3

EXAMPLE II: THE MEAN-FIELD ISING MODEL

Concepts as order parameter, thermodynamic limit, phase transitions, symmetry breaking, universality, relaxation, barrier crossing, metastability, ... are introduced. They are illustrated through the statistical and dynamical features of the Ising model on the complete graph.

3.1 The model, and its phase transition.

We shall now study analytically a model of N spins, called the Ising model, exhibiting a phase transition in the limit $N \to \infty$. The underlying graph is the complete graph K_N; each vertex is labelled by an integer number $i = 1, \ldots, N$ and carries a binary spin σ_i. The energy function is given by the Ising Hamiltonian (1.20) with coupling $J/N > 0$,

$$E(\sigma_1, \ldots, \sigma_N) = -\frac{J}{N} \sum_{i<j} \sigma_i \sigma_j - h \sum_i \sigma_i \qquad , \tag{3.1}$$

3.1.1 *Calculation of the free energy.*

The first term in (3.1) is called the interaction term. The sum runs over all pairs of spins, that is over all edges of K_N. The minus sign ensures that the minimum of energy is reached when all spins are equal to the sign of the “magnetic field” h. In the absence of field ($h = 0$), we know the two ground states. The energy and entropy at zero temperature are thus,

$$\langle E \rangle_{T=0} = -\frac{J}{2}(N-1) \quad , \qquad \langle S \rangle_{T=0} = \ln 2 \quad . \tag{3.2}$$

Notice that the ground state energy is $O(N)$ due to the value of the coupling $J = 1/N$ in (3.1) whereas the entropy is $O(1)$.

At infinite temperature, all configurations are equiprobable. The partition function is simply equal to the total number of configurations: $Z(T = \infty) = 2^N$, leading to

$$\langle E \rangle_{T=\infty} = 0 \quad , \qquad \langle S \rangle_{T=\infty} = N \ \ln 2 \quad . \tag{3.3}$$

The phase transition we are going to study separates two regimes:

- a high temperature phase where entropy effects are dominant: spins configurations are disordered and spins have no priviledged direction (for $h = 0$). The average magnetization per spin, m, vanishes.
- a low temperature phase where energy effects dominate: spins have a tendency to align along each other, resulting in ordered configurations with a non zero magnetization $m = \langle \sigma_i \rangle \neq 0$.

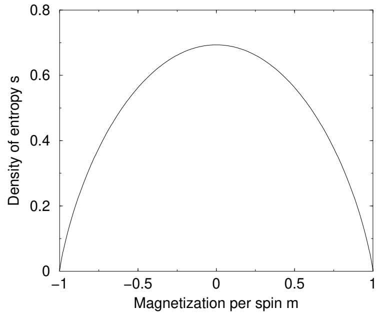

FIG. 3.1. Entropy $s(m)$ of the Ising model on the complete graph as a function of magnetization m. s is an even function of the magnetization, which vