} d^d x \psi_i^* \psi_j = \delta_{ij}$ . Thus in the  $t \rightarrow \infty$  limit we get

$$(4.52) \quad W^* = e^{-V/(2D)} \lim_{t \rightarrow \infty} \hat{W}(\mathbf{x}, t) = c_0 \psi_0 e^{-V/(2D)} = e^{-V/D} \frac{c_0}{\sqrt{Z}} = \frac{1}{Z} e^{-V/D},$$

where we have used that

$$(4.53) \quad c_0 = \int_{\mathbb{R}^d} d^d x \psi_0 \hat{W}_0 = \int_{\mathbb{R}^d} d^d x \hat{W}_0 \exp\{-V/(2D)\}/\sqrt{Z} = 1/\sqrt{Z}.$$

since the initial condition  $W_0$  is normalized, i.e.  $1 = \int_{\mathbb{R}^d} d^d x W_0 = \int_{\mathbb{R}^d} d^d x \hat{W}_0 e^{-\frac{V}{2D}}$ . In conclusion, we have proved that a FP equation with potential force have the time dependent solution that, independently of the initial condition, for large times tend to the Boltzmann distribution. Remember that  $\mathbf{f} = \mathbf{F}_{ext}/\gamma \in \mathbb{R}^d$ . Then if we insist to denote with  $V$  the potential, i.e.  $\mathbf{F}_{ext} = -\nabla V$ , then the  $V$  we have used in the above derivations should have been divided by  $\gamma$ . In this way the stationary distribution would be  $\exp\{-V/(\gamma D)\}$ , which is indeed the Boltzmann distribution due to the Einstein relation (4.19).

<sup>1</sup>This section is optional

<sup>2</sup>Since we want that the eigenfunctions constitute an orthonormal basis we must have that  $1 = \int_{\mathbb{R}^d} d^d x \psi_0^2 = 1$ , which holds with  $Z = \int_{\mathbb{R}^d} d^d x \exp\{-V/D\}$ .

### 4.5. Formal Solution of the FP Equation and the Backward FP Equation

We begin writing the FP eq.(4.34) as follows

$$(4.54) \quad \partial_t w(t) = L_t w(t)$$

where  $L$  is a matrix-like operator such that operating on a generic function  $h$  gives (from now on  $x, y$  etc. will denote  $d$ -dimensional vectors)

$$(4.55) \quad (L_t h)(x) = \int_{\mathbb{R}^d} d^d y L_t(x, y) h(y) = \sum_{\alpha=1}^d \partial_\alpha [-f^\alpha(x, t) + \partial_\alpha (D^\alpha(x, t))] h(x),$$

that is

$$(4.56) \quad L_t(x, y) = \underbrace{\sum_{\alpha=1}^d \frac{\partial}{\partial x_\alpha} \left[ -f^\alpha(x, t) + \frac{\partial}{\partial x_\alpha} D^\alpha(x, t) \right]}_{\mathcal{L}(x, \nabla_x, t)} \delta^d(x - y) \equiv \mathcal{L}(x, \nabla_x, t) \delta^d(x - y)$$

where the derivatives are intended to operate on everything on their right. Integrating eq.(4.54) with the initial condition  $w(t_0) = w_0$ , we have

$$(4.57) \quad w(t) = w_0 + \int_{t_0}^t L_{t_1} w(t_1) dt_1$$

and iterating

$$(4.58) \quad \begin{aligned} w(t) &= w_0 + \int_{t_0}^t L_{t_1} \left( w_0 + \int_{t_0}^{t_1} L_{t_2} w(t_2) dt_2 \right) dt_1 = \\ &= \dots = w_0 + \int_{t_0}^t L_{t_1} w_0 + \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 L_{t_1} L_{t_2} w_0 + \\ &+ \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 L_{t_1} L_{t_2} L_{t_3} w_0 + \dots, \end{aligned}$$

which is the formal solution of (4.54). Indeed if we take the time derivative of the previous equation we have (of course  $\partial_t w_0 = 0$ )

$$(4.59) \quad \begin{aligned} \partial_t w(t) &= \partial_t \int_{t_0}^t L_{t_1} w_0 + \\ &+ \partial_t \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 L_{t_1} L_{t_2} w_0 + \\ &+ \partial_t \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 L_{t_1} L_{t_2} L_{t_3} w_0 + \dots \\ &= L_t w_0 + L_t \int_{t_0}^t dt_2 L_{t_2} w_0 + L_t \int_{t_0}^t dt_2 \int_{t_0}^{t_2} dt_3 L_{t_2} L_{t_3} w_0 + \dots \\ &= L_t \left( w_0 + \int_{t_0}^t dt_2 L_{t_2} w_0 + \int_{t_0}^t dt_2 \int_{t_0}^{t_2} dt_3 L_{t_2} L_{t_3} w_0 + \dots \right) \\ &= L_t w(t). \end{aligned}$$

An equivalent way to write the solution eq.(4.58) is:

$$(4.60) \quad \begin{aligned} w(t) &= w_0 + \int_{t_0}^t L_{t_1} w_0 + \int_{t_0}^t dt_2 \int_{t_2}^{t_1} dt_1 L_{t_1} L_{t_2} w_0 + \\ &+ \int_{t_0}^t dt_3 \int_{t_3}^{t_2} dt_2 \int_{t_2}^{t_1} dt_1 L_{t_1} L_{t_2} L_{t_3} w_0 + \dots. \end{aligned}$$

A much nicer and synthetic way to write the above solution is by introducing the time ordering product operator,  $T$ . Given  $t_1, t_2, \dots, t_n$  and the  $n$  operators  $L_{t_i}$   $i = 1, \dots, n$  we define

$$(4.61) \quad T(L_{t_1} \cdots L_{t_n}) = \begin{cases} L_{t_{i_1}} \cdots L_{t_{i_n}} & \text{if } t_{i_1} > t_{i_2} > \cdots > t_{i_n}, \\ 0 & \text{otherwise.} \end{cases}$$

In terms of  $T$  eq. (4.58), or its equivalent (4.60), can be written as:

$$(4.62) \quad \begin{aligned} w(t) &= w_0 + \int_{t_0}^t L_{t_1} w_0 + \frac{1}{2} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 T(L_{t_1} L_{t_2}) w_0 + \\ &+ \frac{1}{3!} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 T(L_{t_1} L_{t_2} L_{t_3}) w_0 + \cdots = \\ &= \sum_{n \geq 0} \frac{1}{n!} T \left( \prod_{i=1}^n \int_{t_0}^t L_{t_i} dt_i \right) w_0 = T e^{\int_{t_0}^t L_{\tau} d\tau} w_0 \end{aligned}$$

where, by definition,  $T$  operates through the integrals ordering the matrix operators  $L$ 's. Using the last expression and taking into account the time ordering product

$$(4.63) \quad \partial_t T e^{\int_{t_0}^t L_{\tau} d\tau} w_0 = T \left( L_t e^{\int_{t_0}^t L_{\tau} d\tau} \right) w_0 = L_t T e^{\int_{t_0}^t L_{\tau} d\tau} w_0,$$

which, again, prove that eq.(4.62) is the formal solution of (4.54). If we now derive (4.62) or (4.60) with respect to  $t_0$  we obtain

$$(4.64) \quad \partial_{t_0} w(t) = \partial_{t_0} T e^{\int_{t_0}^t L_{\tau} d\tau} w_0 = -T \left( e^{\int_{t_0}^t L_{\tau} d\tau} L_{t_0} \right) w_0.$$

In the relevant case  $w_0(x) = \delta^d(x - x_0)$ , the initial condition corresponding to the propagator  $w(x, t) = W(x, t|x_0, t_0)$  we have

$$(4.65) \quad \begin{aligned} w(x, t) &= W(x, t|x_0, t_0) = \left( T e^{\int_{t_0}^t L_{\tau} d\tau} w_0 \right) (x) = \\ &= \int d^d y \left( T \left( e^{\int_{t_0}^t L_{\tau} d\tau} \right) \right) (x, y) w_0(y) = \left( T \left( e^{\int_{t_0}^t L_{\tau} d\tau} \right) \right) (x, x_0). \end{aligned}$$

that is the propagator is equal to the matrix element of  $T e^{\int_{t_0}^t L_{\tau} d\tau}$ .

$$(4.66) \quad \begin{aligned} \partial_{t_0} W(x, t|x_0, t_0) &= \partial_{t_0} w(x, t) = - \int d^d y \left( T \left( e^{\int_{t_0}^t L_{\tau} d\tau} L_{t_0} \right) \right) (x, y) w_0(y) \\ &= - \left( T \left( e^{\int_{t_0}^t L_{\tau} d\tau} L_{t_0} \right) \right) (x, x_0) = \underbrace{\int d^d y \left( T \left( e^{\int_{t_0}^t L_{\tau} d\tau} \right) \right) (x, y) L_{t_0}(y, x_0)}_{=W(x, t|y, t_0) \text{ by (4.65)}} \\ &= - \int d^d y W(x, t|y, t_0) L_{t_0}(y, x_0) = - \int d^d y W(x, t|y, t_0) \mathcal{L}(y, \nabla_y, t_0) \delta^d(y - x_0) = \\ &= - \mathcal{L}^\dagger(x_0, \nabla_{x_0}, t_0) W(x, t|x_0, t_0) \end{aligned}$$

where

$$(4.67) \quad \mathcal{L}^\dagger(x, \nabla_x, t) = \sum_{\alpha=1}^d \left[ f^\alpha(x, t) \frac{\partial}{\partial x_\alpha} + D^\alpha(x, t) \frac{\partial^2}{\partial x_\alpha^2} \right],$$

Eq.(4.66) is the backward FP equation for the propagator, which, written explicitly, reads

$$(4.68) \quad \begin{aligned} \partial_{t_0} W(x, t|x_0, t_0) &= \\ &= - \sum_{\alpha=1}^d \left[ f^\alpha(x_0, t_0) \frac{\partial}{\partial x_{0,\alpha}} W(x, t|x_0, t_0) + D^\alpha(x_0, t_0) \left( \frac{\partial}{\partial x_{0,\alpha}} \right)^2 W(x, t|x_0, t_0) \right], \end{aligned}$$

If both  $\mathbf{f}$  and  $D^\alpha$  do not depend on time, that is the stochastic process is homogeneous, then there is time translational invariance and  $W(x, t|x_0, t_0) = W(x, t - t_0|x_0, 0)$  implying that  $\partial_{t_0}W(x, t|x_0, t_0) = -\partial_tW(x, t|x_0, t_0)$  and eq.(4.68) have also the alternative expression

$$(4.69) \quad \begin{aligned} \partial_t W(x, t|x_0, t_0) &= \\ &= \sum_{\alpha=1}^d \left[ f^\alpha(x_0, t_0) \frac{\partial}{\partial x_{0,\alpha}} W(x, t|x_0, t_0) + D^\alpha(x_0, t_0) \left( \frac{\partial}{\partial x_{0,\alpha}} \right)^2 W(x, t|x_0, t_0) \right]. \end{aligned}$$

Similar derivations can be carried out also for master equation as shown in exercise 5.7.

## Problems

**Exercise 4.1.** The propagator for a stochastic harmonic oscillator was derived in sec. 4.1. We found  $W(x, t|0, 0) = \sqrt{\frac{k}{2\pi D(1-e^{-2kt})}} e^{-\frac{k}{2D} \frac{x^2}{1-e^{-2kt}}}$ . Derive the analogous result for  $W(x, t|x_0, t_0)$ .

**Exercise 4.2.** Derive the stationary solution of the FP equation for the harmonic oscillator,  $W^*(x)$ , which obeys to the following eq.  $0 = \partial_x [kxW^*(x) + D\partial_x W^*(x)]$ , explain the hypothesis underlying the derivation and its validity for the derived solution.

**Exercise 4.3.** Use Fourier transform to derive the full time dependent propagator  $W(x, t|x_0, t_0)$  of the FP equation of the harmonic oscillator

$$\partial_t W(x, t|x_0, t_0) = \partial_x [kxW(x, t|x_0, t_0) + D\partial_x W(x, t|x_0, t_0)].$$

**Exercise 4.4.** Derive the multidimensional FP equation associated to the Langevin eq.  $dx^\alpha(t) = f^\alpha(\mathbf{x}(t), t)dt + \sqrt{2D_\alpha(\mathbf{x}(t), t)}dB^\alpha(t)$ .

**Exercise 4.5.** Derive the discretized Wiener measure for the under-damped Langevin equation  $m d\mathbf{v}(t) = (-\gamma\mathbf{v} + \mathbf{F}(\mathbf{r}))dt + \gamma\sqrt{2D}d\mathbf{B}$  (see sec. 4.3) and discuss the formal continuum limit eq. (4.42).

**Exercise 4.6.** Verify that the Maxwell-Boltzmann distribution eq. (4.44) satisfies the Kramers equation (4.43) if the noise amplitude  $D$  is given by the Einstein relation.

**Exercise 4.7.** Let  $P_i(t)$  the probability that a system is found in the (discrete) state  $i$  at time  $t$ . If  $dtW_{ij}(t)$  represents the transition probability time to go from state  $j$  to state  $i$  during the time interval  $(t, t + dt)$ , then prove that the master equation governing the time evolution of the system is:

$$(4.70) \quad \dot{P}_i(t) = \sum_j (W_{ij}(t)P_j(t) - W_{ji}(t)P_i(t)) \equiv (H(t)P(t))_i$$

where  $H_{ij}(t) = W_{ij}(t) - \delta_{ij} \sum_k W_{ki}(t)$ .

- (1) If  $a_i$  is an observable quantity (not explicitly dependent on time) of the system when it is in state  $i$ , show that

$$(4.71) \quad \frac{d\langle a \rangle_t}{dt} = \langle H^T a \rangle_t,$$

where  $\langle a \rangle_t = \sum_i P_i(t)a_i$ .

- (2) If the initial condition is  $P_i(t_0) = \delta_{i,i_0}$ , the corresponding solution of the master equation is called propagator and it will be denoted  $P_{i,i_0}(t|t_0)$ . Thus  $P(t|t_0)$  is a matrix satisfying  $\partial P(t|t_0)/\partial t = H(t)P(t|t_0)$ . Show that  $\partial P(t|t_0)/\partial t_0 = -P(t|t_0)H(t_0)$ .
- (3) Assume now that the transition rates do not depend on time and that an equilibrium stationary state exists. A stationary state  $P^*$  satisfies the stationary condition  $HP^* = 0$ . An equilibrium stationary state,  $P^{eq}$ , besides to the stationary condition, satisfies also the so called detailed balance (DB) condition  $W_{ij}P_j^{eq} = W_{ji}P_i^{eq}$  (explain what this means). If  $S$  is the diagonal matrix  $S_{ij} = \delta_{ij}\sqrt{P_i^{eq}}$ , show that, as a consequence of the DB condition, the matrix  $\hat{H} = S^{-1}HS$  is symmetric and semi-negative definite. Under the hypothesis

that each state  $i$  can be reached through a path of non-zero transition rates from any state  $j$  show that the equilibrium state is unique.

**Exercise 4.8.** Show that the matrix  $D^{\omega\nu} = \sum_{\alpha=1}^d g_{\alpha}^{\omega} g_{\alpha}^{\nu}$  is semi-positive definite ( $\omega, \nu = 1, \dots, k$ ) with  $k$  and  $d$  are arbitrary.

**Exercise 4.9.** Consider the Langevin eq.(4.39) and, for  $k = d$  and an invertible matrix  $g(x, t)$ , determine the discretized measure  $d\mathbb{P}_{t_1, \dots, t_N}(\mathbf{x}_1, \dots, \mathbf{x}_N | \mathbf{x}_0, t_0)$  and its formal continuum limit.

**Exercise 4.10.** Derive the FP equation (4.40) from the Langevin equation (4.39).

# The Bloch Equation and the Feynman-Kac formula

In the previous chapter we have seen that in the calculation of the propagator for the harmonic oscillator we end up with the evaluation of an average of the kind  $\langle \exp\{-\int_0^t V(x(\tau))d\tau\} \delta(x - x(t)) \rangle_w$  with the Wiener measure. We show that similar averages are rather common and that they satisfy the Bloch equation, leading to the well known and widely used Feynman-Kac formula. In other words the formula expresses the solution of a differential equation involving a function  $V$ , the Bloch equation, in terms of average of  $\exp\{-\int_0^t V(x(\tau))d\tau\}$  over Brownian trajectories.

## 5.1. Path Integral for Over-damped Langevin Equation with Conservative Force

Consider the overdamped stochastic dynamics of a particle under an external potential  $U(\mathbf{r})$ ; setting  $\mathbf{f} = -\frac{\nabla U(\mathbf{r})}{\gamma}$  the Langevin equation reads:

$$(5.1) \quad d\mathbf{r}(t) = \mathbf{f}(\mathbf{r})dt + \sqrt{2D}d\mathbf{B}$$

whose associated Fokker-Planck equation for the propagator is:

$$(5.2) \quad \partial_t w(\mathbf{r}, t | \mathbf{r}_0) = \nabla [-\mathbf{f}(\mathbf{r})w(\mathbf{r}, t | \mathbf{r}_0) + D\nabla w(\mathbf{r}, t | \mathbf{r}_0)]$$

The solution of this equation is given by a Wiener path integral (see sec.4.2):

$$(5.3) \quad w(\mathbf{r}, t | \mathbf{r}_0, 0) = \int \prod_{\tau=0^+}^t \frac{d^d r(\tau)}{(4\pi D d\tau)^{d/2}} e^{-\frac{1}{4D} \int_0^t d\tau (\dot{\mathbf{r}}(\tau) - \mathbf{f}(\mathbf{r}(\tau)))^2} \delta^d(\mathbf{r}(t) - \mathbf{r})$$

or in terms of its discretized form  $W^{(N)}$  ( $w(\mathbf{r}, t | \mathbf{r}_0, 0) = \lim_{N \rightarrow \infty} W^{(N)}$  with  $t_N = t$  independently of  $N$ ):

$$(5.4) \quad W^{(N)} = \int \prod_{i=1}^N \frac{d^d r_i}{(4\pi D \Delta t_i)^{d/2}} e^{-\sum_{i=1}^N \frac{(\Delta \mathbf{r}_i)^2}{4D \Delta t_i} - \frac{1}{2D} \sum_{i=1}^N \Delta \mathbf{r}_i \mathbf{f}_{i-1} - \frac{1}{4D} \sum_{i=1}^N \mathbf{f}_{i-1}^2 \Delta t_i} \delta^d(\mathbf{r}_N - \mathbf{r})$$

where we have used the general eq.(4.37) with  $D^\alpha = D = \text{constant}$ .  $W^{(N)}$  can also be seen as an expected value over the discrete Wiener measure:

$$(5.5) \quad W^{(N)} = \langle e^{\frac{1}{2D} \sum_{i=1}^N \Delta \mathbf{r}_i \mathbf{f}_{i-1} - \frac{1}{4D} \sum_{i=1}^N \mathbf{f}_{i-1}^2 \Delta t_i} \delta^d(\mathbf{r}_N - \mathbf{r}) \rangle_{N, w}$$

where, by definition,

$$(5.6) \quad \langle \mathcal{O}(\{x_i\}) \rangle_N \equiv \int \prod_{i=1}^N \frac{d^d \mathbf{r}_i}{(4\pi D \Delta t_i)^{d/2}} e^{-\sum_{i=1}^N \frac{(\Delta \mathbf{r}_i)^2}{4D \Delta t_i}} \mathcal{O}(\{x_i\}).$$

The second term in the exponential's argument in the  $N \rightarrow \infty$  limit leads to a standard integral,  $\int_0^t \mathbf{f}^2(\mathbf{r}(\tau)) d\tau$ . To deal the remaining term we use the finite difference analogous of eq.(4.33)<sup>1</sup> for a generic function  $h(\mathbf{r})$

$$(5.7) \quad \begin{aligned} \Delta h(\mathbf{r}) &\equiv h(\mathbf{r} + \Delta \mathbf{r}) - h(\mathbf{r}) = \\ &= \Delta \mathbf{r} \cdot \nabla h(\mathbf{r}) + \sum_{\alpha, \beta} \Delta r^\alpha(t) \Delta r^\beta(t) \partial_\alpha \partial_\beta h(\mathbf{r}) + O(\Delta r^3) = \\ &= \Delta \mathbf{r} \cdot \nabla h(\mathbf{r}) + D \Delta t \nabla^2 h(\mathbf{r}) \end{aligned}$$

Consider the increment between  $\mathbf{r}_N$  and  $\mathbf{r}_0$  and apply the previous formula, using the usual convention  $\Delta \mathbf{r}_i \equiv \mathbf{r}_i - \mathbf{r}_{i-1}$ :

$$(5.8) \quad h(\mathbf{r}_N) - h(\mathbf{r}_0) = \sum_{i=1}^N \underbrace{\Delta h(\mathbf{r}_i)}_{=h(\mathbf{r}_i)-h(\mathbf{r}_{i-1})} = \sum_{i=1}^N \Delta \mathbf{r}_i \cdot \nabla h(\mathbf{r}_{i-1}) + D \Delta t \sum_{i=1}^N \nabla^2 h(\mathbf{r}_{i-1})$$

In the continuum limit the previous equation leads to the following expression for the Ito stochastic integral:

$$(5.9) \quad \int_0^t d\mathbf{r}(\tau) \cdot \nabla h(\mathbf{r}(\tau)) = h(\mathbf{r}(t)) - h(\mathbf{r}(t_0)) - D \int_0^t d\tau \nabla^2 h(\mathbf{r}(\tau)),$$

a version of the fundamental theorem of stochastic Ito calculus. Taking the continuum limit,  $N \rightarrow \infty$ , in eq.(5.5), where eq.(5.9) is used with  $h = -\frac{U(\mathbf{r})}{\gamma}$ , we get:

$$(5.10) \quad w(\mathbf{r}, t | \mathbf{r}_0, 0) = \langle e^{-\frac{U(\mathbf{r})-U(\mathbf{r}_0)}{2D\gamma} + \frac{1}{2\gamma} \int_0^t d\tau \nabla^2 U - \frac{1}{4D\gamma^2} \int_0^t d\tau (\nabla U)^2} \delta^d(\mathbf{r}(t) - \mathbf{r}) \rangle_w$$

If we define

$$(5.11) \quad V(\mathbf{r}) = -\frac{1}{2\gamma} \nabla^2 U(\mathbf{r}) + \frac{1}{4D\gamma^2} (\nabla U(\mathbf{r}))^2$$

and recall that  $\kappa_B T = \beta^{-1} = \gamma D$  we arrive at:

$$(5.12) \quad w(\mathbf{r}, t | \mathbf{r}_0, 0) = e^{-\frac{\beta}{2}(U(\mathbf{r})-U(\mathbf{r}_0))} \langle e^{-\int_0^t V(\mathbf{r}(\tau)) d\tau} \delta^d(\mathbf{r}(t) - \mathbf{r}) \rangle_w$$

where we have taken into account that all Brownian trajectories start at  $\mathbf{r}_0$  at time  $t = 0$  and, due to the presence of  $\delta^d(\mathbf{r}(t) - \mathbf{r})$  in the average, end at  $\mathbf{r}$  at time  $t$ . This is a version for the propagator obeying eq.(5.2), as an average over Brownian trajectories of  $\exp\{-\int_0^t V(\mathbf{r}(\tau)) d\tau\}$ . Notice that the Brownian trajectories entering in the average in eq.(5.12) are the ones obeying the Langevin equation  $d\mathbf{r}(t) = \sqrt{2D} d\mathbf{B}$  whereas the propagator is the one corresponding to the Langevin eq.(5.1), which contains also the force  $\mathbf{f}$ . The above derivation is valid without changes if the force  $\mathbf{f}$  depends on time as far as it is given by  $\mathbf{f}(\mathbf{r}, t) = -\nabla U(\mathbf{r}, t)/\gamma$ . Eq.(5.11) remains the same with the substitution of  $U(\mathbf{r})$  with  $U(\mathbf{r}, t)$  leading to a  $V(\mathbf{r}, t)$  in eq.(5.12).

## 5.2. Feynman-Kac Formula for the Bloch equation

As one may notice, we happened to have to compute more than once eqs. (2.69) (4.12) (5.12) expectation values such as:

$$(5.13) \quad W_B(x, t | x_0, t_0) = \langle e^{-\int_0^t V(x(\tau), \tau) d\tau} \delta(x(t) - x) \rangle_w$$

<sup>1</sup>The rule is simply due to the discrete Wiener weight (5.6): one has that the following substitutions are  $\Delta r^\alpha(t) \Delta r^\beta(t) = 2D \delta^{\alpha\beta} dt$  and  $\Delta r^\alpha(t) \Delta r^\beta(t) \Delta r^\gamma(t) = 0$ , etc. are valid as far as the continuum limit,  $N \rightarrow \infty$ , is concerned

where we now allow  $V$  to have also an explicit time dependence (see observation at the end of previous section). We want to prove, in two different ways, that 5.13 obeys to the so called *Bloch equation*, i.e.:

$$(5.14) \quad \partial_t W_B(x, t|x_0, t_0) = D\partial_x^2 W_B(x, t|x_0, t_0) - V(x, t)W_B(x, t|x_0, t_0)$$

with initial condition  $W_B(x, t_0|x_0, t_0) = \delta(x - x_0)$ . Notice that for  $V = 0$  this is what we have proved already in chapter 2 with the diffusion equation. Eq.(5.13) represent the *Feynman-Kac formula* for the fundamental solution of the Bloch equation (5.14).

**5.2.1. Proof 1.** The first proof starts from eq.(5.13) and derives the Bloch equation (5.14). Start by discretizing  $W_B$ , as we usually do, and introduce  $W_B^{(\epsilon)}$  defined as (for simplicity we choose all  $\Delta t_i = \epsilon = (t - t_0)/N$ , so that  $t_i = t_0 + i\epsilon$  and  $V_i \equiv V(x_i, t_i)$ )<sup>2</sup>:

$$(5.15) \quad W_B^{(\epsilon)}(x, t_{N+1}|x_0, t_0) = \int \prod_{i=1}^{N+1} \frac{dx_i}{\sqrt{4\pi D\epsilon}} e^{-\sum_{i=1}^{N+1} \frac{\Delta x_i^2}{4D\epsilon} - \epsilon \sum_{i=1}^{N+1} V_i} \delta(x_{N+1} - x),$$

so that  $\lim_{\epsilon \rightarrow 0^+} W_B^{(\epsilon)}(x, t|x_0, t_0) = W_B(x, t|x_0, t_0)$ . Integration over  $x_{N+1}$  is immediate, due to the presence of the  $\delta$  of Dirac, and we get:

$$(5.16) \quad \begin{aligned} W_B^{(\epsilon)}(x, t_{N+1}|x_0, t_0) &= \int \prod_{i=1}^N \frac{dx_i}{\sqrt{4\pi D\epsilon}} e^{-\sum_{i=1}^N \frac{\Delta x_i^2}{4D\epsilon} - \epsilon \sum_{i=1}^N V_i} e^{-\frac{(x_N - x)^2}{4D\epsilon} - \epsilon V(x, t_{N+1})} = \\ &= \int \frac{dx'}{\sqrt{4\pi D\epsilon}} \left( \int \prod_{i=1}^N \frac{dx_i}{\sqrt{4\pi D\epsilon}} e^{-\sum_{i=1}^N \frac{\Delta x_i^2}{4D\epsilon} - \epsilon \sum_{i=1}^N V_i} \delta(x_N - x') \right) e^{-\frac{(x' - x)^2}{4D\epsilon} - \epsilon V(x, t_{N+1})} \\ &= \int \frac{dx'}{\sqrt{4\pi D\epsilon}} W_B^{(\epsilon)}(x', t_N|x_0, t_0) e^{-\frac{(x' - x)^2}{4D\epsilon} - \epsilon V(x, t_{N+1})} \end{aligned}$$

Set  $z \equiv \frac{x' - x}{\sqrt{2D\epsilon}}$ :

$$(5.17) \quad W_B^{(\epsilon)}(x, t_{N+1}|x_0, t_0) = \int \frac{dz}{\sqrt{2\pi}} e^{-z^2/2} W_B^{(\epsilon)}(x + z\sqrt{2D\epsilon}, t_N|x_0, t_0) e^{-\epsilon V(x, t_{N+1})}$$

and expand  $W_B^{(\epsilon)}(x + z\sqrt{2D\epsilon}, t_N|x_0, t_0)$  around  $x$  (small  $z\sqrt{2D\epsilon}$ : since the main contributions to the integral come from values of  $|z| \lesssim 1$ , due to the presence of the Gaussian term in  $z$ , then the expansion is allowed). In order to simplify the notation in the following equation we set  $\psi \equiv W_B^{(\epsilon)}(x, t_N|x_0, t_0)$ ,  $\psi' \equiv \partial_x W_B^{(\epsilon)}(x, t_N|x_0, t_0)$ , etc.

$$(5.18) \quad \begin{aligned} W_B^{(\epsilon)}(x, t_{N+1}|x_0, t_0) &= e^{-\epsilon V(x, t_{N+1})} \int \frac{dz}{\sqrt{2\pi}} e^{-z^2/2} \cdot \\ &\cdot \left[ \psi + \psi' z\sqrt{2D\epsilon} + \psi'' z^2 D\epsilon + \dots \right] = \\ &= (1 - \epsilon V(x, t_{N+1}) + O(\epsilon^2)) \left[ \psi + D\epsilon \psi'' + O(\epsilon^2) \right] = \\ &= \psi + \epsilon \left[ D\psi'' - V(x, t_N)\psi \right] + O(\epsilon^2), \end{aligned}$$

where we have taken into account that  $V(x, t_{N+1}) = V(x, t_N + \epsilon) = V(x, t_N) + O(\epsilon)$  from which ( $t_N = t$  and  $x_{N+1} = t + \epsilon$ ):

$$(5.19) \quad \frac{W_B^{(\epsilon)}(x, t + \epsilon|x_0, t_0) - W_B^{(\epsilon)}(x, t|x_0, t_0)}{\epsilon} = (D\partial_x^2 - V(x)) W_B^{(\epsilon)}(x, t|x_0, t_0) + O(\epsilon)$$

For  $N \rightarrow \infty$ , i.e.  $\epsilon \rightarrow 0^+$ , we get the Bloch equation (5.14):

$$(5.20) \quad \partial_t W_B(x, t|x_0, t_0) = (D\partial_x^2 - V(x, t)) W_B(x, t|x_0, t_0)$$

<sup>2</sup>Remember that with the notation  $\Delta x_i^2$  we mean  $(\Delta x_i)^2$  and not  $\Delta(x_i^2)$ .



**5.2.2. Proof 2.** The second proof is based on two observations.

**Observation 1**  $W_B$ , as defined by eq.(5.13), follows ESCK relation (see chapter 2). Indeed if we divide the time interval  $(t_0, t)$ , in  $N + N'$  steps. The discrete propagator from  $t_0$  up to the instant  $t' = t_{N'}$  is given by:

$$(5.21) \quad W_B^{(\epsilon)}(x', t' | x_0, t_0) \equiv \int \prod_{i=1}^{N'} \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} e^{-\sum_{i=1}^{N'} \frac{(\Delta x_i)^2}{4D \Delta t_i} - \epsilon \sum_{i=1}^{N'} V(x_i, t_i)} \delta(x' - x_{N'})$$

The one from  $t' = t_{N'}$  to  $t = t_N$  is:

$$(5.22) \quad W_B^{(\epsilon)}(x, t | x', t') \equiv \int \prod_{i=N'+1}^{N+N'} \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} e^{-\sum_{i=N'+1}^{N+N'} \frac{(\Delta x_i)^2}{4D \Delta t_i} - \epsilon \sum_{i=N'+1}^{N+N'} V(x_i, t_i)} \delta(x - x_{N+N'})$$

Multiplying eqs.(5.21) and (5.22) and integrating over  $x'$  we get:

$$(5.23) \quad \int dx' W_B^{(\epsilon)}(x, t | x', t') W_B^{(\epsilon)}(x', t' | x_0, t_0) =$$

$$(5.24) \quad = \int \prod_{i=1}^{N+N'} \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} e^{-\sum_{i=1}^{N+N'} \frac{(\Delta x_i)^2}{4D \Delta t_i} - \epsilon \sum_{i=1}^{N+N'} V(x_i, t_i)} \delta(x - x_{N+N'}) = W_B^{(\epsilon)}(x, t | x_0, t_0).$$

In the limit  $\epsilon \rightarrow 0^+$  we obtain ESCK relation:

$$(5.25) \quad W_B(x, t | x_0, t_0) = \int dx' W_B(x, t | x', t') W_B(x', t' | x_0, t_0).$$

**Observation 2** If we take  $h \in C(\mathbb{R})$  and set  $u(t) = \exp\left(-\int_{t_0}^t h(s) ds\right)$  we obtain trivially that:

$$\frac{du}{dt} = -h(t)u(t) \quad \text{with} \quad u(t_0) = 1$$

Integrating the differential equation and using the previous solution for  $u(t)$ :

$$(5.26) \quad u(t) = 1 - \int_{t_0}^t h(\tau) u(\tau) d\tau = 1 - \int_{t_0}^t h(\tau) \exp\left(-\int_{t_0}^{\tau} h(s) ds\right) d\tau$$

Given these two observations, set in the previous equation  $h(\tau) = V(x(\tau), \tau)$  and introduce a delta function  $\delta(x - x(t))$ :

$$(5.27) \quad \delta(x - x(t)) e^{-\int_{t_0}^t d\tau V(x(\tau), \tau)} = \delta(x - x(t)) - \delta(x - x(t)) \int_{t_0}^t d\tau V(x(\tau), \tau) e^{-\int_{t_0}^{\tau} ds V(x(s), s)}$$

By taking the averages over Wiener path integral eq.(4.14) on the l.h.s. of the previous equation we get  $W_B$  as defined in (5.13):

$$(5.28) \quad W_B(x, t | x_0, t_0) = \langle \delta(x - x(t)) e^{-\int_{t_0}^t d\tau V(x(\tau), \tau)} \rangle_w = \\ = \langle \delta(x - x(t)) \rangle_w - \int_{t_0}^t d\tau \langle V(x(\tau), \tau) e^{-\int_{t_0}^{\tau} ds V(x(s), s)} \delta(x - x(t)) \rangle_w$$

In the first term,  $\langle \delta(x - x(t)) \rangle_W$ , we recognize  $W(x, t | x_0, t_0)$  i.e. the solution of the diffusion equation with  $W(x, t_0 | x_0, t_0) = \delta(x - x_0)$  (see eqs.(2.43) and (2.34)). The second term can be cast to:

$$(5.29) \quad \int_{t_0}^t d\tau \langle V(x(\tau), \tau) e^{-\int_{t_0}^{\tau} ds V(x(s), s)} \rangle_W = \int_{t_0}^t d\tau \int dx' W_B(x', \tau | x_0, t_0) V(x', \tau) W(x, t | x', \tau),$$

where in the last step we have split the Wiener measure in two pieces, from  $t_0$  to  $t'$  and from  $t'$  to  $t$  (see exercise) To summarize we arrive at:

$$(5.30) \quad W_B(x, t | x_0, t_0) = W(x, t | x_0, t_0) - \int_{t_0}^t dt' \int dx' W(x, t | x', t') V(x', t') W_B(x', t' | x_0, t_0)$$

Taking the time derivative of both sides:

$$(5.31) \quad \begin{aligned} \partial_t W_B(x, t|x_0, t_0) &= \partial_t W(x, t|x_0, t_0) - \int dx' W(x, t|x', t) V(x', t) W_B(x', t|x_0, t_0) \\ &\quad - \int_{t_0}^t dt' \int dx' \partial_t W(x, t|x', t') V(x', t') W_B(x', t'|x_0, t_0) \end{aligned}$$

$$(5.32) \quad \begin{aligned} \partial_t W_B(x, t|x_0, t_0) &= D\partial_x^2 W(x, t|x_0, t_0) - \int dx' \delta(x - x') V(x') W_B(x', t|x_0, t_0) \\ &\quad - \int_{t_0}^t dt' \int dx' D\partial_x^2 W(x, t|x', t') V(x', t') W_B(x', t'|x_0, t_0) \end{aligned}$$

$$(5.33) \quad \begin{aligned} \partial_t W_B(x, t|x_0, t_0) &= \\ &= D\partial_x^2 \left( \underbrace{W(x, t|x_0, t_0) - \int_{t_0}^t dt' \int dx' W(x, t|x', t') V(x', t') W_B(x', t'|x_0, t_0)}_{W_B(x, t|x_0, t_0) \text{ from (5.30)}} \right) + \\ &\quad - V(x) W_B(x, t|x_0, t_0), \end{aligned}$$

we finally obtain the Bloch equation (5.14):

$$(5.34) \quad \partial_t W_B(x, t|x_0, t_0) = (D\partial_x^2 - V(x, t)) W_B(x, t|x_0, t_0).$$

Using the method of section 4.5 or the method of "proof 1" above, one can also derive:

$$(5.35) \quad \partial_{t_0} W_B(x, t|x_0, t_0) = -(D\partial_{x_0}^2 - V(x_0, t_0)) W_B(x, t|x_0, t_0),$$

(see exercise), which might be called *backward Bloch equation*.

**5.2.3. Generalization of the Feynman-Kac Formula.** A more general Bloch equation is

$$(5.36) \quad \begin{aligned} \partial_t W_B(x, t|x_0, t_0) &= \\ &= \left[ \sum_{\omega=1}^k \frac{\partial}{\partial x_\omega} \left( -f(x, t) + \sum_{\nu=1}^k \frac{\partial}{\partial x_\nu} D^{\omega\nu}(x, t) \right) - V(x, t) \right] W_B(x, t|x_0, t_0), \end{aligned}$$

where  $x, x_0 \in \mathbb{R}^k$  and, as usual, the differential operators act on everything on their right. The corresponding backward Bloch equation is

$$(5.37) \quad \begin{aligned} \partial_{t_0} W_B(x, t|x_0, t_0) &= \\ &= - \left[ \sum_{\omega=1}^k \left( f(x_0, t) \frac{\partial}{\partial x_{0\omega}} + \sum_{\nu=1}^k D^{\omega\nu}(x_0, t) \frac{\partial^2}{\partial x_{0\omega} \partial x_{0\nu}} \right) - V(x_0, t) \right] W_B(x, t|x_0, t_0). \end{aligned}$$

One can show that

$$(5.38) \quad W_B(x, t|x_0, t_0) = \left\langle \exp \left\{ - \int_{t_0}^t V(x(s), s) ds \right\} \delta^k(x(t) - x) \right\rangle$$

where the average is taken over the stochastic trajectories obeying the Langevin equation (4.39):

$$(5.39) \quad dx^\omega(t) = f^\omega(x, t) + \sum_{\alpha=1}^d g_\alpha^\omega(x, t) dB^\alpha(t) \quad \omega = 1, \dots, k$$

where  $D^{\omega\nu} = \sum_{\alpha=1}^d g_\alpha^\omega g_\alpha^\nu$  and with  $\mathbf{B}$  being a d-dimensional Brownian motion (see sec. 4.2).

## Problems

**Exercise 5.1.** Write down the details leading to eq.(5.29).

**Exercise 5.2.** Prove the backward Bloch eq. (5.35) in two ways: 1) using eq.(5.34) and the method developed in sec. 4.5; 2) Using the path integral formulation similarly to "proof 1" of eq. (5.34) in sub-sec. 5.2.1.

**Exercise 5.3.** Prove that eq. (5.38) satisfies the backward Bloch eq.(5.37) for the simplest case  $k = d = 1$  and  $D(x, t) > 0$  generic. (Hint: use the discrete measure eq.(4.37) for  $d = 1$ . Notice that it is easier to prove the backward Bloch eq.(5.37) rather than (5.36) since a change of variable involved in the derivation does not need complicated derivations).

**Exercise 5.4.** <sup>3</sup> Prove the results of sec. 5.2.3 in full generality as explained there.

**Exercise 5.5.** Derive the analogous of the Bloch equation and of the backward Bloch equation for the Master equation of exercise 4.7, eq.(4.70). (Hint: Trajectory  $i(t)$  stays constant and suddenly jump at random time. Thus  $\int_{t_0}^t V_{i(s)} ds$  is well defined. When evaluating the average

$$(5.40) \quad W_B(i, t|i_0, t_0) = \left\langle e^{-\int_{t_0}^t V_{i(s)} ds} \delta_{i(t), i} \right\rangle,$$

where  $W_B(i, t_0|i_0, t_0) = \delta_{i, i_0}$  and  $\delta_{i, i_0}$  is the Kronecker delta, at time  $t + dt$  one has to consider two contributions: one from no change of state and the other from the change of state.)

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<sup>3</sup>Optional

# Interesting Stochastic Phenomena

## 6.1. Subdiffusion and superdiffusion

Usual diffusion is one out of many different ways to explore space and time that are found in Nature, as well as in social phenomena and in technological applications. The purpose of this section is to expand the view to anomalous diffusion.

*The part on Levy flights and anomalous diffusion is reviewed in more details in the file “s03\_Levy.pdf” in moodle.*

To start, remember the properties of the fundamental solution  $P(x, t)$  of the diffusion equation for  $x_0 = 0$  and  $t_0 = 0$ :

$$(6.1) \quad P(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

It is obvious, being  $P(x, t)$  a Gaussian distribution, that

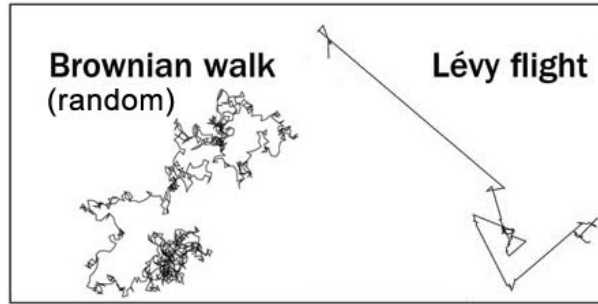
$$(6.2) \quad \langle x^2(t) \rangle = 2Dt$$

Let us try to generalize and consider a number  $\zeta \neq 1$ . We introduce a particle undergoing a diffusion process which is different from the standard Brownian motion. For some  $D_\zeta$  and exponent  $\zeta$ ,

$$(6.3) \quad \langle x^2(t) \rangle = 2D_\zeta t^\zeta$$

If  $0 < \zeta < 1$  we talk about subdiffusion, which is typical of transport of charge carriers in semiconductors and chemicals and monomers of polymer diffusion (at short timescales). Subdiffusion may take place if a particle tends to persist in the same state. For example, the waiting time distribution between particle’s jumps may be proportional to  $t^{-1-\alpha}$  for  $0 < \alpha < 1$ . This distribution has no finite first moment and, as a result, it is not rare in practice to observe trajectories during which the particle remains for an anomalous long time in the same position. The result of this persistence is measured by the anomalous diffusion (6.3) with  $\zeta < 1$ .

If  $\zeta > 1$  we talk about superdiffusion. Levy flights are a phenomenon typically linked with superdiffusion. They are realized by a sequence of jumps whose length could be also large with non-negligible frequency (Figure 1). More precisely, one finds that the distribution of jump displacements  $x$  is proportional to  $|x|^{-1-\mu}$  for large  $x$ , with exponent  $0 < \mu < 2$ . The name “flight” is used to denote quick (instantaneous) jumps. In case the trajectory is performed with finite constant velocity one instead talks of Levy walks.



**Figure 1.** Visual comparison between normal diffusion and a Lévy flight.

In general, one may observe a combination of non-Poissonian waiting times and power-law jump statistics, or other complex features including memory in the process and long range correlations.

To Lévy flights we can associate a generalized diffusion equation,

$$(6.4) \quad \begin{cases} \partial_t P(x, t) = D_\mu \frac{\partial}{\partial |x|^\mu} P(x, t) \\ P(x, 0) = \rho(x) \end{cases}$$

which is understood in the Fourier space,

$$(6.5) \quad \partial_t \tilde{P}(k, t) = -D_\mu |k|^\mu \tilde{P}(k, t)$$

To solve this equation, we note that it is equivalent to

$$\partial_t \left[ e^{D_\mu |k|^\mu t} \tilde{P}(k, t) \right] = 0$$

This implies that the function

$$\tilde{f}(k) = e^{D_\mu |k|^\mu t} \tilde{P}(k, t)$$

is independent of time. By reversing the identity the solution becomes

$$(6.6) \quad \tilde{P}(k, t) = \tilde{f}(k) e^{-D_\mu |k|^\mu t}$$

Here  $\tilde{f}(k)$  is the characteristic function of the initial  $\rho(x)$ , which is obvious by setting  $t = 0$ . This is consistent with having the probability density  $P(x, t)$  as a convolution of  $\rho(x_0)$  and a “propagator”  $W(x|x_0)$  whose characteristic function is  $e^{-D_\mu |k|^\mu t}$ .

For  $k = 2$  we retrieve the usual diffusion. The solution involves a Gaussian  $e^{-Dk^2t}$  and

$$P(x, t) = \int dx_0 \rho(x_0) \frac{1}{4Dt} e^{-(x-x_0)^2/(4Dt)}$$

Note again the convolution structure of this formula. It could be interpreted also as a weighted average for events characterized by different initial positions, where the weight is  $\rho(x_0)$  and the displacement probability density, or propagator, is

$$W(x|x_0) = \frac{1}{4Dt} e^{-(x-x_0)^2/(4Dt)}$$

In general, however, the solution in real space for a generic  $\mu$  is difficult to write explicitly. A few examples below make exception.

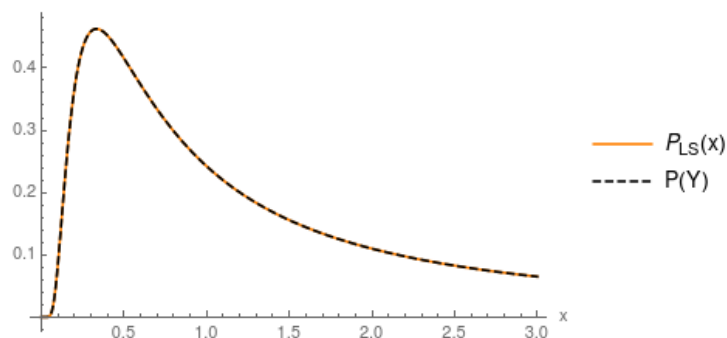
**6.1.1. Cauchy random flights.** The Cauchy random flight is a Lévy flight with  $\mu = 1$ , with

$$(6.7) \quad \tilde{P}_C(k, t) = \tilde{f}(k) e^{-D_1 |k|t}$$

Choosing the initial conditions  $\rho(x) = \delta(x)$  and setting a typical length scale  $x^*(t) = D_1 t$ ,

$$(6.8) \quad P_C(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-x^*(t)|k| + ikx} =$$

$$(6.9) \quad = \frac{1}{\pi} \int_0^{\infty} dk e^{-x^*(t)k} \cos kx = \frac{1}{\pi x^*(t)} \frac{1}{1 + \left(\frac{x}{x^*(t)}\right)^2}$$



**Figure 2.** Levy-Smirnov distribution and the distribution of the sum of two variables  $x, x'$  (each following the Levy-Smirnov), rescaled by  $1/2^2$ , i.e.  $P(Y)$  with  $Y = (x + x')/4$ .

The Cauchy distribution shows explicitly that its variance is not defined,  $\int P_C(x, t)x^2 dx = \infty$ . Indeed, it is a fat-tailed distribution,  $\sigma$  is not finite and the standard central limit theorem cannot be applied (i.e. an average of a lot of samples from a Cauchy flight do not converge to a Gaussian distribution). However, it makes sense to speak of typical scale  $x^*$  even if the variance is infinite.

**6.1.2. Levy stable distributions.** The behavior described above is true in general for a class of distributions called Levy stable distributions, of which the Cauchy is an example. In analogy with the Central Limit Theorem, where the statistics converges to a normal one, one has that each Levy stable distribution is an attractor for a class of single variable distributions, each one characterized by its power-law decay. For example, one might check that the sum of i.i.d. variables with

$$p(x) = \frac{1}{2x^2} \quad \text{for } |x| > 1 \quad \text{and } 0 \text{ otherwise}$$

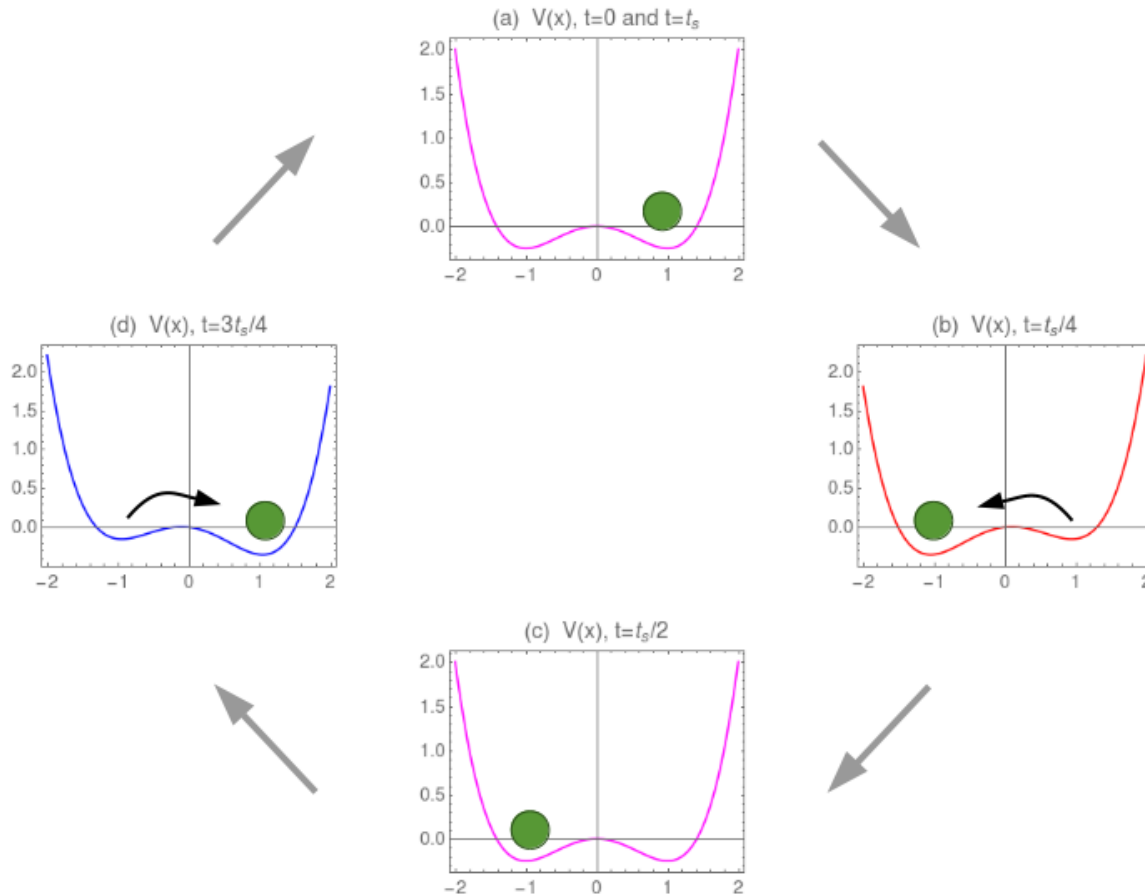
converges to the Cauchy distribution after a suitable rescaling.

In general the Levy stable distributions, which we are briefly mentioning without a detailed mathematical introduction, can be asymmetric. An example of fully asymmetric distribution is the Levy-Smirnov distribution

$$P_{LS}(x) = \frac{1}{\sqrt{2\pi}x^3} e^{-1/(2x)}$$

for  $x > 0$ , and zero otherwise. By summing variables distributed according to  $P_{LS}$  one obtains a result that, after rescaling, is still distributed according to the  $P_{LS}$ . For instance,  $P(Y = \frac{x+x'}{4})$ , obtained from the convolution of  $P_{LS}(x)$  and  $P_{LS}(x')$ , matches  $P_{LS}(Y = x)$  (see Figure 2). Note that the rescaling factor  $1/2^2$  in  $Y$  is not as in the central limit theorem, where it would be  $1/2^{1/2}$  for  $n = 2$ .

The Levy-Smirnov distribution scales as  $P_{LS}(x) \sim x^{-3/2}$  for large  $x$ . By summing variables  $x > 0$  with a  $p(x) \sim x^{-3/2}$  for large  $x$ , one should recover the ‘‘attractor’’  $P_{LS}$  for the rescaled sum. More details can be found in the related literature.



**Figure 3.** Snapshots of the potential  $V(x) = \frac{x^4}{4} - \frac{x^2}{2} + \frac{1}{10} \sin(2\pi t/t_s)$ , with minima in  $x \approx -c = -1$  (state “1”) and  $x \approx c = 1$  (state “2”) separated by a barrier  $\Delta V \simeq 1/4$ . Panels represent four moments of its period following time in clockwise direction.

## 6.2. Stochastic Resonance

Noise, as implied by the word itself, often acts as a perturbation that randomizes the behavior of a system. In this section we discuss a counterexample in which the right amount of noise makes the system more regular in its periodic oscillations. The example concerns the phenomenon of Stochastic Resonance (SR), which was introduced in the 80’s to explain how the climatic oscillations on Earth could be significantly wider than expected by measuring the amplitude of its oscillatory drive, given by the Sun activity over a period of  $\approx 10^5$  years.

Nowadays SR is even used in image reconstruction, and is recognized in many different systems in biology, electronics, and physics. These include lasers, magnetic resonance, and quantum systems. One finds that the transitions between oscillatory energetic levels do follow their periods better when temperature is neither too high nor too low. We illustrate this behavior with a simple two-states model and we show how to quantify the regularity of the periodicity in the system stochastic dynamics. We are going to map a continuous stochastic dynamics (diffusion) to a Markov jumps dynamics (Master equations) between states.

Consider a particle subject to a Mexican hat-like potential with two minima at  $x = c$  and  $x = -c$  as that shown in Figure 3. Suppose that there exists an external driving force that, in a period  $t_s$ , cyclically higher and lowers the relative strength of the potential at  $x = \pm c$ : at time  $t = 0$   $V(c) = V(-c)$ ,  $t = t_s/4$   $V(c) > V(-c)$ ,  $t = t_s/2$   $V(c) = V(-c)$  and  $t = 3t_s/4$   $V(c) < V(-c)$ . Since the shape of the potential varies with time, so does the propensity of the particle to jump either around  $-c$  (state “1”) or  $+c$  (state “2”). Around  $x = 0$  the potential has a local maximum which is unstable and only visited in transients.

In the cycle shown in Figure 3, the particle jumps at about stages  $t = t_s/4$  and  $t = 3t_s/4$ . This behavior is expected to be enhanced by some noise. Without such noise, the system would be too “cold” and unable to jump the barrier. On the other hand, a too “hot” system would jump the barrier regardless of the modulation. Let us see how to find the right balance so that the jumps are better synchronized with the phases of the cycle.

We first model the particle dynamics for a time-independent potential  $V = V_0$ , with a Langevin equation

$$(6.10) \quad \dot{x} = -V_0'(x) + \xi(t) \quad \text{with} \quad \langle \xi(t)\xi(t') \rangle = \kappa\delta(t-t')$$

where  $\kappa$  is the strength of the white noise  $\xi$ . In case of a pure thermodynamic interpretation we would set  $\kappa = 2k_B T$ .

It is possible to prove that the typical jump time scales as

$$(6.11) \quad \langle \tau \rangle_0 = \frac{2}{\kappa} \int_{-c}^c dy \exp\left(\frac{2V_0(y)}{\kappa}\right) \int_{-\infty}^y dz \exp\left(\frac{-2V_0(z)}{\kappa}\right)$$

In the Kramers approximation, the jumping rate  $W_0$  becomes

$$(6.12) \quad W_0 = \langle \tau \rangle_0^{-1} \approx \frac{1}{2\pi} \sqrt{|V''(0)|V''(c)} \exp\left(\frac{-2\Delta V}{\kappa}\right)$$

where  $\Delta V = V(0) - V(c)$ . Due to the symmetry of the system, this rate is the same for transitions  $1 \rightarrow 2$  and  $2 \rightarrow 1$ . In Kramers' formula, there is a strong exponential dependence on the ratio between the barrier height and the noise amplitude. This is modulated by a prefactor taking into account the curvature of the potential in the minimum and at the saddle point. Jumps in this case occur as uncorrelated events, separated by exponentially distributed waiting times with average value  $\langle \tau \rangle_0$ . The system is thus not displaying any regularity in time.

By adding a modulation to the potential, with period  $t_s = 2\pi/\omega_s$

$$(6.13) \quad V(x, t) = V_0(x) + V_1 \frac{x}{c} \sin \omega_s t$$

the jumping rates become asymmetrical at a generic time  $t$ . The exponential dependence on this  $V$  will lead to the sensibility on the phase of the drive. The intuition is that  $\kappa$  should be as large as to barely allow a jump of the potential when the maximum asymmetry is reached.

If  $\Delta V \gg V_1$  and the modulation frequency  $\omega_s$  is much smaller than the rates of intrawell relaxation, the jumping rates can be written as

$$(6.14) \quad W_{1,2} = \frac{1}{2\pi} \sqrt{|V''(0)|V''(c)} \exp\left(-\frac{2}{\kappa} (\Delta V \pm V_1 \sin \omega_s t)\right)$$

where  $W_1$  is the rate for the jump  $1 \rightarrow 2$  and viceversa for  $W_2$ .

**6.2.1. Reduced description.** To achieve some quantitative estimate of the system's regularity, we move to a reduced description with two discrete states and evolution via a master equation:

$$(6.15) \quad \begin{cases} \dot{p}_1 = -W_1(t)p_1 + W_2(t)p_2 \\ \dot{p}_2 = -W_2(t)p_2 + W_1(t)p_1 \end{cases}$$

where  $p_1(t)$  and  $p_2(t)$  are the probabilities to be in the two states. Since  $p_2(t) = 1 - p_1(t)$ ,

$$(6.16) \quad \dot{p}_1 = -\underbrace{(W_1(t) + W_2(t))}_{\equiv W(t)} p_1(t) + W_2(t)$$

We introduce the sum  $W(t) = W_1(t) + W_2(t)$  and by  $\langle W \rangle$  we denote its average over one period. Equation (6.16) approaches a periodic solution,

$$(6.17) \quad p_1(t)^{\text{osc}} = \frac{1}{1 - e^{-\langle W \rangle t_s}} \int_0^{t_s} dt' W_2(t-t') \exp\left(-\int_{t-t'}^t dt'' W(t'')\right)$$



Consider weakly modulated rates:

$$(6.18) \quad \begin{cases} W_1(t) = \frac{W}{2} - \epsilon \sin \omega_s t \\ W_2(t) = \frac{W}{2} + \epsilon \sin \omega_s t \end{cases}$$

Calling  $p_1 = p$ :

$$(6.19) \quad \dot{p}(t) = -Wp(t) + \frac{W}{2} + \epsilon \sin \omega_s t$$

If we just consider the deviations of  $p$  from  $1/2$ , i.e.  $\Delta p = p - \frac{1}{2}$ :

$$(6.20) \quad \dot{\Delta p} = -W \Delta p + \epsilon \sin \omega_s t$$

This has solution  $\Delta p(t) = \Delta p(0)e^{-Wt}$ .

For  $\epsilon = 0$ , one can show (see exercises) that the correlation function  $C(t) = \langle x(t)x(0) \rangle = c^2 e^{-W|t|}$ . Moreover, by means of the Wiener-Kintchine Theorem

$$P(\omega) = 4 \int_0^\infty C(t) \cos(\omega t) dt$$

which relates power spectrum  $P(\omega)$  to  $C(t)$ , one can show that in this case the power spectrum is a Lorentzian

$$P^{(0)}(\omega) = 4c^2 \frac{W}{W^2 + \omega^2}$$

with cutoff angular frequency  $\omega_{cut} = W$ , as shown in Figure 4, left panel.

**6.2.2. Reduced description, for modulated systems.** For  $\epsilon \neq 0$  we change the equation in this way:

$$(6.21) \quad \dot{\Delta p} = -W \Delta p + \epsilon e^{i\omega_s t}$$

Its Fourier transform in time is

$$\begin{aligned} i\omega \Delta \tilde{p} &= -W \Delta \tilde{p} + 2\pi\epsilon \delta(\omega - \omega_s) \\ \Delta \tilde{p} &= \frac{2\pi\epsilon}{i\omega + W} \delta(\omega - \omega_s) \end{aligned}$$

To compute the power spectrum, we note that the signal in  $x$  is determined by the signal in the occupation  $\Delta p$ , times a constant amplitude  $c$ ,  $\tilde{x}(\omega) = c\Delta \tilde{p}(\omega)$ . Then,

$$P(\omega) = |\tilde{x}(\omega)|^2 = S_\epsilon(\omega) \delta(\omega - \omega_s)$$

where

$$(6.22) \quad S_\epsilon(\omega) \equiv \frac{4\pi^2 c^2 \epsilon^2}{\omega^2 + W^2}$$

The signal-to-noise ratio (SNR) in an interval  $\Delta\omega$  including  $\omega = \omega_s$  is

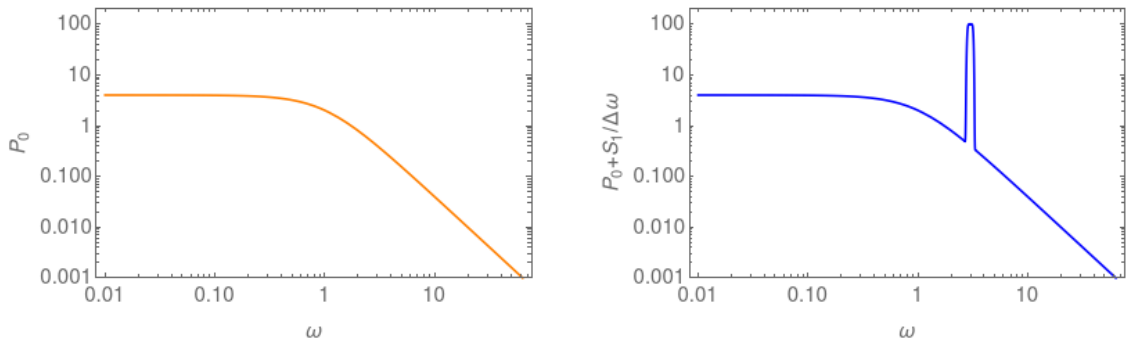
$$\text{SNR}_{\omega_s} = \frac{S_\epsilon(\omega_s) + P^{(0)}(\omega_s)\Delta\omega}{P^{(0)}(\omega_s)\Delta\omega} = 1 + \frac{S_\epsilon(\omega_s)}{P^{(0)}(\omega_s)\Delta\omega}$$

Let us analyze the second term,

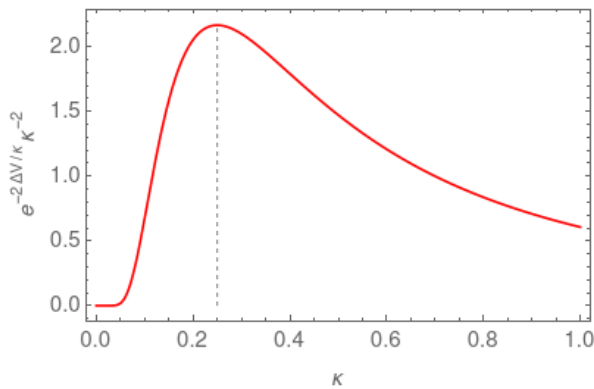
$$\frac{S_\epsilon(\omega_s)}{P^{(0)}(\omega_s)} = \frac{4\pi^2 c^2 \epsilon^2}{W^2 + \omega_s^2} \frac{W^2 + \omega_s^2}{4c^2 W} = \frac{\pi^2 \epsilon^2}{W}$$

and then find where  $\epsilon$  appears in the rates. By setting for simplicity the prefactor  $\frac{1}{2\pi} \sqrt{|V''(0)|V''(c)} = 1$ , we find that the rates for small  $V_1/\Delta V$  can be expanded as

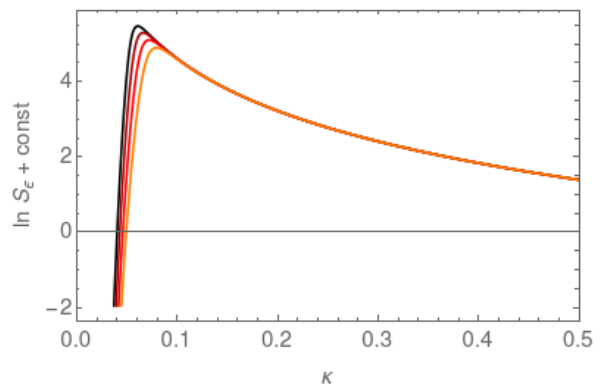
$$\begin{aligned} W_{1,2}(t) &= e^{-\frac{2}{\kappa}(\Delta V \pm V_1 \sin \omega_s t)} = \frac{W}{2} e^{\mp \frac{2V_1}{\kappa} \sin \omega_s t} \approx \\ &\approx \frac{W}{2} \left( 1 \mp \frac{2V_1}{\kappa} \sin \omega_s t \right) \end{aligned}$$



**Figure 4.** Log-log plot of the power spectrum of the system ( $c = 1, W = 1$ ) without modulation (left) and without modulation (right, with  $\omega_s = 3, S_\epsilon/\omega = 100$ ).



**Figure 5.** SNR as a function of  $\kappa$  for  $\Delta V = 1/4$ . The vertical dashed line is at  $\kappa^* = \Delta V$ .



**Figure 6.**  $\ln S_\epsilon$  (plus a constant) as a function of  $\kappa$  for  $\Delta V = 1/4$  and  $W = Ae^{-2\Delta V/\kappa}$  (here  $A = 1$ ). Curves are for four values of  $\omega_s$ :  $10^{-4}$  (black) and its first three multiples of 2.

By comparing this equation with (6.18) we identify  $\epsilon$  with

$$(6.23) \quad \epsilon = \frac{WV_1}{\kappa}$$

Since  $W \sim e^{-\frac{2}{\kappa}\Delta V}$  and  $\epsilon \sim \frac{W}{\kappa}$ , we have

$$\text{SNR}_{\omega_s} \approx \frac{S_\epsilon(\omega_s)}{P^{(0)}(\omega_s)} = \frac{\pi^2 \epsilon^2}{W} \sim \frac{1}{\kappa^2} e^{-\frac{2}{\kappa}\Delta V}$$

The maximum is at  $\kappa^*$  such that

$$\left. \frac{\partial \text{SNR}_{\omega_s}}{\partial \kappa} \right|_{\kappa=\kappa^*} = 0$$

which gives (exercise)  $\kappa^* = \Delta V$ . This holds regardless of the amplitude  $V_1$ , as long as  $V_1 \ll \kappa$ .

In Figure 6 we show an example of the signal (in log scale)

$$\ln S_\epsilon = \ln \frac{W^2/\kappa^2}{W^2 + \omega_s^2} + \text{const}$$

as a function of  $\kappa$ . Curves are for different  $\omega_s \ll A$ , where  $A$  is the prefactor of the rate  $W = Ae^{-2\Delta V/\kappa}$ . The maximum of the signal is at an intermediate value of  $\kappa$ , which is not coincident with  $\Delta V$  but just at an intermediate value not very sensible to  $\omega_s$ . The relevant aspect is that the curve is sharply peaked and that there is a range of  $\kappa$  where the system is very sensible to the drive.

Another feature of SR is the peculiar distribution of waiting times between jumps. Without the periodic signal, the system stays in  $\pm c$  for a time  $\tau$  which is a random quantity exponentially distributed (as in Markov jump systems). The periodic signal deforms the exponential distribution by adding peaks around multiples of a typical time. The first peak at half of the signal period  $t_s$  is enhanced by SR due to the phase synchronization with the drive of the jumps between the two states.

### 6.3. Instantons

Instantons are rare trajectories connecting two states that are not usually found in a typical path. In classical dynamics (instantons exist also in quantum mechanics) the rarity comes from the low noise limit, which limits the ability of the dynamics to visit all states. The typical shape of an atypical trajectory usually contains a sudden transition, hence the name “instanton”. For instance, in the time-scales of the planetary atmospheric evolution, the appearance of a stable giant vortex on the surface of Jupiter (sketched in Figure 7) takes place (rarely) by following an instanton.

We consider a Langevin equation in the low noise limit,

$$(6.24) \quad \dot{x}_\epsilon(t) = F(x_\epsilon) + \sqrt{\epsilon}\xi(t)$$

where  $\xi(t)$  is a standard white noise. In this note we deal with one-dimensional systems while keeping in mind that the approach can be generalized to  $d$  dimensions with some complications (see exercises). A trajectory from this dynamics is denoted by  $[x] = \{x(t)|t_i \leq t \leq t_f\}$ , where  $t_i$  is the initial time and  $t_f$  is the final time. The terminology we borrow from thermodynamic systems is that  $F$  is a “force” and “ $x$ ” a position. However, let us consider a dimensionless  $x$  and  $F$  with dimensions of an inverse time.

The infinitesimal propagator is:

$$(6.25) \quad W(x', t + \Delta t | x, t) = \frac{1}{\sqrt{2\pi\epsilon\Delta t}} e^{-\frac{\Delta t}{2\epsilon} \left( \frac{x' - x}{\Delta t} - F(x) \right)^2}$$

Performing the limit of infinitely many subsequent propagations, the full propagator of a path

$$(6.26) \quad W(x_f, t_f | x_i, t_i) = \int \mathcal{D}[x] e^{-\frac{S[x]}{\epsilon}}$$

can be expressed via an action

$$(6.27) \quad S[x] = \int_{t_i}^{t_f} L(x, \dot{x}) dt$$

with

$$(6.28) \quad L(x, \dot{x}) = \frac{1}{2} (\dot{x} - F(x))^2$$

There is an approximation in the form of the function  $L$  because we are neglecting a term  $\sim \epsilon$  that is irrelevant for small noise. In the limit  $\epsilon \rightarrow 0$ , the weight of most of the trajectories becomes tiny. We use the saddle point approximation and we look for trajectories  $x^*$  that minimize  $S[x]$ . Note that the optimal minimum of  $S[x]$  is where it is zero. Given  $x^*(t)$  with fixed  $x^*(t_i) = x_i$  and  $x^*(t_f) = x_f$ , we get

$$(6.29) \quad W(x_f, t_f | x_i, t_i) \approx e^{-S[x^*]/\epsilon}$$

$$(6.30) \quad S[x^*] = \min_{\substack{x(t_i)=x_i \\ x(t_f)=x_f}} S[x]$$

where the solution  $x^*$  is the instanton.

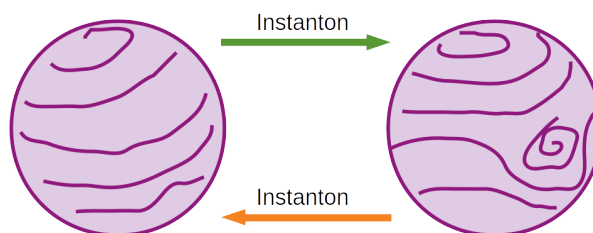


Figure 7. Sketch of instantons at atmospheric scale.

The trajectories extremizing  $S[x]$  solve the Euler-Lagrange equation

$$(6.31) \quad \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x}$$

$$(6.32) \quad \ddot{x} - \dot{x} \frac{dF(x)}{dx} = -(\dot{x} - F(x)) \frac{dF(x)}{dx}$$

$$(6.33) \quad \ddot{x} = \frac{d}{dx} \frac{F(x)^2}{2}$$

Thus, the equation to solve is a second order one, yielding smooth solutions. This might sound strange, given that Brownian trajectories are not differentiable. Yet, this makes sense: the instanton  $x^*$  represents the trajectory followed on average by a real, noisy path during a transition from  $x_i$  to  $x_f$ . A “real” instanton is thus a zigzag around the solution  $x^*$ .

The instanton equation (6.33) may be cast in terms of an effective potential

$$(6.34) \quad V_{\text{eff}}(x) = -\frac{1}{2}F^2(x)$$

in this way

$$(6.35) \quad \ddot{x} = -\frac{d}{dx} V_{\text{eff}}(x)$$

The effective potential is proportional to the negative square of the force. Hence, where forces are changing rapidly with  $x$ , we should expect more acceleration in the solution for  $x^*$ . On the contrary, where forces are not so sensible on  $x$ , the instanton gets less accelerated.

For instance, if  $F = -dV/dx$  is a conservative force, the effective potential is zero (hence maximum) at all stationary points of the potential  $V$ , being them minima, maxima, or saddles! This leads to some counterintuitive behavior of instantons. To gain more insight into this, below we discuss two examples.

Finally, we note that (6.35) is an equation conserving a total “energy”  $E$ ,

$$(6.36) \quad E = \frac{1}{2}\dot{x}^2 + V_{\text{eff}}(x)$$

This may offer a route for finding an analytical solution for  $x^*$  that is alternative to the solution of (6.35).

**6.3.1. Instanton, example 1.** We consider a one-dimensional system where the force  $F$  derives from a potential  $V(x) = \frac{\kappa}{2}x^2$ , namely  $F(x) = -\kappa x$ . The stochastic process related to this linear force is called the Ornstein-Uhlenbeck process

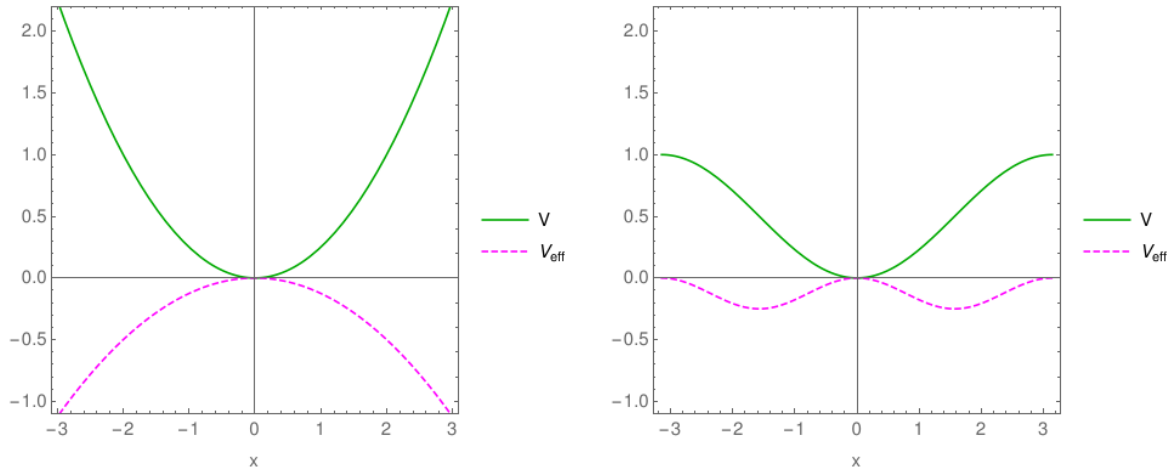
$$(6.37) \quad \dot{x} = -\kappa x + \sqrt{\epsilon}\xi(t)$$

The effective potential in this case is  $V_{\text{eff}}(x) = -\frac{1}{2}\kappa^2 x^2$ , which is a reversed parabola (see Figure 8). We ask which trajectory is typically followed from  $x_i = 0$  at  $t_i = -\infty$  to a final  $x_0$  at  $t_f = 0$ . The instanton solution is given by

$$(6.38) \quad \ddot{x} = \frac{d}{dx} \left( \frac{\kappa^2 x^2}{2} \right) = \kappa^2 x$$

The instanton thus is  $x^*(t) = x_0 e^{\kappa t}$ . Most of the time it sits close to the minimum of the well. Only at the very last moment it raises to reach the point  $x_0$ . We stress that  $x_0$  could be even a very unusual point given a low noise strength  $\epsilon$ . By raising the value of  $x_0$ , the shape of the instanton is only amplified and the time spent far from the minimum of  $V$  is not becoming extensive with respect to the time close to it.

Noting that the initial velocity in the  $x^*$  is  $\dot{x}_i = 0$ , it is possible to find the same instanton solution by the conservation of energy (exercise).



**Figure 8.** Harmonic potential and its effective potential for  $V(x) = \frac{\kappa}{2}x^2$  (left) and  $V(x) = \kappa(1 - \cos x)$  (right). In these examples,  $\kappa = 1/2$ .

**6.3.2. Instanton, example 2.** We consider another one-dimensional system with potential  $V(x) = \kappa(1 - \cos x)$ , giving  $F(x) = -\kappa \sin x$  and effective potential  $V_{\text{eff}}(x) = -\frac{1}{2}\kappa^2 \sin^2 x$ . For  $x \approx 0$  this potential overlaps with the  $V$  in the previous example (see Figure 8).

In this case we ask which trajectory is typically followed from  $x_i, \dot{x}_i = 0$  at  $t_i = -\infty$  to a final  $x_f = \pi$  at  $t_f$ , given that the trajectory is midway ( $x(0) = \pi/2$ ) at  $t = 0$ .

To find the instanton solution this time we use energy conservation. We start from a finite  $t_i$  (to be sent to  $-\infty$ ) and small yet finite  $x_i, \dot{x}_i = \delta \gtrsim 0$ , for reasons emerging during the following calculation. Due to these assumptions, at most the initial energy  $E \sim \delta^2 \gtrsim 0$  (it will turn out to be zero exactly). For analytical purposes, we adopt  $E = 0$  from the beginning. Thus,  $\frac{1}{2}\dot{x}^2 = -V_{\text{eff}}(x)$  yields

$$(6.39) \quad \dot{x} = \sqrt{-2 \left( -\frac{1}{2}\kappa^2 \sin^2 x \right)} = \kappa \sin x \quad \text{for} \quad 0 \leq x \leq \pi$$

Separating variables,

$$(6.40) \quad \kappa dt = \frac{dx}{\sin x}$$

and integrating up to time  $t$ ,

$$(6.41) \quad \begin{aligned} \kappa(t - t_i) &= \int_{x_i}^x \frac{dx'}{\sin x'} \\ &= \log \tan \frac{x}{2} \Big|_{x_i}^x \\ &= \log \frac{\tan x/2}{\tan x_i/2} \end{aligned}$$

which can be inverted to find

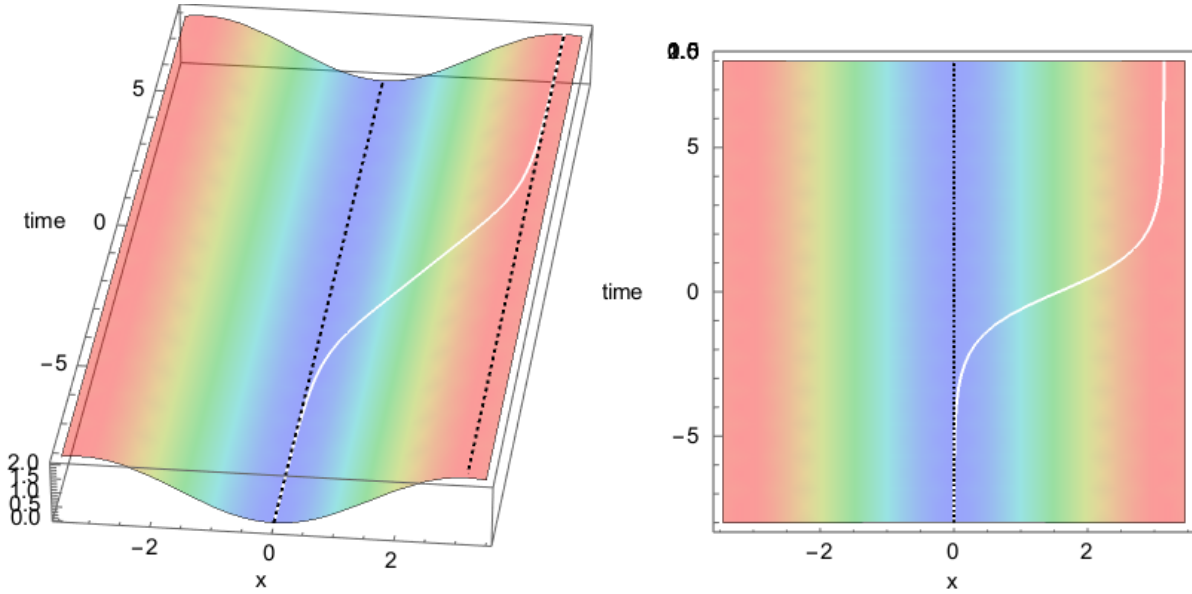
$$(6.42) \quad x(t) = 2 \arctan \left[ \tan \frac{x_i}{2} e^{\kappa(t-t_i)} \right]$$

The condition  $x(0) = \pi/2$  requires

$$(6.43) \quad \begin{aligned} \arctan \left[ \tan \frac{x_i}{2} e^{-\kappa t_i} \right] &= \frac{\pi}{4} \\ \rightarrow \tan \frac{x_i}{2} e^{-\kappa t_i} &= 1 \end{aligned}$$

which simplifies the equation for the instanton to

$$(6.44) \quad x^*(t) = 2 \arctan \left[ e^{\kappa t} \right]$$



**Figure 9.** Example of instanton for the dynamics with  $V(x) = \kappa(1 - \cos x)$  (with  $\kappa = 1/2$ ) for  $t_i = -\infty, x_i = 0$  and  $t_f = \infty, x_f = \pi$ , passing from  $x = \pi/2$  at  $t = 0$ .

This solution is compatible with the initial requirements but would not have made sense without a finite  $x_i$  because of the division by  $\tan x_i/2$ . The condition (6.43) indeed allows a simultaneous limit  $t_i \rightarrow -\infty, x_i \rightarrow 0$ .

The instanton (6.44) has a shape shown in Figure 9. Note that it spends as much time close to the bottom of the well as it spends close to the saddle  $x \approx \pi$ . This can be also understood by the shape of the effective potential (Figure 8). An initial slow roll down  $V_{\text{eff}}(x)$  from  $x = 0$  is then maximally accelerated around  $x = \pi/2$  and returns to zero velocity at large times around  $x \lesssim \pi$  due to the negative acceleration from the increase of  $V_{\text{eff}}(x)$  in  $x \in [\pi/2, \pi]$ . As anticipated, the instanton is not accelerating around saddle points of the potential  $V$ .

In practice the same shape of the instanton can be reversed on the side  $x > \pi$  of the saddle. A realistic transition from the first well  $x = 0$  to the second well  $x = 2\pi$  would look like a noisy instanton around a curve as (6.44) but eventually translated in time, followed by a similar curve down the hill at  $x > \pi$ . However, the time spent on top of the saddle would be not negligible, as indicated by the shape of the ideal solution  $x^*$ .

The proof that  $E = 0$  for the solution  $x^*$  in (6.44) is left as an exercise.

**6.3.3. Other applications of instantons.** The low noise limit has a statistics characterized the dominant paths. In this sense, calculations along the lines of those above show that:

- a stationary distribution emerges as

$$(6.45) \quad P(x) \approx e^{-V_{\text{inst}}(x)/\epsilon}$$

where

$$(6.46) \quad V_{\text{inst}}(x_f, t_f | x_i, t_i) = S[x^*]$$

$$(6.47) \quad V_{\text{inst}}(x) = \lim_{\substack{t_i \rightarrow -\infty \\ x_i \rightarrow x_m \\ t_f \rightarrow 0 \\ x_f \rightarrow x}} V_{\text{inst}}(x_f, t_f | x_i, t_i)$$

is a potential corresponding to the action from an instanton path starting at a reference  $x_m$  (e.g. a stationary point visited normally by the low noise dynamics).

- Given  $x_m$  within a domain  $D$  with boundary  $\partial D$ , the exit time from  $x_m$  to any point  $x$  on the boundary is

$$(6.48) \quad \tau_\epsilon \approx e^{V_{\text{inst}}^*/\epsilon}$$

with

$$(6.49) \quad V_{\text{inst}}^* = \min_{x \in \partial D} \min_{t \geq 0} V_{\text{inst}}(x, t | x_m, 0)$$

The exit point  $x$  is where there is a minimum in the action  $S$  joining it to the initial  $x_m$ , and the exit time is the duration of the corresponding instanton, which would thus be the exit path from  $D$ . Note that the optimal time  $\tau_\epsilon$  gets longer in a modified system in which the optimal path needs to reach a point with higher  $V_{\text{inst}}^*$ .

## Problems

### Problems on Levy flights.

**Exercise 6.1.** Expand the details of these passages

$$(6.50) \quad P(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-x^*|k| + ikx} = \frac{1}{\pi} \int_0^{\infty} dk e^{-x^*k} \cos kx = \frac{1}{\pi x^*} \frac{1}{1 + \left(\frac{x}{x^*}\right)^2}$$

used to find the one-dimensional Cauchy distribution. Finding the last term by skipping entirely the  $\cos kx$  step is also an option. Here  $x = 0$  at  $t = 0$  and  $x^* = D_1 t$ .

**Exercise 6.2.** With the Cauchy jump distribution with typical displacement  $x^* = D_1 t$  at time  $t$  (see previous exercise, setting  $x = \text{displacement}$ ), compute the probability  $P(x, t)$  to find the particle at position  $x$  at time  $t$  for such a Levy process, when the initial distribution is uniform and bound as  $P(x, 0) = \rho(x) = 1/(2a)$  for  $x \in [-a, a]$  and  $\rho(x) = 0$  otherwise.

**Exercise 6.3.** (optional) Check numerically that the sum  $S_n = x_1 + \dots + x_n$  of  $n$  i.i.d. variables  $x \in \mathbb{R}$ , each one distributed according to

$$p(x) = \frac{1}{4x^2} \quad \text{for } |x| > 1, \quad p(x) = 1/4 \quad \text{for } |x| \leq 1$$

converges to a Cauchy distribution

$$P_{\text{Cauchy}}(Y) = \frac{1}{\pi(1 + Y^2)}$$

after a suitable rescaling  $Y_n = \gamma S_n / n^\beta$ . What are  $\gamma$  and  $\beta$ ?

**Problems on stochastic resonance.** Consider the two-state model with states at position  $x_1 = -c$  and  $x_2 = +c$  and probability  $p$  to be in state  $-c$ , which evolves according to

$$\dot{p} = -Wp + \frac{W}{2} + \epsilon \sin(\omega_s t)$$

(see the notes of the lecture for more details)

**Exercise 6.4.** For  $\epsilon = 0$ , show that the correlation function  $C(t) = \langle x(t)x(0) \rangle = c^2 e^{-W|t|}$ .

**Exercise 6.5.** For  $\epsilon = 0$ , use the Wiener-Kintchine Theorem

$$P(\omega) = 4 \int_0^{\infty} C(t) \cos(\omega t) dt$$

to show that the power spectrum in this case is

$$P^{(0)}(\omega) = 4c^2 \frac{W}{W^2 + \omega^2}$$

**Exercise 6.6.** For  $\epsilon \neq 0$ , show that the *signal-to-noise ratio* is maximum at  $\kappa^* = \Delta V$  if the rates follow the Kramers formula

$$W_{1,2} = \exp \left[ -\frac{2\Delta V}{\kappa} \mp \frac{2V_1}{\kappa} \sin(\omega_s t) \right] = \frac{W}{2} \exp \left[ \mp \frac{2V_1}{\kappa} \sin(\omega_s t) \right]$$

with  $V_1 \ll \Delta V$  and using the correct identification for  $\epsilon$  in this case.



**Problems on instantons.** For the one-dimensional stochastic motion

$$\dot{x} = F(x) + \sqrt{\epsilon} \xi$$

with white noise  $\xi$  and drift  $F$ , the instantons ( $\epsilon \rightarrow 0$  limit) follow the equation

$$\ddot{x} = -\frac{dV_{\text{eff}}}{dx} \quad \text{with} \quad V_{\text{eff}}(x) = -F^2(x)/2$$

which implies a conservation of the “energy”

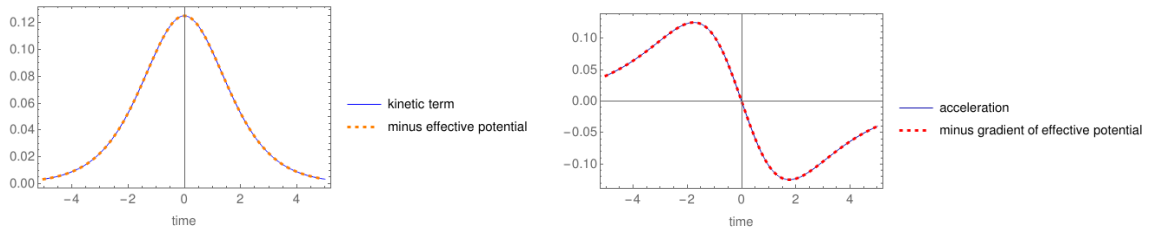
$$E = \frac{1}{2}\dot{x}^2 + V_{\text{eff}}(x)$$

**Exercise 6.7.** Find the instanton for  $F = -\kappa x$  by using the conservation of energy, for initial condition  $t_i = 0, x_i = 0, \dot{x}_i = 0$  and final condition  $x_0$  at  $t = 0$ .

**Exercise 6.8.** For  $F = -\kappa \sin x$  (see lecture notes) show that the instanton

$$x^*(t) = 2 \arctan [e^{\kappa t}]$$

has “energy”  $E = 0$  at every instant  $t$ .



**Figure 10.** For  $\kappa = 1/2$ , graphical examples of the conservation of “energy” (both terms in  $E$  are equal) and of the solution of the instanton equation.

Consider a  $N$ -dimensional system with  $i \leq N$  components. Each component of  $\vec{x} = (x_i)$  follows a stochastic motion

$$\dot{x}_i = F_i(\vec{x}) + \sqrt{\epsilon} \xi_i$$

with independent white noises  $\langle \xi_i(t) \xi_j(t') \rangle = \delta_{ij} \delta(t - t')$ .

**Exercise 6.9.** By starting from the Euler-Lagrange equation per component, show that the instanton equations become

$$(6.51) \quad \ddot{x}_i = \frac{\partial}{\partial x_i} \frac{|F|^2}{2} + \sum_{j=1}^N \left( \frac{\partial F_i}{\partial x_j} - \frac{\partial F_j}{\partial x_i} \right) \dot{x}_j$$

where  $|F|^2 = \sum_{j=1}^N F_j^2$ .

**Exercise 6.10.** Show that

$$E = \frac{1}{2}|\dot{x}|^2 + V_{\text{eff}}(x)$$

with  $V_{\text{eff}}(x) = -\frac{1}{2}|F|^2$ , is constant for the solution of the instanton equations (6.51).

# Disordered systems

For systems in equilibrium at a temperature  $T$  (and  $\beta = 1/T$ , with Boltzmann constant  $k_B = 1$ ), average quantities in the canonical ensemble are obtained by running weighted sums over all possible configurations  $S$ ,

$$(7.1) \quad \langle X \rangle = \frac{\sum_S X[S] e^{-\beta H[S]}}{\sum_S e^{-\beta H[S]}}$$

The denominator is the partition function

$$(7.2) \quad Z = \sum_S e^{-\beta H[S]}$$

and  $H[S]$  is the Hamiltonian, or energy function of the system. The free energy is  $F = -T \log Z$ . If we have  $X$  coupled to a parameter  $\alpha$  in  $H' = H + \alpha X$ , we see from the structure of (7.1) that  $\langle X \rangle = \frac{1}{\beta} \partial F / \partial \alpha |_{\alpha=0}$  derives from a suitable derivative of the free energy, which acts as a generating function. Hence, the knowledge of  $F$  allows to predict the mean behavior of the system.

One of the standard theoretical models of condensed matter is the Ising model for ferromagnets, which is the paradigm of a system displaying a phase transition by varying the temperature. In the following we use this model to show how the free energy should be evaluated in systems with some quenched disorder. To emphasize the similarities and the differences from the non-disordered system, we start by recalling the solution of the mean field Ising model.

## 7.1. A simple non-disordered system: the mean field Ising Model

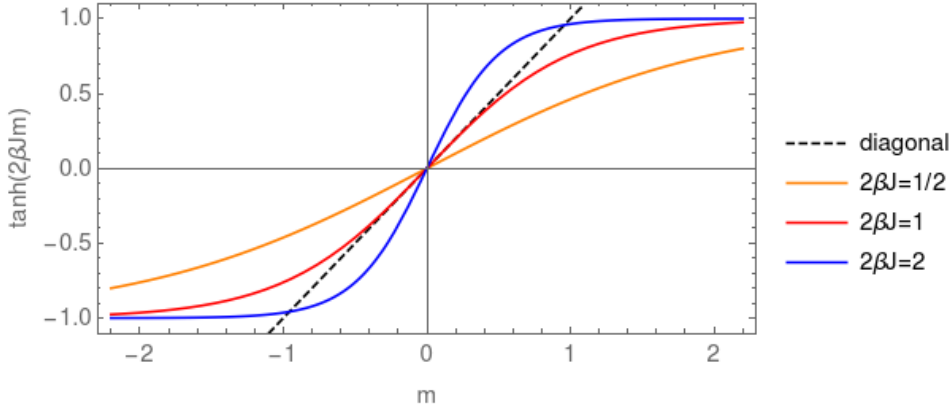
A standard Ising model, with spins  $S_i \in \{-1, 1\}$  for  $i = 1 \dots N$  and Hamiltonian

$$(7.3) \quad H = -\frac{J}{N} \sum_{i \neq j} S_i S_j - h \sum_i S_i$$

is in a “mean-field” version if the sum runs over all possible pairs of  $1 \leq i \leq N$  and  $1 \leq j \leq N$  with  $i \neq j$  (in the next section also the  $(i, i)$  pair will be included for simplifying the calculations; such constant energy shift is irrelevant thermodynamically). The system is ferromagnetic if  $J > 0$  and hence  $-J < 0$  favors the alignment of the spins. The external field  $h$  is the same for all spins.

We are interested in the thermodynamic limit  $N \rightarrow \infty$ . From the point of view of a given spin  $j$ , a myriad of other spins should contribute with an average effect due to the central limit theorem. The average magnetization

$$(7.4) \quad m = \frac{1}{N} \sum_i \langle S_i \rangle$$



**Figure 1.** The graphical solution of (7.12) is obtained by finding the intersections of the  $\tanh(2\beta Jm)$  function with the function  $m$ . The three curves are for low, critical, and large  $\beta$ .

should thus play a relevant role. Indeed, it enters in the calculation of the typical energetic contribution from  $j$ ,

$$(7.5) \quad H_j = S_j \left[ -\frac{2J}{N} \sum_i S_i - h \right]$$

$$(7.6) \quad \simeq S_j \left[ -\frac{2J}{N} \sum_i \langle S_i \rangle - h \right] \quad (\text{for large } N)$$

$$(7.7) \quad \equiv -h_m S_j \quad \text{with average field } h_m = 2Jm + h$$

(we would have had  $J$  and not  $2J$  if pairs  $i < j$  were considered).

The mean field approximation yields a non-interacting system of a single spin  $S_j$  in a field  $h_m$ . Its two possible states at inverse temperature  $\beta = 1/T$  thus appear with probability given by Boltzmann weights normalized by the partition function  $Z$ ,

$$(7.8) \quad P(S_j) = \frac{e^{-\beta H_j}}{Z} = \frac{e^{\beta h_m S_j}}{e^{\beta h_m} + e^{-\beta h_m}}$$

There is still a self-consistency condition to impose on  $h_m$  and thus on the magnetization  $m$ :

$$(7.9) \quad m = \sum_{S_j=\pm 1} P(S_j) S_j$$

$$(7.10) \quad = \frac{e^{\beta h_m} - e^{-\beta h_m}}{e^{\beta h_m} + e^{-\beta h_m}}$$

$$(7.11) \quad = \tanh(\beta h_m)$$

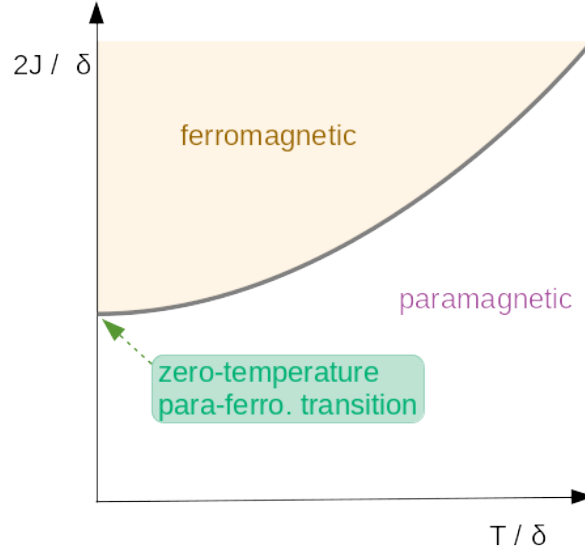
and by recalling what is  $h_m$ , the self-consistent equation becomes

$$(7.12) \quad m = \tanh(\beta 2Jm + \beta h)$$

Even for the simplest case  $h = 0$  without external field, one should find the solution graphically as shown in Figure 1. At low  $\beta$  (high temperature) the function  $\tanh(\beta 2Jm)$  is quite flat and stays below the function  $m$ , hence there is only one solution at  $m = 0$ . At a critical  $\beta_c$ , three solutions merge at  $m = 0$  and they split above  $\beta_c$  into  $m = -m^*, 0, +m^*$  because  $\tanh(\beta 2Jm)$  is steep enough to cross the diagonal  $m$  three times. The critical  $\beta_c$  is found by requiring that the tangent of  $\tanh(\beta 2Jm)$  is equal to 1 at  $m = 0$ , which yields  $\beta_c = 1/(2J)$ .

## 7.2. Random Field Ising Model (RFIM)

We aim at understanding what changes from the standard Ising model if the field  $h_i$  is now randomly assigned to each site  $i$ . To stress that this random field is a fixed feature of each



**Figure 2.** Phase diagram of the RFIM.

system, we call it *quenched disorder*. We may expect that this disorder added to the thermal randomness is a crucial factor when much stronger than the total ferromagnetic coupling with the other spins. In this sense, we could have a paramagnetic phase also if the temperature is very low because the spins prefer to follow their own local  $h_i$  rather than the global trend given by the magnetization.

We thus study a Random Field Ising Model (RFIM): the ferromagnetic coupling between spins  $S_i \in \{-1, 1\}$  (in a configuration denoted by  $S = (S_1, \dots, S_N)$ ) is as in the standard Ising model and the interaction is again not limited to nearest neighbor but runs over all pairs  $i, j$ ,

$$(7.13) \quad H_h[S] = -\frac{J}{N} \sum_{i,j} S_i S_j - \sum_i h_i S_i$$

including the  $i, i$  interaction, for later convenience. Here, as a novelty, the disorder is realized by picking each local field  $h_i$  from the same Gaussian distribution with variance  $\delta^2$ ,

$$(7.14) \quad p(h_i) = \frac{1}{\sqrt{2\pi\delta^2}} e^{-h_i^2/2\delta^2} \quad \forall i \leq N$$

and fixing it. Thus, every system is characterized by a given quenched disorder  $h = \{h_i | i = 1, \dots, N\}$  (of i.i.d. random variables) with full probability

$$(7.15) \quad p(h) = \prod_{i=1}^N p(h_i)$$

We would like to prove that the phase diagram of the RFIM is as that shown in Figure 2, where two phases (ferromagnetic with a macroscopic magnetization, and paramagnetic) appear. The diagram is as a function of the ratios  $T/\delta$  and  $J/\delta$ . The value  $T/\delta$  quantifies how thermal energy is relevant with respect to the disorder. The value  $J/\delta$  quantifies the relevance of the ferromagnetic coupling with respect to the disorder, and obviously the ferromagnetic phase appears where  $J/\delta$  is sufficiently large, where “sufficiently” is quantified by the dense line separating the phases (note its monotonic increase with  $T$ : why?). The phase diagram also shows that, for given values of  $J$  and  $T$ , there is always a value of  $\delta$  that can randomize the system enough to make it paramagnetic. Even for  $T = 0$  we may see a para-ferromagnetic phase transition by varying  $\delta$ .

The new issue is to find the typical behavior of a system by averaging its behavior over the realizations of the disorder. As discussed later, this centers around averaging the free energy

$$(7.16) \quad F_h = -T \log Z_h$$

over the disorder, rather than averaging the partition function

$$(7.17) \quad Z_h = \sum_S e^{-\beta H_h[S]}$$

An average over the disorder is denoted by an overline in the following. For example,

$$(7.18) \quad \overline{F} = -T \overline{\log Z_h} = -T \int \prod_i dh_i p(h) \log Z_h$$

The average of a nonlinear function as the log is problematic and it turns out to be simpler to average the  $n$ -th power  $(Z_h)^n$ . Because of this, it is useful to follow the *replica trick*. In its various forms, it reads

$$(7.19) \quad \overline{\log Z_h} = \lim_{n \rightarrow 0} \frac{\overline{Z_h^n} - 1}{n},$$

$$(7.20) \quad \overline{\log Z_h} = \lim_{n \rightarrow 0} \frac{1}{n} \log \overline{Z_h^n},$$

$$(7.21) \quad \overline{\log Z_h} = \left. \frac{\partial}{\partial n} \overline{Z_h^n} \right|_{n=0}$$

This is a useful mathematical step that, however, comes at the price of performing a weird limit of  $n \rightarrow 0$  replicas. Each replica is one out of  $n$  copies of the system, all sharing the same disorder  $h$ .

We label each replica by an index  $a = 1, \dots, n$  let it understood that  $Z = Z_h$  and  $H_h[S] = H[S]$  both depend on a quenched disorder  $h$ . The  $n$ -th power of the partition function is then

$$(7.22) \quad \begin{aligned} \overline{Z_h^n} &= \overline{\sum_{\{S^a\}} \exp\left(\frac{\beta J}{N} \sum_a \sum_{ij} S_i^a S_j^a\right) \exp\left(\beta \sum_i \sum_a S_i^a h_i\right)} \\ &= \sum_{\{S^a\}} \exp\left(\frac{\beta J}{N} \sum_a \sum_{ij} S_i^a S_j^a\right) \underbrace{\overline{\exp\left(\beta \sum_i \sum_a S_i^a h_i\right)}}_{\equiv e^{\sum_i \lambda_i h_i}} \end{aligned}$$

where  $\sum_{\{S^a\}}$  means sum over all possible configurations of all replicas and

$$(7.23) \quad \lambda_i = \beta \sum_a S_i^a$$

Since the average over disorder is limited to the last term with  $h_i$ 's, and since each term yields its own average via a Gauss integral,

$$(7.24) \quad \overline{e^{\lambda_i h_i}} = \int dh_i p(h_i) e^{\lambda_i h_i} = e^{\delta^2 \lambda_i^2 / 2},$$

we may rewrite

$$(7.25) \quad \overline{Z_h^n} = \sum_{\{S^a\}} \exp \left[ \frac{\beta J}{N} \sum_a \sum_{ij} S_i^a S_j^a + \frac{\beta^2 \delta^2}{2} \sum_i \left( \sum_a S_i^a \right)^2 \right]$$

$$(7.26) \quad = \sum_{\{S^a\}} \exp \left[ \frac{\beta J}{N} \sum_a \left( \sum_i S_i^a \right)^2 + \frac{\beta^2 \delta^2}{2} \sum_i \left( \sum_a S_i^a \right)^2 \right]$$

where we noted that the first term in the exponential is just the square of  $\sum_i S_i^a$ . This is possible thanks to the choice of running the interactions also over the  $(i, i)$  pairs.

By inspecting the structure of (7.26) we note that we arrived at a system with interacting replicas! At the same time, the disorder has disappeared from the formulas. This trade of complications will finally lead to a solution of the RFIM.

Next we use the Hubbard-Stratonovich (HS) transformation,

$$(7.27) \quad e^{\frac{b}{2}z^2} = \frac{1}{\sqrt{2\pi b}} \int dx e^{-\frac{x^2}{2b} \pm zx}$$

(for negative exponent it becomes  $e^{-\frac{b}{2}z^2} = \frac{1}{\sqrt{2\pi b}} \int dx e^{-\frac{x^2}{2b} \pm izx}$ ) which is useful for transforming squares in exponentials. In physical terms, this is translated to a replacement of interactions between degrees of freedom ( $z^2$ ) by interactions with a mediating field  $x$  (the term  $zx$ ) which follows a Gaussian statistics ( $x^2$ ). The left-hand side of the HS formula can be seen in (7.26) if we identify

$$(7.28) \quad z_a = \sqrt{2J\beta} \sum_i S_i^a$$

$$(7.29) \quad b = \frac{1}{N}$$

$$(7.30) \quad e^{\frac{b}{2}z_a^2} = \frac{1}{\sqrt{2\pi b}} \int dx_a e^{-\frac{x_a^2}{2b} + z_a x_a}$$

By performing the HS transformation we get a version of  $\overline{Z}^n$  in which spins  $S_i$  appear decoupled from the others,

$$(7.31) \quad \overline{Z}^n = \left(\frac{N}{2\pi}\right)^{n/2} \sum_{\{S^a\}} \int \prod_a dx_a \exp \left[ -\frac{N}{2} \sum_a x_a^2 + \underbrace{\sqrt{2J\beta} \sum_i \sum_a S_i^a x_a + \frac{\beta^2 \delta^2}{2} \sum_i \left( \sum_a S_i^a \right)^2}_{\sum_i \dots \text{ gives } N \text{ times the same object } \log Z_1} \right]$$

$$(7.32) \quad = \left(\frac{N}{2\pi}\right)^{n/2} \int \prod_a dx_a \exp \left[ N \left( -\frac{1}{2} \sum_a x_a^2 + \log Z_1(x_a) \right) \right]$$

with

$$(7.33) \quad Z_1(x_a) = \sum_{\{S^a=\pm 1\}} \exp \left( \sqrt{2\beta J} \sum_a x_a S^a + \frac{\beta^2 \delta^2}{2} \left( \sum_a S^a \right)^2 \right)$$

where we set  $S_i^a \rightarrow S^a$  due to the independence of  $Z_1$  on the index  $i$ .

The exponent  $\sim N$  in (7.32) shows that we can now use the saddle point approximation for large  $N$ . In doing this, we also assume that all replicas share the same  $x_a = x$  (like in a replica symmetric solution), hence  $\sum_a x_a = nx$ , and  $\sum_a x_a^2 = nx^2$ . The saddle point, denoted by  $x_m$ , solves the equation

$$(7.34) \quad \frac{\partial}{\partial x} \left[ -\frac{1}{2}nx^2 + \log Z_1(x) \right] = 0 \quad \rightarrow \quad nx = \frac{\partial}{\partial x} \log Z_1(x)$$

hence

$$(7.35) \quad nx_m = \sqrt{2\beta J} \frac{\sum_{\{S^a=\pm 1\}} (\sum_a S^a) e^{A[S, x_m]}}{\sum_{\{S^a=\pm 1\}} e^{A[S, x_m]}}$$

where

$$(7.36) \quad A[S, x] = \sqrt{2\beta J} x \sum_a S^a + \frac{\beta^2 \delta^2}{2} \left( \sum_a S^a \right)^2$$

The structure of (7.35) reveals that  $x_m$  is proportional to the average over the replicas of the spins, i.e. the magnetization  $m$ , in an ensemble where the Boltzmann weight  $e^A$  determines

averages  $\langle \dots \rangle$ ,

$$(7.37) \quad \frac{x_m}{\sqrt{2\beta J}} = \left\langle \frac{1}{n} \sum_a S^a \right\rangle \equiv m$$

We can thus rewrite everything by using  $m = x_m/\sqrt{2\beta J}$ :

$$(7.38) \quad \overline{Z^n} \propto e^{N[-n\beta J m^2 + \log Z_1(m)]}$$

$$(7.39) \quad Z_1(m) = \sum_{\{S^a = \pm 1\}} e^{A[S, m]}$$

$$(7.40) \quad A[S, m] = 2\beta J m \sum_a S^a + \frac{\beta^2 \delta^2}{2} \left( \sum_a S^a \right)^2$$

$$(7.41) \quad m = \frac{1}{Z_1(m)} \sum_{\{S^a = \pm 1\}} \left( \frac{1}{n} \sum_a S^a \right) e^{A[S, m]}$$

where  $A[S, m]$  still couples the statistics of the replicas.

We recall that we are looking for a self-consistent equation for the magnetization, in analogy to the solution of the standard mean field Ising model. The square  $(\sum_a S^a)^2$  that resisted so far in the exponent is removed by means of another HS transformation,

$$(7.42) \quad e^{A[S, m]} = \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2 + (2\beta J m + \beta \delta \nu) \sum_a S^a}$$

This brings the advantage of finally decoupling the replicas. With this HS transformation,  $Z_1(m)$  becomes

$$(7.43) \quad \begin{aligned} Z_1(m) &= \sum_{\{S^a = \pm 1\}} e^{A[S, m]} \\ &= \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2} \prod_a \sum_{S^a = \pm 1} e^{(2\beta J m + \beta \delta \nu) S^a} \quad (n \text{ decoupled replicas}) \\ &= \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2} [2 \cosh(2\beta J m + \beta \delta \nu)]^n \\ &= \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2 + n \log[2 \cosh(2\beta J m + \beta \delta \nu)]} \end{aligned}$$

We are finally able to perform the limit  $n \rightarrow 0$  dictated by the replica trick, for which  $Z_1 \rightarrow 1$ .

In analogy, we can prove that also the formula for  $m$  can be rewritten without any explicit reference to each replica but with just the number  $n$  of replicas appearing (exercise). It turns out that

$$(7.44) \quad m = \frac{1}{Z_1(m)} \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2 + n \log[2 \cosh(2\beta J m + \beta \delta \nu)]} \tanh(2\beta J m + \beta \delta \nu)$$

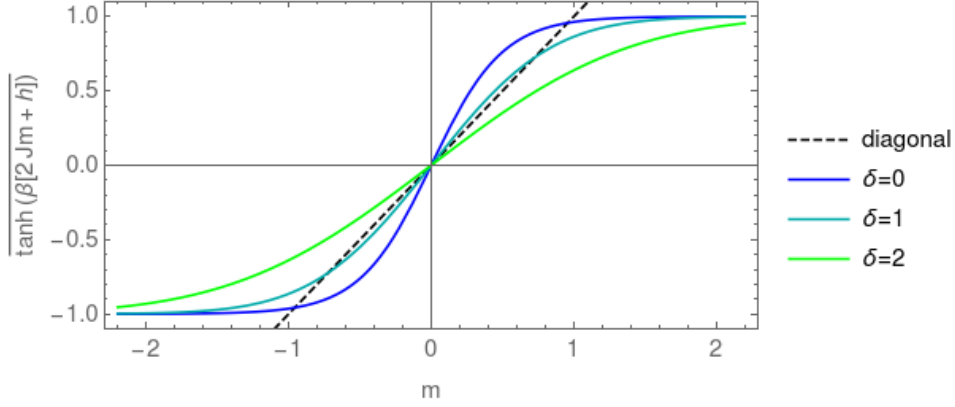
which, for  $n \rightarrow 0$ , gives

$$(7.45) \quad m = \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2} \tanh(2\beta J m + \beta \delta \nu)$$

This further appearance of a Gaussian distribution for  $\nu$  (unit variance) is welcome as one can convert it to a Gaussian distribution for  $h = \delta \nu$  and translate the formula to an average over disorder [see (7.15)],

$$(7.46) \quad \begin{aligned} m &= \int \frac{dh}{\sqrt{2\pi\delta^2}} e^{-\frac{h^2}{2\delta^2}} \tanh(2\beta J m + \beta h) \\ &= \overline{\tanh(\beta(2Jm + h))} \end{aligned}$$

This self-consistent equation for  $m = m_{sc}(m)$  with  $m_{sc}(m)$  given by the right-hand side of (7.46) is solved graphically, as shown for the Ising model. The critical line in the phase diagram of



**Figure 3.** Plot of the self-consistent magnetization (7.46) vs  $m$ , for  $\beta = J = 1$ . The three curves are for different noise strengths:  $\delta = 0$  (standard Ising),  $\delta = 1$  and  $\delta = 2$ . Note that the system without disorder is ferromagnetic for these parameters but becomes paramagnetic at sufficiently high  $\delta$ .

Figure 2 corresponds to the points where  $\partial m_{sc}/\partial m = 1$ , that the values of  $(T, \delta, J)$  for which the curve is tangent to the diagonal line  $m = m$ . One can prove (exercise) that this condition turns into the equation

$$(7.47) \quad 2\beta J \int dh p(h) \frac{1}{[\cosh(\beta h)]^2} = 1$$

which can be recast in several forms; for example, by using reduced variables  $J' = J/\delta$ ,  $\beta' = \beta\delta$ ,  $\tilde{h} = \beta h$  related to those in the axis of the phase diagram of Figure 2, we get

$$(7.48) \quad 2\beta' J' \int \frac{d\tilde{h}}{\sqrt{2\pi}} e^{-\frac{\tilde{h}^2}{2\beta'^2}} \frac{1}{[\cosh \tilde{h}]^2} = 1$$

Using this condition, one can show that even for zero temperature one has a para-ferromagnetic transition by varying the ratio  $2J/\delta = 2J'$ . The transition takes place (exercise) at  $2J/\delta = \sqrt{\pi/2}$ . Note that the self-consistent equation of the mean field Ising model is recovered from (7.46) for  $\delta \rightarrow 0$ . In Figure 3 there is an example of ferromagnetic phase disappearing by increasing  $\delta$ .

The free energy averaged over the disorder in the end is

$$(7.49) \quad \begin{aligned} \bar{F} &= -T \overline{\log Z} \\ &= -T \left. \frac{\partial}{\partial n} Z^n \right|_{n=0} \\ &\simeq -T \left. \frac{\partial}{\partial n} \left[ e^{N(-n\beta J m^2 + \log Z_1)} \right] \right|_{n=0} \\ &= -TN \left[ -\beta J m^2 + \left. \frac{\partial}{\partial n} \log Z_1 \right]_{n=0} \right. \\ &= N \left[ J m^2 - \left. \frac{T}{Z_1} \frac{\partial}{\partial n} Z_1 \right]_{n=0} \right. \\ &= N \left[ J m^2 - T \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2} \log[2 \cosh(2\beta J m + \beta \delta \nu)] \right] \\ &= N \left[ J m^2 - T \int \frac{dh}{\sqrt{2\pi\delta^2}} e^{-\frac{h^2}{2\delta^2}} \log[2 \cosh(\beta(2Jm + h))] \right] \end{aligned}$$

To wrap up, after deciding that the correct quantity to average is the free energy, one uses the replica trick to convert the computation to that of a system of interacting replicas without disorder. By some massage including two Hubbard-Stratonovich steps (to get rid of quadratic



forms in the exponent till we get to the right quadratic form, i.e. the disorder average) and by the identification of some quantities with others having physical meaning (magnetization, average over disorder), one finds a self-consistent equation for the magnetization that represents the generalization to a system with quenched disorder of its version for the Ising model. This magnetization enters in the solution for the free energy. The phase diagram of the RFIM follows from these equations, with boundary between phases given by the points where the self-consistent function of the magnetization has derivative 1.

As a final point, let us highlight that the limits  $\lim_{N \rightarrow \infty} \lim_{n \rightarrow 0}$  have been inverted in the above calculations, becoming  $\lim_{n \rightarrow 0} \lim_{N \rightarrow \infty}$ . Performing the thermodynamic limit before the limit to zero replicas is fine for the RFIM.

### 7.3. Neural networks and Hopfield model

The RFIM does not have a very interesting low temperature phase. In the ferromagnetic state it displays the two possible magnetizations and even in the paramagnetic case it stays around a single characteristic state which converges, for  $T \rightarrow 0$ , to a single state with spins fully aligned with local fields. This is not the case, in general, for disordered systems, which usually display a complex low temperature phase, or phases, with many basins of the free energy.

Our first example of disordered spin system with many nontrivial minima is a neural network where patterns are intentionally generated by an external agent, by encoding them in the coupling  $J_{ij}$  between neurons, which are biologically realized by axons. In this case each  $J_{ij}$  represents a *synaptic efficiency*, i.e. the kind of transmission of the axon from neuron  $j$  to neuron  $i$ . We will map neurons to spins and  $J_{ij}$  to their coupling, thus translating patterns into energetic minima.

Biologically, a neuron is activated when the incoming electrical signal overcomes a threshold. We define neuron states as

$$(7.50) \quad S_i = +1 \quad (\text{excited}), \text{ and} \quad S_i = -1 \quad (\text{at rest})$$

and a local field collecting all other impulses as

$$(7.51) \quad h_i = \sum_{j=1}^N J_{ij}(S_j + 1)$$

where also  $J$ 's take  $\pm 1$  values,

$$(7.52) \quad \begin{aligned} J_{ij} &= +1 && (\text{excitatory synapse}) \\ J_{ij} &= -1 && (\text{inhibitory synapse}) \end{aligned}$$

These  $J$ 's are quenched. The dynamical variables are the  $S_i$ , evolving by defining a new value of each  $S_i$  given the local excitation  $h_i$  determined by all values of other  $S_j$ 's.

The dynamical rule, defined in discrete time  $t = 1, 2, 3, \dots$ , is the following:

$$(7.53) \quad S_i(t+1) = \text{sgn}(h_i(t) - \theta_i^*) \quad \text{with} \quad h_i(t) = \sum_{j=1}^N J_{ij}(S_j(t) + 1)$$

and local threshold  $\theta_i^*$ . A simplifying hypothesis

$$(7.54) \quad \theta_i^* = \sum_{j=1}^N J_{ij}$$

leads to

$$(7.55) \quad S_i(t+1) = \text{sgn} \left[ h_i(t) - \sum_{j=1}^N J_{ij} \right] = \text{sgn} \left[ \sum_{j=1}^N J_{ij} S_j(t) \right]$$

We have all  $J_{ij} \neq 0$  and thus the system is densely connected. However, we impose the  $J_{ii} = 0$  (Hebb rule).

The purpose of this neural network is to store  $P$  patterns. By indexing the patterns with  $\mu = 1, \dots, P$ , we have that each pattern

$$(7.56) \quad \vec{\xi}^\mu = \{\xi_1^\mu, \dots, \xi_N^\mu\} \quad \text{with} \quad \xi_i^\mu = \{+1, -1\}$$

is essentially a spin configuration. We choose

$$(7.57) \quad \begin{aligned} J_{ii} &= 0 \quad (\text{Hebb rule}) \\ J_{ij} &= \frac{1}{N} \sum_{\mu=1}^P \xi_i^\mu \xi_j^\mu \end{aligned}$$

The second requirement defines the Hopfield model and introduces *memory* in the neural network: each pattern turns out to be a fixed point of the activation dynamics,

$$(7.58) \quad S_i(t) = \xi_i^\mu \rightarrow S_i(t+1) = \xi_i^\mu$$

This means that patterns are solutions of the equation

$$(7.59) \quad \xi_i^\mu = \text{sgn} \left[ \sum_{j=1}^N J_{ij} \xi_j^\mu \right]$$

This can be seen by first noting that the *scalar product* between two patterns,

$$(7.60) \quad \frac{1}{N} \sum_{j=1}^N \xi_j^\mu \xi_j^\nu \simeq \delta_{\mu\nu} + O(N^{-1/2})$$

yields essentially zero for  $\mu \neq \nu$  if the number of pattern is small compared to the system size,  $P/N \rightarrow 0$  for  $N \rightarrow \infty$  even if  $P \gg 1$ . This limitation for  $P$  is assumed hereafter. The second term in the previous equation takes into account the random overlap of patterns. Hence,

$$(7.61) \quad \begin{aligned} \text{sgn} \left[ \sum_{j=1}^N J_{ij} \xi_j^\mu \right] &= \quad (\text{with the definition of } J_{ij}, (7.57) ) \\ \text{sgn} \left[ \sum_{j=1}^N \left( \frac{1}{N} \sum_{\nu=1}^P \xi_i^\nu \xi_j^\nu \right) \xi_j^\mu \right] &= \quad (\text{rearranging}) \\ \text{sgn} \left[ \sum_{\nu=1}^P \xi_i^\nu \left( \frac{1}{N} \sum_{j=1}^N \xi_j^\nu \xi_j^\mu \right) \right] &= \quad (\text{using } (7.60) ) \\ \text{sgn} \left[ \sum_{\nu=1}^P \xi_i^\nu \delta_{\mu\nu} \right] &= \\ \text{sgn} [\xi_i^\mu] &= \xi_i^\mu \end{aligned}$$

which proves (7.59).

What happens if we start from a configuration slightly different from a pattern? The dynamics is mapped to that of a disordered Ising model with energy

$$(7.62) \quad \begin{aligned} E[\vec{S}] &= -\frac{1}{2} \sum_{i,j=1}^N J_{ij} S_i S_j \\ &= -\frac{1}{2} \sum_i S_i h_i \end{aligned}$$

that is minimized by a configuration  $\vec{S}$  aligned with its local field  $\vec{h}$ . At finite temperature  $T = 1/\beta$  the probability of a configuration  $\vec{S} = \{S_1, \dots, S_N\}$  is

$$(7.63) \quad p(\vec{S}) = \frac{1}{Z} \exp\{-\beta E[\vec{S}]\}$$

where as usual  $Z$  stands for the partition function

$$(7.64) \quad Z = \sum_{\vec{S}} \exp\{-\beta E[\vec{S}]\}$$

A zero temperature dynamics, when updating  $\vec{S}(t)$ , leads always to a new  $\vec{S}(t+1)$  with energy  $E[\vec{S}(t+1)] \leq E[\vec{S}(t)]$ . When starting from an initial  $\vec{S}(0)$  not too different from a given pattern  $\vec{\xi}^\mu$ , the energy minimization brings to  $S(t) = \vec{\xi}_\mu$  at some finite time  $t$ . The configurations  $\vec{S}(0)$  falling back to such pattern are in its basin of attraction, or free energy local minimum.

As an application in computer science, one may think of the neural network as a storage of  $P$  images, and of  $\vec{S}(0)$  as an image copied from a  $\vec{\xi}^\mu$  but with corrupted pixels. The original image may be recognized among the others by energy minimization.

Next we show that the number of energy minima of an Hopfield model is essentially the number  $P$  of patterns. The free energy per spin is

$$(7.65) \quad f = -\frac{1}{N\beta} \log Z$$

The  $P$  patterns are stationary points of the landscape of the energy function  $E$ .

By using the approximation

$$(7.66) \quad J_{ij} = (1 - \delta_{ij}) \frac{1}{N} \sum_{\mu=1}^P \xi_i^\mu \xi_j^\mu$$

$$(7.67) \quad \simeq \frac{1}{N} \sum_{\mu=1}^P \xi_i^\mu \xi_j^\mu$$

which is a modification forgetting about Hebb's rule encoded in (7.66) and with little relevance  $\sim N$  in a sum  $\sim N^2$ , we rewrite  $J_{ij}$  via (7.57) in the partition function,

$$(7.68) \quad Z = \sum_{\vec{S}} \exp \left\{ \frac{\beta}{2N} \sum_{ij} S_i S_j \sum_{\mu=1}^P \xi_i^\mu \xi_j^\mu \right\}$$

$$(7.69) \quad = \sum_{\vec{S}} \exp \left\{ \frac{\beta}{2N} \sum_{\mu=1}^P \left( \sum_i S_i \xi_i^\mu \right)^2 \right\}$$

$$(7.70) \quad = \sum_{\vec{S}} \int \prod_{\mu} dq_{\mu} \exp \left\{ -\frac{1}{2} N \beta \sum_{\mu=1}^P q_{\mu}^2 + \beta \sum_{\mu=1}^P q_{\mu} \left( \sum_i S_i \xi_i^\mu \right) \right\}$$

where in the last step we removed the square by a HS transformation, for which we are forgetting the prefactors (they would be irrelevant for our purposes). Now each of the terms with  $1 \leq i \leq N$  is independent on the others. The last term in the previous exponential becomes

$$(7.71) \quad \sum_{S_i=\pm 1} \exp \left\{ \beta \left( \sum_{\mu=1}^P q_{\mu} \xi_i^{\mu} \right) S_i \right\} = \quad \left( \text{defining } \vec{q} \cdot \vec{\xi}_i = \sum_{\mu=1}^P q_{\mu} \xi_i^{\mu} \right)$$

$$(7.72) \quad 2 \cosh(\beta \vec{q} \cdot \vec{\xi}_i) =$$

$$(7.73) \quad \exp\{\log[2 \cosh(\beta \vec{q} \cdot \vec{\xi}_i)]\}$$

and the partition function turns into

$$(7.74) \quad Z = \int \prod_{\mu} dq_{\mu} \exp \{-N\beta u(\vec{q})\}$$

with

$$(7.75) \quad u(\vec{q}) = \frac{1}{2} \sum_{\mu=1}^P q_{\mu}^2 - \frac{1}{\beta N} \sum_{i=1}^N \log[2 \cosh(\beta \vec{q} \cdot \vec{\xi}_i)]$$

to be expanded around its stationary point  $\vec{q}^*$  (minimizing  $u(q)$ ) for performing a saddle point approximation. In fact, the free energy coincides with the  $u$  function at the saddle point,

$$(7.76) \quad f = -\frac{1}{N\beta} \log Z = u(\vec{q}^*)$$

The stationary point is found by requiring

$$(7.77) \quad \left\{ \frac{\partial u}{\partial q_1} = 0, \dots, \frac{\partial u}{\partial q_P} = 0 \right\} \Big|_{\vec{q}=\vec{q}^*}$$

For any component this means

$$(7.78) \quad \frac{\partial u}{\partial q_{\mu}} = q_{\mu} - \frac{1}{N\beta} \sum_{i=1}^N \frac{1}{\cosh(\beta \vec{q} \cdot \vec{\xi}_i)} \sinh(\beta \vec{q} \cdot \vec{\xi}_i) \beta \xi_i^{\mu} = 0$$

leading to

$$(7.79) \quad q_{\mu}^* = q_{\mu} = \frac{1}{N} \sum_{i=1}^N \tanh(\beta \vec{q} \cdot \vec{\xi}_i) \xi_i^{\mu} \quad \forall \mu = 1, \dots, P$$

(we are dropping the star from the notation). The sum over all neurons  $i = 1, \dots, N$  for  $N \rightarrow \infty$  becomes an average over the possible values of  $\xi$ ,

$$(7.80) \quad \frac{1}{N} \sum_i f(\xi_i) \equiv \langle f \rangle = \int d\xi P(\xi) f(\xi)$$

$P(\xi)$ , the probability density of  $\xi$ , is found by noting that  $\xi_i = \pm 1$  with equal chance:

$$(7.81) \quad \int d\xi P(\xi) \dots = \frac{1}{2} \delta(\xi - 1) \dots + \frac{1}{2} \delta(\xi + 1) \dots \equiv \mathbb{E}(\dots)$$

The solution (7.79) is thus rewritten without the index  $i$  in the notation,

$$(7.82) \quad q_{\mu} = \mathbb{E} \left[ \tanh(\beta \vec{q} \cdot \vec{\xi}) \xi^{\mu} \right] \quad \forall \mu$$

To find a solution, we assume that  $\vec{q} = (q, 0, \dots, 0)$  with  $P-1$  null values and only one nontrivial  $q$  value, and later check if it works.

The physical meaning of  $q$  is better understood by stepping back to the sum over discrete variables (7.70) but with function  $u$  replaced by  $\tilde{u}$

$$(7.83) \quad \tilde{u}(\vec{q}, S_1, \dots, S_N) = \frac{1}{2} \sum_{\mu=1}^P q_{\mu}^2 - \frac{1}{\beta N} \sum_{\mu=1}^P q_{\mu} \left( \sum_{i=1}^N \xi_i^{\mu} S_i \right)$$

In this case, the saddle point solution  $\vec{q}$  where  $\partial u / \partial q_{\mu} = 0$  for all  $\mu$ 's yields

$$(7.84) \quad q_{\mu} = \frac{1}{N} \sum_{i=1}^N \xi_i^{\mu} S_i$$

which reveals that  $q_{\mu}$  is the *overlap* of the spins with the  $\mu$ -th pattern of the neural network. This explains that  $\vec{q} = (q_1, 0, \dots, 0)$  for  $\mu = 1$  makes sense, and similarly for all other patterns  $\nu \neq 1$  we should set  $\vec{q} = (0, \dots, 0, q_{\nu}, 0, \dots, 0)$ .

Focusing on the first pattern, from the above structure for  $q$  we get  $P$  equations,

$$(7.85) \quad q_1 = \mathbb{E} [\tanh(\beta q_1 \xi^1) \xi^1] \quad (1 \text{ equation})$$

$$(7.86) \quad q_\nu = \mathbb{E} \left[ \underbrace{\tanh(\beta q_1 \xi^1)}_{\text{odd}} \underbrace{\xi^\nu}_{\text{odd}} \right] \quad (P - 1 \text{ equations for } \nu > 1)$$

Each of the  $P - 1$  equations (7.86) is an expectation of independent odd terms with an even probability distribution for  $\xi$ 's, hence for parity it gives  $q_\nu = 0$ , consistently with the hypothesis that  $\vec{q}$  contains only one nonzero element. This is given by (7.85), which explicitly is

$$(7.87) \quad \begin{aligned} q_1 &= \frac{1}{2} \tanh(\beta q_1) - \frac{1}{2} \tanh(\beta q_1) \times (-1) \\ &= \tanh(\beta q_1) \end{aligned}$$

Since this is true for all patterns, in summary the only relevant saddle point equation for the Hopfield model is

$$(7.88) \quad q = \tanh(\beta q)$$

which resembles that of the mean field Ising model, with the overlap  $q$  replacing the magnetization  $m$ . In a sense, the overlap is a generalization of the concept of magnetization, to systems where a global magnetization does not appear, but where the overlap still quantifies some local order emerging within the state space.

Similarly to what seen for the Ising model, from the saddle point equation (7.88) we learn that there is a (second order) phase transition, here at  $\beta_c = 1$  where  $\tanh(q)$  is tangent to the  $q = q$  line. Of the two nonzero solutions  $\pm \hat{q}$  appearing at  $\beta > \beta_c$ , the one at  $-\hat{q}$  does not tell us anything more than that at  $+\hat{q}$  because fully anticorrelated and fully correlated have the same information content. By going to  $T \rightarrow 0$  we are left with  $P$  ground states, one for every pattern.

## 7.4. Sherrington-Kirkpatrick (SK) model

Here we discuss the Sherrington-Kirkpatrick (SK) model, a central model in the field of disordered systems (perhaps the “*Ising model of disordered systems*”), allowing us to introduce some ideas and techniques central in this field. In particular we will explain the reason why it is possible to compute *exactly* the free-energy of this model and how to cast this calculation into a variational problem. By doing this we will introduce the characteristic order parameter of disordered systems: the *overlap matrix*  $q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^N S_i^\alpha S_i^\beta$ . While a complete account of the (quite technical) intermediate steps of the free-energy calculation can be found in [“*Spin Glass Theory and Beyond*”, Marc Mézard, Giorgio Parisi and Miguel A. Virasoro, Wiley] and [“*Statistical Physics of Spin Glasses and Information Processing*”, Hidetoshi Nishimori, Oxford University Press], the present lesson will be concluded by an informal physical explanation of how the *hierarchical* ansatz for the matrix  $q_{\alpha\beta}$  captures the hierarchical nature of the free-energy landscape (minima nested into minima) typical of the spin-glass low-temperature phase. The presence of a multi-valley free-energy landscape is indeed the characteristic feature of systems with *quenched disorder* as the SK model. While the hierarchical structure of the landscape of the SK model is represented by the highly non trivial *full* replica-symmetry-breaking ansatz (full-RSB), the more simple *one-step* replica-symmetry-breaking ansatz will be discussed in the next lecture on the *p-spin* model.

**7.4.1. Details on the SK model.** We consider a magnetic system where each spin can take the values  $S_i = \{+1, -1\}$ , as for the Ising and Hopfield model. Again, the Hamiltonian

$$(7.89) \quad H[\vec{S}] = - \sum_{i < j} J_{ij} S_i S_j$$

contains all possible interactions between spins and is thus of fully long-range kind.

Now the couplings are quenched but not to store patterns, they are chosen at random from a Gaussian distribution

$$(7.90) \quad P(J_{ij}) = \sqrt{\frac{N}{2\pi\delta^2}} \exp\left\{-\frac{N}{2\delta^2}(J_{ij})^2\right\}$$

with zero mean (thus, no ferromagnetism is present) and variance  $\langle J^2 \rangle = \delta^2/N$  with constant  $\delta$ . This choice leads to a free energy

$$(7.91) \quad F_J = -\frac{1}{\beta} \log Z_J \sim N$$

that is extensive for every realization of the disorder  $J$ . We can fix  $\delta = 1$  and check this with a high-temperature expansion (small  $\beta$  expansion) of  $Z_J$ :

$$(7.92) \quad \begin{aligned} Z_J &= \sum_{\vec{s}} \exp\left\{\beta \sum_{i<j} J_{ij} S_i S_j\right\} \\ &\simeq \sum_{\vec{s}} \left[1 + \beta \sum_{i<j} J_{ij} S_i S_j\right] + \sum_{\vec{s} \times \vec{s}} \frac{\beta^2}{2} \sum_{i<j} \sum_{k<l} J_{ij} J_{kl} S_i S_j S_k S_l \end{aligned}$$

where the sum  $\sum_{\vec{s}} 1 = 2^N$  because it runs over all possible  $2^N$  spin states. The sums with spins are zero whenever a spin, say  $S_i$ , appears an odd number of times in the summand because every contribution with  $S_i = +1$  is canceled by another one with  $S_i = -1$ . This is the case for the sum  $\sum_{i<j} J_{ij} S_i S_j$ . For the same reason, in the  $\beta^2$  sum there survives a nonzero term when  $i = k$  and  $j = l$ , so that

$$(7.93) \quad Z_J \simeq 2^N \left[1 + \frac{\beta^2}{2} \sum_{i<j} J_{ij}^2\right]$$

whose logarithm is

$$(7.94) \quad \begin{aligned} \log Z_J &\simeq N \log 2 + \log \left[1 + \frac{\beta^2}{2} \sum_{i<j} J_{ij}^2\right] \\ &\simeq N \log 2 + \underbrace{\frac{\beta^2}{2} \sum_{i<j} J_{ij}^2}_{\text{must be of order } N} \end{aligned}$$

In the last term there appear the variance of the disorder,  $\sim N^2$  times. Imposing extensivity,  $N^2 \langle J^2 \rangle \sim N$ , we see that it must be  $\langle J^2 \rangle \sim N^{-1}$ . This is common to many disordered systems with long-range couplings.

The goal of our calculation is to compute the free energy in the thermodynamic limit

$$(7.95) \quad F_J = \lim_{N \rightarrow \infty} -\frac{1}{\beta} \log Z_J.$$

This task might look at a first glance as a hopeless one since the partition function  $Z_J$  depends on quenched random variables. How is it possible to compute  $F_J$  while keeping the random couplings  $J_{ij}$  fixed in the Hamiltonian? And even if it was possible, how general will be the result? I.e., will it depend on the specific disorder instance, namely the choice of the coefficients  $\{J_{ij}\}_{i<j}$ , or will be *universal* with respect to any choice of the coefficients? The solution to all this problems/questions comes in the form of the *self-averaging* property of the free energy with respect to the disorder instance. The question on how relevant is the dependence of  $F_J$  on  $\{J_{ij}\}_{i<j}$  is indeed a well posed one: considered as a function of random couplings,  $F_J$  is itself a fluctuating random variable. Two different choices of the random coupling sets, which in practice

correspond to *experiments* on two different samples, let us label them as  $J^{(0)} = \{J_{ij}^{(0)}\}_{i<j}$  and  $J^{(1)} = \{J_{ij}^{(1)}\}_{i<j}$ , yields in general two different values of the free-energy, i.e.,

$$(7.96) \quad F_{J^{(0)}} \neq F_{J^{(1)}}.$$

The self-averaging property of the free energy tells us precisely that the difference between these two values is irrelevant in the thermodynamic limit, i.e., the standard deviation of  $F_J$  is negligible with respect to its average value. By denoting the average of  $F_J$  with respect to the probability distribution of random couplings as

$$(7.97) \quad \overline{F_J} = \int_{-\infty}^{\infty} \prod_{i<j} dJ_{ij} P(J_{ij}) F_J,$$

and the standard deviation as

$$(7.98) \quad \sigma(F_J) = \sqrt{(\overline{F_J^2}) - (\overline{F_J})^2}$$

we have that the self-averaging property reads in formula as

$$(7.99) \quad \lim_{N \rightarrow \infty} \frac{\sigma(F_J)}{\overline{F_J}} \sim \frac{1}{\sqrt{N}}$$

The self-averaging property of the free energy is thus crucial: in practice it tells us that in the thermodynamic limit, *up to negligibly small fluctuations*, any choice of the disordered couplings yields the same result. From the point of view of our calculation it means that in the thermodynamic limit we can *average* over the disorder instances:

$$(7.100) \quad \lim_{N \rightarrow \infty} -\frac{1}{N\beta} \log Z_J = \lim_{N \rightarrow \infty} -\frac{1}{N\beta} \overline{\log Z_J} \equiv f,$$

where  $f_J = F_J/N$  is the free energy per spin.

As for the RFIM, here it is useful to use the replica trick, here in the version based on the math identity  $\log x = \lim_{n \rightarrow 0} (x^n - 1)/n$ . Hence, we focus on  $\overline{Z_J^n}$  rather than  $\overline{\log Z_J}$ . For  $n$  replicas indexed by  $\alpha$  or  $\beta$  (with  $n$  remaining integer till the very last step of the calculation), we have

$$(7.101) \quad \begin{aligned} \overline{Z_J^n} &= \int_{-\infty}^{\infty} \prod_{i<j} dJ_{ij} P(J_{ij}) (Z_J)^n \\ &= \int_{-\infty}^{\infty} \prod_{i<j} dJ_{ij} P(J_{ij}) \sum_{\{S_1^\alpha, \dots, S_N^\alpha | \alpha=1, \dots, n\}} \exp \left\{ \beta \sum_{\alpha=1}^n \sum_{i<j} J_{ij} S_i^\alpha S_j^\alpha \right\} \end{aligned}$$

This formula contains a nice linear contribution of random  $J_{ij}$ 's. In (7.101) replicas share the same disorder but are uncoupled (no  $\alpha$  and  $\beta$  together) and spins are coupled.

For a single  $J_{ij}$  with an explicit version of  $P(J)$ , the resulting Gaussian integral yields

$$(7.102) \quad \int_{-\infty}^{\infty} dJ_{ij} \exp \left\{ -\frac{N}{2\delta^2} (J_{ij})^2 + \beta J_{ij} \sum_{\alpha=1}^n S_i^\alpha S_j^\alpha \right\} = \exp \left\{ \frac{\beta^2 \delta^2}{2N} \sum_{\alpha, \beta=1}^n S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta \right\}$$

( $\beta$  as an index of a replica should be not confused with the inverse temperature). Note that this average over disorder is coupling replicas. Moreover, it is decoupling spins because  $\sum_{i<j} \approx$

$\frac{1}{2} \sum_{i,j}$  and back to the full (7.101) this gives

$$\begin{aligned} \overline{Z^n} &= \sum_{\{S_1^\alpha, \dots, S_N^\alpha | \alpha=1, \dots, n\}} \exp \left\{ \frac{\beta^2 \delta^2}{2N} \sum_{\alpha, \beta=1}^n \sum_{i < j}^N S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta \right\} \\ &= \exp \left\{ \frac{nN\beta^2 \delta^2}{4} \right\} \sum_{\{S_1^\alpha, \dots, S_N^\alpha | \alpha=1, \dots, n\}} \exp \left\{ \frac{\beta^2 \delta^2}{2N} \sum_{\alpha < \beta}^n \left( \sum_{i=1}^N S_i^\alpha S_i^\beta \right)^2 \right\}, \end{aligned} \quad (7.103)$$

which contains no  $J$ 's and displays only single site spins  $S_i$ . In order to obtain the second line from the first one of Eq. (7.103) we played a little bit with the summation indices and made an approximation which is valid only in the large  $N$  limit. For the double summation over (latin) spin indices we used

$$\begin{aligned} \sum_{i < j}^N S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta &= \frac{1}{2} \left( \sum_{i,j=1}^N S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta - N \right) \\ &\cong \frac{1}{2} \left( \sum_{i=1}^N S_i^\alpha S_i^\beta \right) \left( \sum_{j=1}^N S_j^\alpha S_j^\beta \right) = \frac{1}{2} \left( \sum_{i=1}^N S_i^\alpha S_i^\beta \right)^2, \end{aligned} \quad (7.104)$$

where we have dropped the term  $N$  because it is subleading with respect to the double sum, which contains  $\mathcal{O}(N^2)$  terms. We can thus write:

$$\begin{aligned} \sum_{\alpha, \beta=1}^n \sum_{i < j}^N S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta &\cong \sum_{\alpha, \beta=1}^n \frac{1}{2} \left( \sum_{i=1}^N S_i^\alpha S_i^\beta \right)^2 \\ &= \sum_{\alpha=1}^n \frac{1}{2} \left( \sum_{i=1}^N S_i^\alpha S_i^\alpha \right)^2 + \frac{1}{2} \sum_{\alpha \neq \beta}^n \left( \sum_{i=1}^N S_i^\alpha S_i^\beta \right)^2 \\ &= \frac{nN}{2} + \sum_{\alpha < \beta}^n \left( \sum_{i=1}^N S_i^\alpha S_i^\beta \right)^2, \end{aligned} \quad (7.105)$$

which is what needed to go from the first to the second line of Eq. (7.103). Note that the argument used to neglect the diagonal elements of the double summation  $\sum_{i,j}$ , i.e. that they are  $N$  terms with respect to an overall amount of  $\mathcal{O}(N^2)$  terms, cannot be applied to the double summation over replica indices  $\sum_{\alpha, \beta}$ , where the diagonal elements are  $n$  and the off-diagonal ones are  $n(n-1)$ , for the simple reason that we are going to take the limit  $n \rightarrow 0$  and not the limit  $n \rightarrow \infty$ , as we did for number of spins in the systems: in the case of replica indices the diagonal elements do not represent a subleading contribution.

Let us spend few words of comment on the last two equations: it is only thanks to the fact that in the original Hamiltonian the summation  $\sum_{i < j}$  goes over *all independent pairs of indices*, i.e., over  $\mathcal{O}(N^2)$  terms, that we could write the double summation typical of any model with a two-body interaction as a single summation squared. Models where this kind of simplification is possible are usually known as *mean-field* models, i.e., models where, due to the large number of mutual interactions between the degrees of freedom, one is able, after a certain number of manipulations, to write the free-energy of the systems in terms of an order parameter which carries no spatial index (the latin index  $i$  in the present case). This means that in mean-field models any information and/or dependence on spatial dimensions is lost. Such models yield thus only an *approximate description* of real physical model—try to figure out for a moment the difference between our SK model and a disordered Ising model on a 2D or a 3D lattice—but enjoy a very nice feature: they can be solved exactly. The possibility to unfold the double



summation as shown above is thus crucial because this allows us to introduce a *global order parameter* of the kind

$$(7.106) \quad q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^N S_i^\alpha S_i^\beta.$$

We will comment further on the meaning of  $q_{\alpha\beta}$  in what follows, here let us just note that if we plug the definition  $\sum_{i=1}^N S_i^\alpha S_i^\beta = Nq_{\alpha\beta}$  into (7.103) we get for the exponential term of the partition function

$$(7.107) \quad \exp \left\{ \frac{N\beta^2\delta^2}{2} \sum_{\alpha<\beta}^n q_{\alpha\beta} \right\},$$

which puts in evidence that the argument of the exponential is an extensive function, i.e., it is proportional to the number of spin  $N$  in the system, and that it depends only on a global order parameter,  $q_{\alpha\beta}$ . Nevertheless, this naive replacement of  $\sum_{i=1}^N S_i^\alpha S_i^\beta$  with  $q_{\alpha\beta}$  is mathematically wrong, because the spins  $S_i^\alpha$  are summation variables inside the partition function and we must do a proper change of variables, like in an integral. The correct way to introduce the order parameter  $q_{\alpha\beta}$  is by means of the Hubbard-Stratonovich transformation that we have already met discussing the Random-Field Ising Model and the Hopfield model. By doing this, the quantity  $q_{\alpha\beta}$  appears simply as an auxiliary variable to linearize the squared sum  $(\sum_{i=1}^N S_i^\alpha S_i^\beta)^2$ ; we will demonstrate later that, in the large- $N$  limit, the definition of  $q_{\alpha\beta}$  is really the one given in (7.106).

In the following we adopt the shorthand notation

$$(7.108) \quad \sum_{\{S_1^\alpha, \dots, S_N^\alpha | \alpha=1, \dots, n\}} \rightarrow \sum_{\S}.$$

As we have said, the square in (7.103) is thus unfolded by a HS transformation,

$$(7.109) \quad \overline{Z}_J^n \approx \sum_{\S} \int_{-\infty}^{\infty} \prod_{\alpha<\beta} dq_{\alpha\beta} \underbrace{\exp \left\{ -\frac{N\beta^2\delta^2}{2} \sum_{\alpha<\beta} q_{\alpha\beta}^2 \right\}}_{[1]} \underbrace{\exp \left\{ \beta^2\delta^2 \sum_{\alpha<\beta} q_{\alpha\beta} \sum_{i=1}^N S_i^\alpha S_i^\beta \right\}}_{[2]}$$

At this step, It is worth noting that in the first line of (7.103) we had a double summation over replica indices of the kind  $\sum_{\alpha, \beta=1}^n$  which we replaced with  $2 \sum_{\alpha<\beta}^n$ , to that only independent couple of indices were effectively considered. Although we still have to prove the identity in (7.106), from it we can argue quite naturally that the matrix  $q_{\alpha\beta}$  is symmetric, i.e.  $q_{\alpha\beta} = q_{\beta\alpha}$ , so that only half of its off-diagonal elements are independent integration variables. The appearance of terms linear in the index  $i$  allows to factorize the trace operator. Focusing on the

second term [2],

$$\begin{aligned}
& \sum_{\S} \exp \left\{ \beta^2 \delta^2 \sum_{\alpha < \beta} q_{\alpha\beta} \underbrace{\sum_{i=1}^N (S_i^\alpha S_i^\beta)}_{\text{identical for all } i} \right\} \\
&= \prod_{i=1}^N \left[ \sum_{\S} \exp \left\{ \beta^2 \delta^2 \sum_{\alpha < \beta} q_{\alpha\beta} (S_i^\alpha S_i^\beta) \right\} \right] \\
&= \left[ \sum_{\S} \exp \left\{ \beta^2 \delta^2 \sum_{\alpha < \beta} q_{\alpha\beta} S^\alpha S^\beta \right\} \right]^N \\
&\equiv \left[ \sum_{\S} \exp \{L(q_{\alpha\beta})\} \right]^N \\
&= \left[ \text{Tr} e^{L(q_{\alpha\beta})} \right]^N \\
(7.110) \quad &= \exp \left\{ N \log \left[ \text{Tr} e^{L(q_{\alpha\beta})} \right] \right\}
\end{aligned}$$

with operator  $L(q_{\alpha\beta}) = \beta^2 \delta^2 \sum_{\alpha < \beta} q_{\alpha\beta} S^\alpha S^\beta$ . The form of (7.110) is ready for the not-so-unexpected saddle point approximation, as is the full formula for the partition function,

$$\begin{aligned}
\overline{Z}_J^n &= \exp \left\{ nN\beta^2\delta^2/4 \right\} \int_{-\infty}^{\infty} \prod_{\alpha < \beta} dq_{\alpha\beta} \\
&\quad \exp \left\{ -\frac{N\beta^2\delta^2}{2} \sum_{\alpha < \beta} q_{\alpha\beta}^2 + N \log \left[ \text{Tr} e^{L(q_{\alpha\beta})} \right] \right\} \\
(7.111) \quad &= \int_{-\infty}^{\infty} \prod_{\alpha < \beta} dq_{\alpha\beta} e^{-nNA[q_{\alpha\beta}]}
\end{aligned}$$

with the function  $A[q_{\alpha\beta}]$  defined as

$$(7.112) \quad A[q_{\alpha\beta}] = \underbrace{-\frac{\beta^2\sigma^2}{4} + \frac{\beta^2\delta^2}{2n} \sum_{\alpha < \beta} q_{\alpha\beta}^2}_{\text{energetic}} - \underbrace{\frac{1}{n} \log \left[ \text{Tr} e^{L(q_{\alpha\beta})} \right]}_{\text{entropic}},$$

where we have emphasized which are the *energetic* and the *entropic* contributions to  $A[q_{\alpha\beta}]$ . Note the  $1/n$  factor embedded in  $A$ .

At this point we are not at all done, but we can say that the remaining part of the calculation is only technical: we must find the correct ansatz for the structure of the matrix  $q_{\alpha\beta}$  and take the limit  $n \rightarrow 0$  in the appropriate way. This last part of the work is usually the subject of graduate courses and can be found in PhD summer schools lecture-notes like [“*Replica Theory and Spin Glasses*”, F. Morone, F. Caltagirone, E. Harrison, G. Parisi, *arXiv:1409.2722*]. The purpose of this lecture was just to show that the calculation of the SK free-energy can be cast as a variational problem where the variational parameter, which is, not by chance, the order parameter of the systems, is a matrix. Indeed what we are left with in (7.111) is just the integration over the matrix elements  $q_{\alpha\beta}$ , of which, due to the overall prefactor  $N$ , we can get rid with a saddle-point approximation. That is, we write

$$(7.113) \quad \overline{Z}_J^n = \int_{-\infty}^{\infty} \prod_{\alpha < \beta} dq_{\alpha\beta} e^{-nNA[q_{\alpha\beta}]} \approx \exp \left\{ -nNA[q_{\alpha\beta}^*] \right\},$$

where the matrix elements  $q_{\alpha\beta}^*$  are the solution of the saddle-point equations

$$(7.114) \quad \frac{\partial A}{\partial q_{\alpha\beta}} = 0, \quad \forall q_{\alpha\beta} \quad \Longrightarrow \quad q_{\alpha\beta}^*$$

To check the correctness of the calculation when plugging an ansatz for  $q_{\alpha\beta}^*$  in  $A$ , one must always take care that in all terms of  $A$  which depend on  $q_{\alpha\beta}$  a prefactor  $n$  can be singled out, so that it simplifies with the  $1/n$  outside brackets on the right-hand side of (7.112). The final step to compute the free energy per spin amounts to the switching of the two limits  $N \rightarrow \infty$  and  $n \rightarrow 0$ , which allows us to write:

$$(7.115) \quad \begin{aligned} f &= \lim_{\substack{N \rightarrow \infty \\ n \rightarrow 0}} -\frac{1}{N\beta} \frac{\overline{Z^n} - 1}{n} \\ &= \lim_{\substack{n \rightarrow 0 \\ N \rightarrow \infty}} -\frac{1}{nN\beta} (\overline{Z^n} - 1) \\ &= \lim_{\substack{n \rightarrow 0 \\ N \rightarrow \infty}} -\frac{1}{nN\beta} (1 - nNA[q_{\alpha\beta}^*] - 1) \\ f &= \frac{1}{\beta} A[q_{\alpha\beta}^*] \end{aligned}$$

This swap of limits is a risky step that everybody is normally willing to take because mathematicians then cover it rigorously. To recover the notion of overlap in  $q_{\alpha\beta}$ , note that at some point after the HS transformation we had (7.109), which we rewrite as

$$(7.116) \quad \begin{aligned} \overline{Z_j^n} &= \exp \{nN\beta^2\delta^2/4\} \sum_{\S} \int_{-\infty}^{\infty} \prod_{\alpha < \beta} dq_{\alpha\beta} \\ &\quad \exp \left\{ -\frac{N\beta^2\delta^2}{2} \sum_{\alpha < \beta} q_{\alpha\beta}^2 + \beta^2\delta^2 \sum_{\alpha < \beta} q_{\alpha\beta} \sum_{i=1}^N S_i^\alpha S_i^\beta \right\} \\ &= \exp \{nN\beta^2\delta^2/4\} \sum_{\S} \int_{-\infty}^{\infty} \prod_{\alpha < \beta} dq_{\alpha\beta} \exp \{-Nu(q_{\alpha\beta}, S_1^\alpha, \dots, S_N^\alpha)\} \end{aligned}$$

with  $u$  defined as

$$(7.117) \quad u(q_{\alpha\beta}, S_1^\alpha, \dots, S_N^\alpha) = \beta^2\delta^2 \left[ \frac{1}{2} \sum_{\alpha < \beta} q_{\alpha\beta}^2 - \sum_{\alpha < \beta} q_{\alpha\beta} \frac{1}{N} \sum_{i=1}^N S_i^\alpha S_i^\beta \right]$$

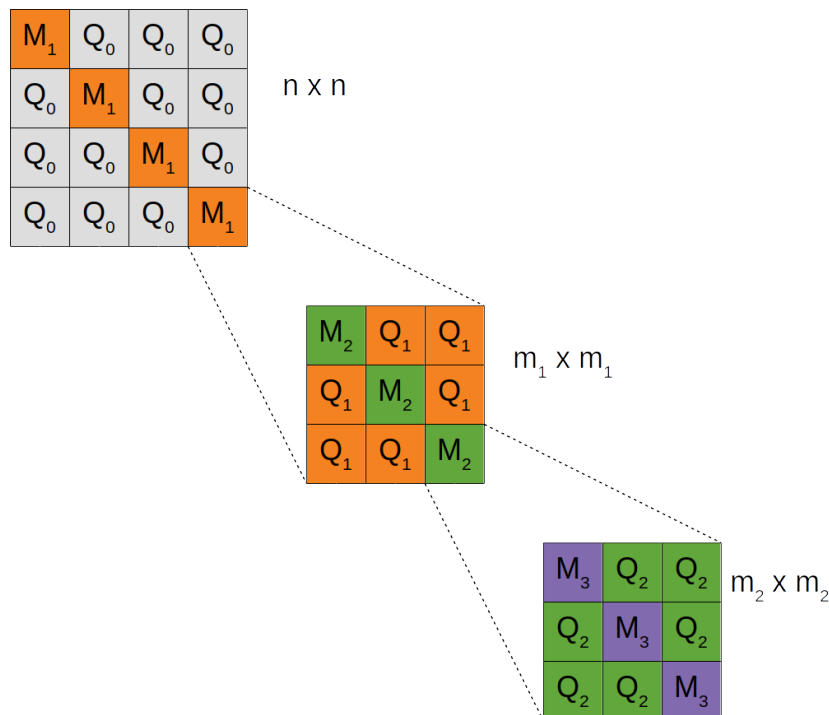
The saddle point requires

$$(7.118) \quad \frac{\partial u}{\partial q_{\alpha\beta}} = 0, \quad \forall q_{\alpha\beta} \quad \Longrightarrow \quad q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^N S_i^\alpha S_i^\beta$$

This  $q_{\alpha\beta}$  is the overlap, i.e., again the scalar product between spins of two replicas (in the Hopfield model it was between a replica and a pattern). Therefore, the physical meaning of  $q_{\alpha\beta}$  is the quantification of replicas similarity. Due to this,  $q_{\alpha\beta}$  must be a real symmetric matrix.

We cannot give all the details of the calculation of the SK behavior. It turns out that the model has a phase transition of the second order at a critical temperature  $T_c$ , between and ergodic phase at high temperature and a non-ergodic phase at low  $T$ . In the latter case, the phase space of all possible spin configurations splits into disjoint ergodic components. A realization of the system sits in one of these isolated pieces of the phase space forever if the temperature stays low.

There remains to choose the best ansatz for  $q_{\alpha\beta}$ . A possibility is the *replica symmetric ansatz*:  $q_{\alpha\alpha} = 1$  and  $q_{\alpha\beta} = q_0$  for  $\alpha \neq \beta$ . This ansatz means that a replica is maximally identical to itself while equally dissimilar to all other ones. It works well for  $T > T_c$ , where all states are



**Figure 4.** Sketch of the hierarchical overlap of replicas in the SK model at low temperature in the non-ergodic phase. The matrix in the top-left corner is the overlap matrix  $q_{\alpha\beta}$ . The diagram should be continued iterating indefinitely the magnifications.

more or less equally probable, but in the non-ergodic phase it does not capture the complexity of the phase space.

At low temperature the SK model displays a fascinating hierarchy of replica similarities, which is summarized by a label: *full replica symmetry breaking*. It is better to think of  $n$  very large, even if the  $n \rightarrow 0$  is mandatory at the end. As we have said, according to a very reasonable physical intuition, the matrix  $q_{\alpha\beta}$  must be a symmetric one. Furthermore, let us notice that each row of the matrix  $q_{\alpha\beta}$  represents all the possible values of the overlap between a given replica of the system, say  $\alpha$ , with other replicas of the system, say  $\beta \neq \alpha$ . Since we ask that no replica is privileged with respect to the others, it is also reasonable to ask that all the elements appearing in a row of the matrix  $q_{\alpha\beta}$  also appear in all the others, up to a permutation. The only degree of freedom we are left with is thus the rule to assign the matrix elements in a row. The mesmerizing discovery of Parisi in the late '70 was that the only symmetry which is broken at the critical temperature  $T_c$  and represents the breaking of ergodicity is the *permutation symmetry* of the matrix elements within a single row of the matrix  $q_{\alpha\beta}$ , i.e., *different replicas might have different overlaps*. In this perspective let us fix the row index of the matrix element  $q_{\alpha\beta}$  in order to parameterize the elements on a row with only one index:  $q_{1i} = q_i$ , where  $i$  runs from 1 to  $n$  and we have dropped the row index. The way permutation symmetry is broken is decided by the assignment rule:

$$(7.119) \quad i \longrightarrow q_i$$

Once this rule is fixed for one row of the matrix, the structure of the other rows follows, since they are just a permutation of the first. This leads to the so-called *Parisi's matrix*, which we briefly discuss in what follows.

A large  $n$  allows to introduce a sequence of similarity levels. In the first stage of symmetry breaking, the  $n \times n$  matrix  $q_{\alpha\beta}$  is represented as composed of  $m_1 \times m_1$  submatrices  $M_1$  and  $Q_0$  (Figure 4). The matrix  $Q_0$  is fully composed of elements equal to  $q_0$ , the typical lowest overlap between replicas. The matrix  $M_1$  is found  $n/m_1$  times on the diagonal of  $q_{\alpha\beta}$ .

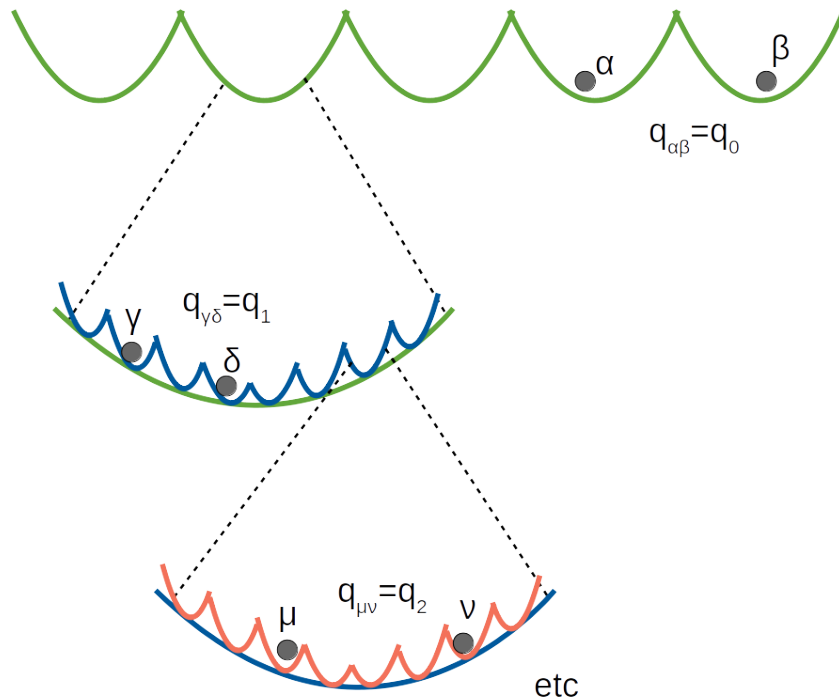
At a second stage, by inspecting the structure of  $M_1$ , one finds that it resembles that of  $q_{\alpha\beta}$  in the first stage. It is composed of submatrices  $M_2$  and  $Q_1$  of size  $m_2 \times m_2$ , where  $Q_1$  is filled by elements  $q_1 > q_0$  while  $M_2$ 's are sequenced on the diagonal of  $M_1$ . The story goes on like this, forming a sequence  $q_0 < q_1 < q_2 < q_3 < \dots < q_k$  and correspondingly  $n > m_1 > m_2 > m_3 > \dots > m_k$ . In order to reconnect with the discussion above on the elements of a single row, let us notice that a  $k$ -steps breaking of the permutation symmetry between replicas corresponds to the assignment of  $k$  different values to the  $n$  elements of a row for the matrix  $q_{\alpha\beta}$ . As long as  $k$  is finite the *number of elements*  $m_i$  in the row (with  $1 < i < n$ ) which take the value  $q_i$  can be interpreted as being proportional to the *probability* that two replicas have the overlap  $q_i$ .

A question is then immediately in order: how to recognize which is the the correct level  $k$  of breaking of the replica permutation symmetry? And why a breaking should be considered at all?

The first thing to say is that the replica-symmetric ansatz, i.e., the assumption that all the off-diagonal elements of  $q_{\alpha\beta}$  are identical ( $q_{\alpha\beta} = q$  for all  $\alpha$  and  $\beta$  such that  $\alpha \neq \beta$ ), leads to a negative entropy at zero temperature:  $S(0) = -\frac{1}{2\pi} \approx -0.17$ . This is clearly a wrong result because we have discrete variables and the entropy has a unique and unequivocal meaning: it is the logarithm of the number  $\mathcal{N}$  of microstates accessible at a given temperature and since  $\mathcal{N} \geq 1$  we have  $S = \log \mathcal{N} \geq 0$ . If one then tries to compute the free-energy assuming one level of breaking of the permutation symmetry between replicas, i.e., to subdivide the  $n \times n$  matrix in blocks of size  $m_1$  and with possible value of the overlap  $q_1$  and  $q_0$ , obtaining the correct value of  $q_0$ ,  $q_1$  and  $m_1$  from the extremization of the free-energy, one finds that at  $T = 0$  the entropy is still negative but *less* negative, i.e. with the *one-step-replica-symmetry-breaking* ansatz it takes the value  $S(T = 0) = -0.1$ . Although the result is still incorrect, this tells us that we are moving in the right direction, because the *negative* entropy has become less negative, hence less wrong. We will discuss in the next lecture a model where the assumption of only one step of replica symmetry breaking is the correct one: the  $p$ -spin model, which has two main differences with the SK model presented here, continuous variables and non-linear interactions. By increasing further the number of levels  $k$  at which the symmetry between replicas can be broken in the SK model, one obtains a zero-temperature entropy which is closer and closer to zero. This suggested to consider the possibility of an *infinite number of breakings* of the permutation symmetry between replicas, which, at least for the SK model, turns out to be the correct assumption. Before commenting further on this, let us just quote the formal and unequivocal criterion to discriminate whether the assumption of *breaking at "k" levels* is right or wrong. The criterium to say whether a saddle-point solution is good is that it must be *stable*, namely it must be a *minimum* of the free energy. The stability of the stationary point is decided by the eigenvalues spectrum of the Hessian

$$(7.120) \quad M_{(\alpha\beta),(\gamma\delta)} = \frac{\partial^2 A}{\partial q_{\alpha\beta} \partial q_{\gamma\delta}}$$

It is only when this Hessian matrix has all the eigenvalues positive that we have a stable solution. If one computes the eigenvalues of  $M_{(\alpha\beta),(\gamma\delta)}$  one finds that the smallest one, the *replicon*, is negative for any finite number  $k$  of breakings. In the SK model any saddle-point solution with a finite number of breakings is *unstable*. The name *replicon* comes from the famous paper of J.R.L de Almeida and D.J. Thouless where the (un-)stability of the replica-symmetric solution of the SK model was studied for the first time [“*Stability of the Sherrington-Kirkpatrick solution of a spin glass model*”, J.R.L. de Almeida and D.J. Thouless, *J. Phys. A* **13** (1978)] (D.J Thouless was precisely the same guy awarded with Nobel prize in 2016 for the Kosterlitz-Thouless transition). For the details of all this analysis we refer the curious student to the literature quoted at the beginning of this lecture. The final outcome is, as anticipated, that the correct ansatz sends  $k \rightarrow \infty$ , which is called the *full-replica-symmetry-breaking* (full-RSB) ansatz. The infinite number of elements in the sequence of overlaps  $q_1 < \dots < q_k$  suggested as well the title of the paper where the full-RSB was proposed for the first time [“*Infinite number of order parameters*”



**Figure 5.** Sketch of the hierarchical energy landscape of the SK model at low temperature in the non-ergodic phase:  $q_0 < q_1 < q_2 < \dots$

for *spin-glasses*, Giorgio Parisi, *Phys. Rev. Lett.* **43**, 1754 (1979)].

Such infinite number of order parameters reflects the hierarchical multi-valley structure of the SK energy landscape at low  $T$ , as sketched in Figure 5, with an infinite sequence of minima nested into others. Clearly, by zooming out the details of this *fractal* structure of nested minima, we find that the typical overlap between configurations trapped within the same minimum is larger the smaller is the scale at which we have zoomed the landscape, as shown in Fig. 5.

Our last comment is on the  $n \rightarrow 0$  limit, on which we did not spend (on purpose) a lot of words so far. We warn the curious students that this is a highly a technical part, which might be challenging for a naive intuition of what is going on. In any case, all details are given in the references at the beginning of the lecture.

When  $k \rightarrow \infty$  and at the same time  $n \rightarrow 0$  one has to plug an infinite number of different choices  $q_1 < \dots < q_k$  into a zero dimensional matrix. It turns out that the most convenient thing to do ( ... and it works!) is to replace the numerable sequence  $q_1 < \dots < q_k$  with a continuous function

$$(7.121) \quad q(x) : [0, 1] \rightarrow [0, 1],$$

where the role played by the subscript index  $i$  in  $q_i$  has been taken up by the real variable  $x$ , of which the overlap  $q$  becomes a function. A function  $q(x)$  in the unit interval  $[0, 1]$  is an element of an infinite-dimensional space, i.e., there is an infinite number of choices to define it: this is OK, because it is in fair agreement with the infinite number of order parameters we were after. Then, it can be shown (see the references) that the role played by the *breaking parameter*  $m_k$ , i.e., that of representing the probability to find the overlap  $q_k$  between two replicas, is played in this sort of continuum limit by the variable  $x$  in the domain of  $q(x)$ . In particular it can be shown that the function  $q(x) : x \in [0, 1] \rightarrow q \in [0, 1]$  has a well defined inverse

$$(7.122) \quad x[q] : q \in [0, 1] \rightarrow x \in [0, 1],$$

which can be identified as the *cumulative distribution of the overlap*, i.e., the probability density distribution  $P(q)$  of the overlap turns out to be

$$(7.123) \quad P(q) = \frac{dx}{dq}$$

To conclude, let us just quote the final result, i.e., the form of the free-energy per spin when the two limits of an infinite number of breakings,  $k \rightarrow \infty$ , and of zero size of the overlap matrix,  $n \rightarrow 0$ , are taken:

$$(7.124) \quad \beta f = -\frac{\beta^2 \sigma^2}{4} \left[ 1 + \int_0^1 dx q(x)^2 - 2q(1) \right] - \int_{-\infty}^{\infty} \frac{du}{\sqrt{2\pi}} e^{-u^2/2} f_0(0, u\sqrt{q(0)}),$$

where the function  $f_0$  is the solution of the so-called *Parisi equation*,

$$(7.125) \quad \frac{\partial f_0(x, h)}{\partial x} = -\frac{\sigma^2}{2} \frac{dq}{dx} \left[ \frac{\partial^2 f_0}{\partial h^2} + x \left( \frac{\partial f_0}{\partial h} \right)^2 \right],$$

where  $h$  is a magnetic field which has to be in general taken into account in the Hamiltonian, i.e.,  $H = -\sum_{i<j} J_{ij} S_i S_j - h \sum_{i=1}^N S_i$ . In all the calculations presented in this lectures we set  $h = 0$  for simplicity, but the generalization to the case of  $h > 0$  is straightforward.

To conclude, let us just try to recognize the origin of the terms of the full-RSB free energy in (7.125). It is quite easy to recognize the contribution of the *energetic* term of (7.112):

$$(7.126) \quad -\frac{\beta^2 \sigma^2}{4} + \frac{\beta^2 \delta^2}{2n} \sum_{\alpha<\beta} q_{\alpha\beta}^2 \implies -\frac{\beta^2 \sigma^2}{4} \left[ 1 + \int_0^1 dx q(x)^2 - 2q(1) \right].$$

Just recall that  $\sum_{\alpha<\beta} = n(n-1)/2$  and that all the  $n$  rows of the matrix  $q_{\alpha\beta}$  are identical up to a permutation, so that it is not difficult to believe that in the limit  $n \rightarrow 0$  one has

$$(7.127) \quad \sum_{\alpha<\beta} q_{\alpha\beta}^2 \approx n(n-1) \int dq q(x)^2 \rightarrow -n \int dq q(x)^2$$

Much less recognizable—indeed it requires several intermediate steps and tricks to be derived—is the connection of the entropic contribution with its original form at finite  $n$ :

$$(7.128) \quad \frac{1}{n} \log \left[ \text{Tr} e^{L(q_{\alpha\beta})} \right] \approx \int_{-\infty}^{\infty} \frac{du}{\sqrt{2\pi}} e^{-u^2/2} f_0(0, u\sqrt{q(0)})$$

## 7.5. Spherical p-spin model

In the previous lecture we have studied the Sherrington-Kirkpatrick (SK) model, which is the mean-field version of the disordered Ising model. The most puzzling result is that the correct way to represent the breaking of ergodicity in the SK model is by an infinite sequence of breakings of the permutation symmetry between replicas, which, on physical grounds, corresponds to a low temperature phase characterized by fractal free-energy landscape with an infinite hierarchy of minima nested into each other.

The situation is in a sense much simpler in the so called spherical  $p$ -spin model, another disordered model with quenched random couplings characterized by continuous *spins* and non-linear couplings, i.e., in the Hamiltonian it is assumed  $p > 2$  for the order of the nonlinear  $p$ -body interaction:

$$(7.129) \quad H(\sigma) = - \sum_{i_1 > \dots > i_p = 1} J_{i_1, \dots, i_p} \sigma_{i_1} \dots \sigma_{i_p}$$

where the  $N$  continuous spin variables are subject to the global *spherical* constraint

$$(7.130) \quad \sum_{i=1}^N \sigma_i^2 = N,$$

Each of the quenched couplings  $J_{i_1, \dots, i_p}$  follows a Gaussian distribution

$$(7.131) \quad p(J) = \frac{N^{\frac{p-1}{2}}}{\sqrt{p!}\pi} \exp \left\{ -\frac{J^2 N^{p-1}}{p!} \right\},$$

where, as we are going to show, the scaling of the variance with  $N$  is chosen precisely as to have extensive free-energy.

The peculiarity of this model, attracting a lot of interest since the end of the the 80s, is its low-temperature ergodicity-breaking transition characterized by a one-step replica-symmetry-breaking ansatz at the critical temperature  $T_K$ , which is known for this model as the Kauzmann temperature. At  $T_K$  phase space splits many disjoint ergodic components, each corresponding to a minimum of the free energy. In the large  $N$  limit there are only two possibilities: two configurations of the system sampled with the Boltzmann probability

$$(7.132) \quad P_J(\sigma) = e^{-\beta H_J[\sigma]} \delta \left( N - \sum_{i=1}^N \sigma_i^2 \right)$$

can be either belonging to the same ergodic component, i.e., the basin of the same free-energy minimum, hence their overlap is  $q_1 > 0$ , or belonging to different minima, so that their overlap is  $q_0 = 0$ . As we are going to see the probability to have overlap  $q_0$  or  $q_1$  depends on the breaking parameter  $m$ , which is of course a real number in the interval  $m \in [0, 1]$ . Within the large- $N$  saddle-point approximation there is no other option, not a possible continuum degree of similarity  $q(x)$  like in the SK model, no structure of nested minima. Also, the different minima of the free-energy are separated by extensive, i.e.,  $\sim N$ , free-energy barriers, at variance with the SK model.

**7.5.1. Free-energy calculation.** Much in the same way as in the SK model, also in the  $p$ -spin model the free-energy is *self-averaging*, so that it can be computed as the result of a saddle-point calculation of the replicated partition function:

$$(7.133) \quad f = \lim_{N \rightarrow \infty} -\frac{1}{N\beta} \overline{\log Z} = \lim_{\substack{n \rightarrow 0 \\ N \rightarrow \infty}} -\frac{1}{nN\beta} (\overline{Z^n} - 1)$$

Let us now consider the case  $p = 3$  till some point of the calculation because the formulae are shorter, but please keep in mind that the steps are identical for any  $p$  and so do the result. We thus assume the interaction

$$(7.134) \quad H = - \sum_{i < j < k} J_{ijk} \sigma_i \sigma_j \sigma_k,$$

The partition function reads as

$$(7.135) \quad \begin{aligned} \overline{Z^n} &= \int_{-\infty}^{\infty} \prod_{i < j < k} dJ_{ijk} P(J_{ijk}) \left[ \int_{-\infty}^{\infty} \prod_{i=1}^N d\sigma_i e^{\beta \sum_{i < j < k} J_{ijk} \sigma_i \sigma_j \sigma_k} \delta \left( N - \sum_{i=1}^N \sigma_i^2 \right) \right]^n \\ &= \int_{-\infty}^{\infty} \prod_{i < j < k} dJ_{ijk} P(J_{ijk}) \int_{-\infty}^{\infty} \mathcal{D}\sigma e^{\beta \sum_{i < j < k} J_{ijk} \sum_{\alpha=1}^n \sigma_i^\alpha \sigma_j^\alpha \sigma_k^\alpha}, \end{aligned}$$

where we have used the symbol

$$(7.136) \quad \mathcal{D}\sigma = \prod_{i=1}^N \prod_{\alpha=1}^n d\sigma_i^\alpha \prod_{\alpha=1}^n \delta \left( N - \sum_{i=1}^N (\sigma_i^\alpha)^2 \right),$$



to denote, with a compact notation, an integration over spin variables satisfying the spherical constraint for each replica  $\alpha$ . It is more convenient to leave the spherical constraint hidden in the integration measure symbol.

In the Hamiltonian there is a number  $\sum_{i<j<k} = N(N-2)(N-3)/3!$  of independent triplets of interacting spins, and we have a corresponding number of integrations over the disorder coefficients  $J_{ijk}$  to do. Each of them is a simple Gaussian integral, which, dropping prefactors, is

$$\begin{aligned}
& \int_{-\infty}^{\infty} dJ_{ijk} \exp \left\{ -J_{ijk}^2 \frac{N^{p-1}}{p!} + J_{ijk} \beta \sum_{\alpha=1}^n \sigma_i^\alpha \sigma_j^\alpha \sigma_k^\alpha \right\} = \\
& = \exp \left\{ \frac{\beta^2 p!}{4N^{p-1}} \left( \sum_{\alpha=1}^n \sigma_i^\alpha \sigma_j^\alpha \sigma_k^\alpha \right)^2 \right\} \\
(7.137) \quad & = \exp \left\{ \frac{\beta^2 p!}{4N^{p-1}} \sum_{\alpha, \beta=1}^n \sigma_i^\alpha \sigma_i^\beta \sigma_j^\alpha \sigma_j^\beta \sigma_k^\alpha \sigma_k^\beta \right\},
\end{aligned}$$

from which, by collecting all the  $\mathcal{O}(N^3)$  integrations and by recalling that

$$(7.138) \quad p! \sum_{i<j<k}^N \approx \sum_{ijk}^N$$

we get

$$\begin{aligned}
\overline{Z^n} &= \int_{-\infty}^{\infty} \mathcal{D}\sigma \exp \left\{ \frac{\beta^2 p!}{4N^{p-1}} \sum_{i<j<k} \sum_{\alpha, \beta=1}^n \sigma_i^\alpha \sigma_i^\beta \sigma_j^\alpha \sigma_j^\beta \sigma_k^\alpha \sigma_k^\beta \right\} \\
&= \int_{-\infty}^{\infty} \mathcal{D}\sigma \exp \left\{ \frac{\beta^2}{4N^{p-1}} \sum_{\alpha, \beta=1}^n \left( \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta \right) \left( \sum_{j=1}^N \sigma_j^\alpha \sigma_j^\beta \right) \left( \sum_{k=1}^N \sigma_k^\alpha \sigma_k^\beta \right) \right\} \\
(7.139) \quad &= \int_{-\infty}^{\infty} \mathcal{D}\sigma \exp \left\{ \frac{\beta^2 N}{2} \sum_{\alpha < \beta} \left( \frac{1}{N} \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta \right)^p \right\}
\end{aligned}$$

In the expression of the replicated partition in the last line of Eq. (7.139) it is easy to recognize the expression of the matrix order parameter that we have already introduced in the discussion of the SK model, the *overlap*:

$$(7.140) \quad Q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta,$$

As in the case of the SK, this expression shows that the overlap is a quantity (a) free from spin indices, i.e., a *global* order parameter; and (b) of order  $\mathcal{O}(1)$ , so that we correctly have that the argument of the exponential is an extensive function, i.e.,  $\beta^2 N/2 \sum_{\alpha < \beta} Q_{\alpha\beta}^p$ . The possibility to write things in terms of a global order parameter comes once again due to the fact that the sum in the Hamiltonian of Eq. (7.134) is over all the independent  $p$ -uplets of spins, whose number is of order  $\mathcal{O}(N^p)$ . Hence each spin participates to a number of interactions of order  $\mathcal{O}(N^{p-1})$ , i.e., infinite in the thermodynamic limit  $N \rightarrow \infty$ . Due to this property, we know that once again we are dealing with a *mean-field* model, which has no space structure but can be solved exactly.

Since  $p > 2$ , in the  $p$ -spin model we cannot introduce anymore the variables  $Q_{\alpha\beta}$  by means of a Hubbard-Stratonovich transformation, as we did for the RFIM, Hopfield model and the SK model. The change of variables from spins to overlaps is pursued by exploiting the formal

identity:

$$(7.141) \quad 1 = \int dQ_{\alpha\beta} \delta \left( N Q_{\alpha\beta} - \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta \right),$$

where we have assumed the following normalization for the Dirac-delta integral

$$(7.142) \quad \int_{-\infty}^{\infty} dx \delta(x - x_0) = N,$$

so that

$$(7.143) \quad \int_{-\infty}^{\infty} dx \delta(Nx - x_0) = \frac{1}{N} \int_{-\infty}^{\infty} dx \delta \left( x - \frac{x_0}{N} \right) = 1$$

To carry on easily the integration over the spins, it is worth recalling the integral representation of the Dirac delta,

$$(7.144) \quad \delta(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx}.$$

For the purpose of the following calculation it is convenient to regard the integral on the right-hand side of Eq. (7.144) as an integral over a contour in the complex  $k$  plane, but rotated of  $\pi/2$  radians (Wick rotation), which amounts to change variables from  $k$  to  $s = e^{i\pi/2}k$ , and then shift the (now parallel to the  $Im(k)$  axis) contour to the point  $s_0$ , which is assumed to be on the *right* of any singularity in the complex  $k$  plane (any deformation of the integration contour which does not pass through singular point is allowed by complex analysis). This means we can rewrite

$$(7.145) \quad \delta(x) = \int_{s_0-i\infty}^{s_0+i\infty} \frac{ds}{2\pi i} e^{sx}.$$

The need to account for a shift of the contour to a (still) unknown value of  $s_0$  is due to the following reason. In general the Dirac delta is used within an expression of the kind,

$$(7.146) \quad \begin{aligned} \mathcal{I}(\beta) &= \int dx f_\beta(x) \delta(x) \\ &= \int_{s_0-i\infty}^{s_0+i\infty} \frac{ds}{2\pi i} \int dx f_\beta(x) e^{sx} \\ &= \int_{s_0-i\infty}^{s_0+i\infty} \frac{ds}{2\pi i} g(s), \end{aligned}$$

where  $g(s)$  is, in full generality, a function in the complex  $s$  plane which might have singularities. In order for the Wick rotation to be done correctly the value  $s_0$  must lie on right of any singularity of  $g(s)$ . Since the analytic structure of  $g(s)$  depends on  $f_\beta(x)$ , which is not yet intervening when the integral definition of  $\delta(x)$  is introduced first, one must leave the value  $s_0$  generic. By repeating the above steps with the Dirac delta appearing in Eq. (7.141) and taking into account that we need to introduce the integration over  $n(n-1)/2$  elements of matrix  $Q_{\alpha\beta}$ , we get:

$$(7.147) \quad \begin{aligned} 1 &= \int_{-\infty}^{\infty} \prod_{\alpha < \beta} dQ_{\alpha\beta} \prod_{\alpha < \beta} \delta \left( N Q_{\alpha\beta} - \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta \right) \\ &= \int_{-\infty}^{\infty} \prod_{\alpha < \beta} dQ_{\alpha\beta} \int_{\lambda_{\alpha\beta}^0 - i\infty}^{\lambda_{\alpha\beta}^0 + i\infty} \prod_{\alpha < \beta} d\lambda_{\alpha\beta} \exp \left\{ N \sum_{\alpha < \beta} \lambda_{\alpha\beta} Q_{\alpha\beta} - \sum_{\alpha < \beta} \lambda_{\alpha\beta} \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta \right\}, \end{aligned}$$

where the meaning of the extremes of integration for  $\lambda_{\alpha\beta}$  variables should be clear from the previous discussion. Summarizing, we get:

$$(7.148) \quad \overline{Z^n} = \int \mathcal{D}Q \mathcal{D}\lambda \mathcal{D}\sigma \exp \left\{ \frac{\beta^2 N}{2} \sum_{\alpha < \beta} Q_{\alpha\beta}^p + N \sum_{\alpha < \beta} Q_{\alpha\beta} \lambda_{\alpha\beta} - \sum_{\alpha < \beta} \lambda_{\alpha\beta} \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta \right\},$$

where we have used the abbreviation

$$(7.149) \quad \int_{-\infty}^{\infty} \prod_{\alpha < \beta} dQ_{\alpha\beta} \int_{\lambda_{\alpha\beta}^0 - i\infty}^{\lambda_{\alpha\beta}^0 + i\infty} \prod_{\alpha < \beta} d\lambda_{\alpha\beta} = \int \mathcal{D}Q \mathcal{D}\Lambda$$

From the expression in Eq. (7.148) it is clear that the integration over the spin variables can be easily carried on and amounts to  $N$  identical integrals. By recalling that  $\sum_{\alpha < \beta} = \frac{1}{2} \sum_{\alpha, \beta=1}^n$  we can write

$$(7.150) \quad \begin{aligned} & \int_{-\infty}^{\infty} \prod_{i=1}^N \prod_{\alpha=1}^n d\sigma_i^\alpha \exp \left\{ -\frac{1}{2} \sum_{\alpha, \beta=1}^n \lambda_{\alpha\beta} \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta \right\} \\ &= \prod_{i=1}^N \left[ \int_{-\infty}^{\infty} \prod_{\alpha=1}^n d\sigma_i^\alpha \exp \left\{ -\frac{1}{2} \sum_{\alpha, \beta=1}^n \lambda_{\alpha\beta} \sigma_i^\alpha \sigma_i^\beta \right\} \right] \\ &= \left[ \int_{-\infty}^{\infty} \prod_{\alpha=1}^n d\sigma^\alpha \exp \left\{ -\frac{1}{2} \boldsymbol{\sigma}^T \Lambda \boldsymbol{\sigma} \right\} \right]^N \\ &= \left( \frac{1}{\sqrt{\det \Lambda}} \right)^N, \end{aligned}$$

where  $\boldsymbol{\sigma} = (\sigma^1, \dots, \sigma^n)$  indicates a vector in replica space and  $\Lambda$  is the  $n \times n$  matrix with elements  $\lambda_{\alpha\beta}$ . By finally exponentiating the determinant in Eq. (7.150) our replicated partition function has become an integral where, due to the  $N$  factor appearing in front of every term in the argument of the exponential, the possibility to complete the calculation with a saddle-point approximation seems really at hand. Indeed we have the expression:

$$(7.151) \quad \overline{Z^n} = \int \mathcal{D}Q \mathcal{D}\Lambda \exp [-NS(Q, \Lambda)] \prod_{\alpha=1}^n \delta(1 - Q_{\alpha\alpha}),$$

with

$$(7.152) \quad S(Q, \Lambda) = -\frac{\beta^2}{4} \sum_{\alpha\beta=1}^n Q_{\alpha\beta}^p - \frac{1}{2} \text{Tr}(Q\Lambda) + \frac{1}{2} \log \det \Lambda,$$

at which we arrive via the following identities, we have also used the symmetry property of the matrix  $\Lambda$  (or  $Q$ , equivalently):

$$(7.153) \quad \sum_{\alpha < \beta} Q_{\alpha\beta} \lambda_{\alpha\beta} = \frac{1}{2} \sum_{\alpha\beta=1}^n Q_{\alpha\beta} \lambda_{\alpha\beta} = \frac{1}{2} \sum_{\alpha\beta=1}^n Q_{\alpha\beta} \lambda_{\beta\alpha} = \frac{1}{2} \text{Tr}(Q\Lambda)$$

Since we are interested in the large- $N$  limit we can evaluate the integration over the elements of  $\Lambda$  by means of a saddle point approximation:

$$(7.154) \quad \int \mathcal{D}\Lambda \exp [-NS(Q, \Lambda)] \approx \exp [-NS(Q, \Lambda^*[Q])],$$

where the symbol  $\Lambda^*[Q]$  indicates the dependence of  $\Lambda$  on  $Q$  single out by the saddle-point equations:

$$(7.155) \quad \frac{\partial S}{\partial \lambda_{\alpha\beta}} = 0 \quad \Longrightarrow \quad \Lambda^*[Q].$$

By then recalling the identity

$$(7.156) \quad \log \det \Lambda = \text{Tr} \log \Lambda,$$

and letting the derivation operator  $\partial/\partial\lambda_{\alpha\beta}$  pass through the “Tr” operator for both the two terms  $\text{Tr}(Q\Lambda)$  and  $\text{Tr} \log \Lambda$  one can finally obtain the identity

$$(7.157) \quad Q_{\alpha\beta} = \frac{\partial}{\partial\lambda_{\alpha\beta}} \log \Lambda = (\Lambda^{-1})_{\alpha\beta}.$$

The reader has to recall at this point that the elements of the matrix  $Q$  are real numbers. This means, as soon as we set  $\lambda_{\alpha\beta}^* = (Q^{-1})_{\alpha\beta}$ , that the saddle-point of the function  $\exp\{-NS(Q, \Lambda)\}$  with respect to each integration  $\int_{\lambda_{\alpha\beta}^0 - i\infty}^{\lambda_{\alpha\beta}^0 + i\infty} d\lambda_{\alpha\beta}$  lies precisely at the intersection between the (vertical) integration contour and the real axis, i.e. a point which is shifted with respect to the origin. Finally, according to a somehow *a posteriori* argument, we have an explanation of why to choose  $\lambda_{\alpha\beta}^0 \neq 0$  in the integration symbol of Eq. (7.147) and that this quantity turns out to be precisely

$$(7.158) \quad \lambda_{\alpha\beta}^0 = \lambda_{\alpha\beta}^* = (Q^{-1})_{\alpha\beta}.$$

As a conclusion we can simply replace  $\Lambda$  with  $Q^{-1}$  into the expression of  $S(Q, \Lambda)$  of Eq. (7.152), getting (apart from terms constant with respect to  $Q$  and  $\beta$ )

$$(7.159) \quad \overline{Z}^n \approx \int \mathcal{D}Q \exp[-NS(Q)] \prod_{\alpha=1}^n \delta(1 - Q_{\alpha\alpha}) \approx \exp[-nNA(Q^*)],$$

with

$$(7.160) \quad A(Q) = \underbrace{-\frac{\beta^2}{4n} \sum_{\alpha\beta=1}^n Q_{\alpha\beta}^p}_{\text{energetic}} - \underbrace{\frac{1}{2n} \log \det Q}_{\text{entropic}},$$

and where  $Q^*$  in the last term of Eq. (7.159) is the solution of the saddle-point equations

$$(7.161) \quad \frac{\partial A}{\partial Q_{\alpha\beta}} = 0 \quad \Longrightarrow \quad Q_{\alpha\beta}^*.$$

As we did in the SK model, also here in Eq. (7.160) we have emphasized which are the *energetic* and the *entropic* contributions to the free energy. Let us also stress that the matrix  $Q^*$  that satisfies the saddle-point equations must also satisfy the spherical constraint conditions implemented by the Dirac deltas in Eq. (7.159): whatever is the ansatz for the matrix  $Q^*$ , it must be one with all elements equal to 1 on the diagonal.

The free-energy of the system is retrieved by taking the limit  $n \rightarrow 0$  of the replicated partition function:

$$(7.162) \quad \beta f = \lim_{\substack{n \rightarrow 0 \\ N \rightarrow \infty}} -\frac{1}{nN} (\overline{Z}^n - 1) = \lim_{\substack{n \rightarrow 0 \\ N \rightarrow \infty}} -\frac{1}{nN} (e^{-nNA(Q^*)} - 1) =$$

$$(7.163) \quad = \lim_{\substack{n \rightarrow 0 \\ N \rightarrow \infty}} -\frac{1}{nN} (1 - nNA(Q^*) - 1) = A(Q^*)$$

**7.5.2. Replica Symmetric Solution.** In order to write the free energy in Eq. (7.160) one needs an assumption on the matrix  $Q_{\alpha\beta}$ . The simplest is a replica-symmetric assumption, i.e., all elements outside the diagonal are identical to each other and equal to  $q_0$ , whereas on the diagonal they are equal to 1:

$$(7.164) \quad Q_{\alpha\beta} = \text{Diag}_n(1 - q_0, \dots, 1 - q_0) + q_0 \mathbf{1}_n \otimes \mathbf{1}_n,$$

where  $\text{Diag}_n(1 - q_0, \dots, 1 - q_0)$  denotes a  $n \times n$  diagonal matrix with all elements equal to  $1 - q_0$  on the diagonal, while  $\mathbf{1}_n \otimes \mathbf{1}_n$  denotes an  $n \times n$  matrix with *all* elements identical to 1.

In order to compute the free-energy one takes advantage of the known formula for the determinant of a matrix with elements identical outside the diagonal, i.e., a matrix  $A$  of the kind

$$(7.165) \quad A = \text{Diag}_n(a_1 - b, \dots, a_n - b) + b \mathbf{1}_n \otimes \mathbf{1}_n.$$

There is a general formula for the determinant of the matrix  $A$ , which reads:

$$(7.166) \quad \det(A) = \prod_{i=1}^n (a_i - b) + b \sum_{i=1}^n \prod_{\substack{j=1 \\ j \neq i}}^n (a_j - b)$$

Adapting the result for the determinant of  $A$  to the replica symmetric matrix  $Q$  of Eq. (7.164) one gets

$$(7.167) \quad \det(Q) = (1 - q_0)^n + nq_0(1 - q_0)^{n-1} = (1 - q_0)^n \left( 1 + n \frac{q_0}{1 - q_0} \right),$$

so that

$$(7.168) \quad \begin{aligned} \lim_{n \rightarrow 0} \frac{1}{n} \log \det(Q) &= \lim_{n \rightarrow 0} \frac{1}{n} \left[ n \log(1 - q_0) + \log \left( 1 + n \frac{q_0}{1 - q_0} \right) \right] \\ &= \log(1 - q_0) + \frac{q_0}{1 - q_0} \end{aligned}$$

Much more easily we obtain the *energetic* contribution in the limit  $n \rightarrow 0$ :

$$(7.169) \quad \sum_{\alpha\beta=1}^n Q_{\alpha\beta}^p = n + n(n-1)q_0^2.$$

Putting together the pieces we thus have:

$$(7.170) \quad \begin{aligned} f &= \lim_{n \rightarrow 0} -\frac{1}{\beta} \left\{ \frac{\beta^2}{4n} \sum_{\alpha\beta=1}^n Q_{\alpha\beta}^p + \frac{1}{2n} \log \det Q \right\} \\ &= -\frac{1}{2\beta} \left\{ \frac{\beta^2}{2} [1 - q_0^p] + \log(1 - q_0) + \frac{q_0}{1 - q_0} \right\}. \end{aligned}$$

The value of the free energy in the replica symmetric phase can be finally obtained by replacing  $q_0$  in Eq. (7.170) with the value  $q_0^*$  which satisfies the saddle point equation  $\partial f / \partial q_0 = 0$ . A peculiarity of the number of replicas  $n \rightarrow 0$  is that the correct  $q_0^*$  in this limit *maximizes* rather than *minimizes* the expression in Eq. (7.170). This can be intuitively understood in light of the *change of sign* of the energetic contribution implied by the limit  $n \rightarrow 0$ . Very heuristically, one has that the analytic continuation to values  $n < 1$  implies

$$(7.171) \quad -\frac{1}{4\beta} Q_{\alpha\beta}^p \implies \frac{1}{4\beta} q_0^p.$$

Then, we must recall the general thermodynamic relation

$$(7.172) \quad F = U - TS$$

where  $F$  is free energy,  $U$  the internal energy and  $TS$  the temperature times entropy. From Eq. (7.172) it is clear that the *convexity* of free energy function must have the same sign as that of the energy, thus a change of sign of the latter implies the same for the former.

**7.5.3. Replica Symmetry Breaking.** It is well known that the  $p$ -spin model has a critical temperature  $T_K$  at which ergodicity is broken: phase space splits in a multiplicity of disjoint ergodic components corresponding to different free-energy minima. In particular, what happens at  $T_K$  is that the free-energy obtained with a one-step replica symmetry breaking (1-RSB) ansatz becomes lower than the replica-symmetric energy. Not only, but it can be checked that the 1-RSB saddle point is a *stable one*, so that no further levels of breakings of the permutation symmetry between replicas are needed to characterize the glassy phase at  $T < T_K$ .



Then in the limit  $n \rightarrow 0$  we have, using the properties of the logarithm,

$$\begin{aligned}
& \lim_{n \rightarrow 0} \log[1 - mq_0 - (1 - m)q_1 + n q_0] = \\
& \lim_{n \rightarrow 0} \log[1 - mq_0 - (1 - m)q_1] + \log \left( 1 + n \frac{q_0}{1 - mq_0 - (1 - m)q_1} \right) = \\
(7.178) \quad & = \log[1 - mq_0 - (1 - m)q_1] + n \frac{q_0}{1 - mq_0 - (1 - m)q_1},
\end{aligned}$$

The contribution  $\log[1 - mq_0 - (1 - m)q_1]$  not proportional to  $n$  coming from the last term added on the right hand side of Eq. (7.177) cancels with the same term with opposite sign coming from the second addendum on the right of Eq. (7.177). In conclusion, as expected within a 1-RSB scheme, we have that the entropic term is proportional to  $n$ ,

$$\begin{aligned}
(7.179) \quad \log \det(Q) = & n \left[ \frac{m-1}{m} \log(1 - q_1) + \frac{1}{m} \log \left( 1 + n \frac{q_0}{1 - mq_0 - (1 - m)q_1} \right) + \right. \\
& \left. + \frac{q_0}{1 - mq_0 - (1 - m)q_1} \right]
\end{aligned}$$

Putting together the pieces, in the limit  $n \rightarrow 0$  the free energy from the 1-RSB ansatz formally reads as:

$$\begin{aligned}
(7.180) \quad -2\beta F = & \frac{\beta^2}{2} [1 - mq_0^p - (1 - m)q_1^p] + \frac{m-1}{m} \log(1 - q_1) + \\
& + \frac{1}{m} \log(1 - mq_0 - (1 - m)q_1) + \frac{q_0}{1 - mq_0 - (1 - m)q_1}.
\end{aligned}$$

The expression in Eq. (7.180) is of course a formal one for the reason that we have not yet decided which physical meaning to attach to the number  $m$ . Indeed, for integer  $n$ , the parameter  $m$  is such that  $1 < m \leq n \dots$  but what about the limit  $n \rightarrow 0$ ?

**7.5.4. The breaking parameter  $m$ .** In order to provide a correct interpretation for  $m$  in the limit  $n \rightarrow 0$  let us stick on its meaning when  $n$  is integer and large. Already in the case of the SK model we have mentioned that “*the number  $m_k$  of times that the value  $q_k$  appears in a row of the matrix  $Q_{\alpha\beta}$  is proportional to its probability*”. Being  $q_{\alpha\beta}^*$  a solution of the saddle-point equations we have thus that a meaningful definition of the overlap probability reads as

$$(7.181) \quad \overline{P_J(q)} = \frac{2}{n(n-1)} \sum_{\alpha < \beta} \delta(q - q_{\alpha\beta}^*),$$

where the average over the disorder for  $P_J(q)$  is mandatory for two reasons: 1) first, the probability of the overlap is not a self-averaging quantity (not proved here), which means that even in the  $N \rightarrow \infty$  limit it depends on the instance of random couplings, hence the subscript  $J$  is needed; 2) second, since the 1-RSB (or whatever  $k$ -RSB) ansatz for  $Q_{\alpha\beta}$  is made inside formulas coming *when the free energy has been already averaged over the disorder*, for consistency the overlap matrix  $q_{\alpha\beta}^*$  chosen for the saddle point must be related to the *disorder average* of the overlap probability distribution  $\overline{P_J(q)}$ . This said, let us show how  $\overline{P_J(q)}$  reads explicitly according to its definition in Eq. (7.181) in the case of a 1-RSB ansatz:

$$\begin{aligned}
(7.182) \quad \overline{P_J(q)} = & \frac{1}{n(n-1)} \sum_{\alpha \neq \beta} \delta(q - q_{\alpha\beta}^*) \\
= & \frac{m-1}{n-1} \delta(q - q_1) + \frac{n-m}{n-1} \delta(q - q_0).
\end{aligned}$$

From the expression in Eq. (7.182) we have that the *naïve* way to take the limit  $n \rightarrow 0$ , i.e., sending  $n$  to zero while leaving  $m$  untouched, which seems in contradiction with the inequality  $m < n$ , leads to:

$$(7.183) \quad \lim_{n \rightarrow 0} \overline{P_J(q)} = m \delta(q - q_0) + (1 - m) \delta(q - q_1)$$

We are thus at the end. From the expression of  $\overline{P_J(q)}$  in Eq. (7.183) it is clear that in order to have it well defined as a normalized probability distribution there is only one possible interpretation for the parameter  $m$ : it must be a number in the interval  $[0, 1]$ .

We have thus learned that the limit  $n \rightarrow 0$  implies a kind of *switch* in the definition of  $m$ , i.e., from a natural number in the interval  $1 < m \leq n$  to a real number in the interval  $m \in [0, 1]$ . At this stage, in order to completely solve the thermodynamics of the  $p$ -spin we just have to fix  $q_0$ ,  $q_1$  and  $m$  at the different temperatures.

**7.5.5. The critical temperatures  $T_K$  and  $T_d$ .** Now that the nature of the variational parameter  $m$  has been established we have to look for solutions of the 1-RSB equations:

$$(7.184) \quad \frac{\partial f}{\partial q_0} = 0, \quad \frac{\partial f}{\partial q_1} = 0, \quad \frac{\partial f}{\partial m} = 0.$$

The usual strategy is to solve the first two equations at fixed  $m$ , and then plug  $m$ ,  $q_0(m)$  and  $q_1(m)$  into the free-energy, inspecting numerically for which value  $m = m^*$  it has a *maximum*. Clearly  $m$ ,  $q_0$  and  $q_1$  are variational parameters that depend on the temperature. A peculiarity of the  $p$ -spin model is that, at variance with the SK, the study of the mean-field equations for  $m$ ,  $q_0$  and  $q_1$  tells us that there are two critical temperatures,  $T_d$  and  $T_K$  with  $T_d > T_K$ , which represent respectively the critical temperature for *dynamical ergodicity breaking* ( $T_d$ ) and the critical temperature for *thermodynamic ergodicity breaking* ( $T_K$ ), also known as the *ideal glass transition* temperature.

Before studying the saddle-point equations there is an aspect worth noticing, namely that by plugging  $m = 1$  into the 1-RSB free energy of Eq. (7.180) we get back exactly the RS free energy of Eq. (7.170). It was therefore more economic to study directly the 1-RSB free energy, keeping in mind that the RS free energy is its special case.

Summarizing, from the study of the 1-RSB saddle-point equations in (7.184) there are three interesting regimes emerging:

- $T > T_d$ : The saddle-point equations admit only one trivial solution:  $q_1 = q_0 = 0$  and  $m = 1$ . This is the ergodic replica symmetric phase. There are no free energy minima in the landscape.
- $T_K < T < T_d$ : There is still the trivial solution that we have for  $T > T_d$  but also a new non-trivial one appears:  $q_1 > q_0$  and  $m = 1$ . This solution, which has the same free-energy of that at  $T > T_d$ , is the signature that *many* free-energy minima separated by extensive *energetic* barriers arise as soon as  $T < T_d$ . For a detailed study of this regime, a more advanced course is needed. Here we can only say (without proving it) that the number of such minima at a given free energy,  $\mathcal{N}(f)$ , is found to be *exponentially large* in the size of the system, i.e.

$$(7.185) \quad \mathcal{N} \approx \exp [N\Sigma(f)],$$

where  $\Sigma(f)$  is a quantity known in the jargon of glassy systems as *configurational entropy*. One can attach to these minima the notion of *states*, much like the positive or negative magnetization *states* of a ferromagnet at low temperature. The reason for this is that, due to the infinite energy barrier separating them, any dynamics starting with an initial condition in one of these states remains trapped there forever (no tunneling is allowed, at least in a mean-field model). They thus represent *disjoint ergodic components* of phase space, a sort of prelude of the ergodicity breaking transition taking place at the lower temperature  $T_K < T_d$ . Nevertheless, from a thermodynamic point of view, states are irrelevant above  $T_K$  since the probability that the system ends up into one of them is exponentially small, precisely in force of their exponential abundance, i.e.,

$$(7.186) \quad p_{state} \sim \exp [-N\Sigma(f)]$$



This thermodynamic *irrelevance* of the states above  $T_K$  is reflected precisely by the fact that the solution with  $q_1 > q_0$  and  $m = 1$  has the same free-energy of the one with  $q_0 = q_1 = 0$  and that if we ask for the probability to find two configurations at overlap  $q_1 > 0$  this is zero even according to the definition of  $\overline{P}_J(q)$  given in Eq. (7.183).

- $T < T_k$ : In this regime we find both the solution with  $q_0 = q_1 = 0$  and  $m = 1$  and the replica-symmetry-broken one with  $q_1 > q_0$  and  $m < 1$ , corresponding to finding with finite probability two configurations of the system at finite overlap, see Eq. (7.183). In particular, if one compares the free energy of the RS solution and of the 1-RSB one, when  $T < T_K$  the 1-RSB solution has a smaller free energy,

$$(7.187) \quad T \leq T_K \quad \Longrightarrow \quad f(q_1 > q_0, m < 1) < f(q_1 = q_0 = 0, m = 1).$$

Hence, for temperatures below  $T_K$ , thermodynamic equilibrium is determined by the glass phase, where the systems remains trapped forever in one of the states. The ergodicity-breaking transition taking place in the  $p$ -spin model at  $T_K$  is usually known as the *ideal glass transition* or, more precisely the *Random First-Order Transition* (RFOT). The RFOT name comes from the fact that the ergodicity-breaking transition at  $T_K$  has a mixed character between a first and second order transition. This happens because the distribution  $\overline{P}_J(q)$  is bimodal already at the transition temperature  $T = T_K$ , with a secondary peak at a finite distance from the origin, corresponding to  $q_1 > q_0$  already at  $T = T_K$  [see Eq.(7.183)]—a feature typical of a *first-order* transition—while at the same time for the transition at  $T_K$  there is no latent heat, much like a *second-order* or *continuous* transition. “Random First-Order” was therefore introduced to refer to something which is a kind of “smoothed first-order transition”.

**7.5.6. Appendix.** Consider an  $m \times m$  matrix:

$$\begin{pmatrix} \alpha & \beta & \cdots & \beta \\ \beta & \alpha & \cdots & \beta \\ \vdots & \vdots & \ddots & \vdots \\ \beta & \beta & \cdots & \alpha \end{pmatrix}$$

Its generic element can be written as:

$$(7.188) \quad c_{ij} = \alpha\delta_{ij} + \beta(1 - \delta_{ij})$$

The eigenvalues equation reads:

$$(7.189) \quad \sum_{j=1}^n c_{ij}v_j = \sum_{j=1}^n \alpha\delta_{ij}v_j + \beta(1 - \delta_{ij})v_j = \lambda v_i$$

$$(7.190) \quad (\alpha - \beta)v_i + \beta \sum_{j=1}^m v_j = \lambda v_i$$

If  $\sum_{j=1}^n v_j = 0$  (can be done in  $m - 1$  ways by choosing different values for  $v_j$ ):

$$\lambda = \alpha - \beta$$

else sum over  $i$  (and  $\sum_{j=1}^m v_j \neq 0$ ):

$$(7.191) \quad (\alpha - \beta) \sum_{i=1}^m v_i + \beta \sum_{i=1}^m \sum_{j=1}^m v_j = \lambda \sum_{i=1}^m v_i$$

$$(7.192) \quad (\alpha - \beta) \sum_{i=1}^m v_i + m\beta \sum_{i=1}^m v_i = \lambda \sum_{i=1}^m v_i$$

divide by  $\sum_{j=1}^m v_j$ :

$$\lambda = \alpha + (m - 1)\beta$$

So we have  $\lambda_1 = \alpha - \beta$  with  $\deg \lambda_1 = m - 1$  and  $\lambda_2 = \alpha + (m - 1)\beta$  with  $\deg \lambda_2 = 1$ . The replica symmetric matrix is a block circulant matrix where the first row block is:

$$\begin{pmatrix} A & \underbrace{B \dots B}_{f-1 \text{ times}} \end{pmatrix}$$

$$A_{ij} = \delta_{ij} + q_1 (1 - \delta_{ij})$$

$$B_{ij} = q_0$$

$$f = n/m$$

where  $n$  is the number of replicas. The eigenvalues of  $A$  are:

$$\lambda_{1A} = 1 - q_1 \quad \deg_1 = m - 1$$

$$\lambda_{2A} = 1 + (m - 1)q_1 \quad \deg_2 = 1$$

The eigenvalue of  $B$  are:

$$\lambda_{1B} = 0 \quad \deg_1 = m - 1$$

$$\lambda_{2B} = mq_0 \quad \deg_2 = 1$$

Now  $A$  and  $B$  commute and they are the same kind of circulant matrix of first row  $(\alpha, \beta, \dots, \beta)$  solved above. The block matrix is the block analogue of this kind of circular matrix and because  $A$  and  $B$  commute the eigenvalues of this matrix have the same form when we make the substitution  $\alpha \rightarrow \lambda_A$  and  $\beta \rightarrow \lambda_B$ ; there is only one requirement: we can mix only eigenvalues having the same set of eigenvectors. In the end we get

$$(7.193) \quad \lambda_A = 1 - q_1 \quad \lambda_B = 0$$

$$(7.194) \quad \lambda_1 = \lambda_A - \lambda_B = 1 - q_1$$

$$(7.195) \quad \lambda_1 = \lambda_A + (f - 1)\lambda_B = 1 - q_1$$

and

$$(7.196) \quad \lambda_A = 1 + (m - 1)q_1 \quad \lambda_B = mq_0$$

$$(7.197) \quad \lambda_2 = \lambda_A - \lambda_B = 1 + (m - 1)q_1 + mq_0 = 1 - q_1 + m(q_1 - q_0)$$

$$(7.198) \quad \lambda_3 = \lambda_A + (f - 1)\lambda_B = 1 - q_1 + m(q_1 - q_0) + nq_0$$

The eigenvalue  $\lambda_2$  has degeneracy  $f - 1 = \frac{n}{m} - 1$  and  $\lambda_3$  has 1; since it is assured that the matrix is diagonalizable the degeneracy of  $\lambda_1$  is  $n - \frac{n}{m}$ .

## Problems

Following the notation of the lecture notes:

**Exercise 7.1.** Consider the Random Field Ising Model (RFIM), in which the disorder has variance  $\delta^2$ . Proceed to arrive at the formula where the number  $n$  of replicas appears explicitly in the magnetization  $m$ ,

$$m = \frac{1}{Z_1(m)} \int \frac{d\nu}{\sqrt{2\pi}} \exp \left[ \frac{1}{2} \nu^2 + n \ln 2 \cosh(2\beta J m + \beta \delta \nu) \right] \tanh(2\beta J m + \beta \delta \nu)$$

**Exercise 7.2.** With the self-consistent solution  $m_{SC}(m) = m$  of the RFIM, by using the condition  $\partial m_{SC} / \partial m = 1$  for the critical point, show that the phase transition between paramagnetic phase and ferromagnetic phase takes place where this condition is satisfied:

$$(7.199) \quad 2\beta J \int dh p(h) \frac{1}{[\cosh(\beta h)]^2} = 1$$

**Exercise 7.3.** Show that at zero temperature in the RFIM there is a disorder-driven para-ferromagnetic transition where the random field standard deviation  $\delta$  and the coupling  $J$  satisfy  $2J/\delta = \sqrt{\pi/2}$ . For simplicity one may take  $\delta = 1$ .

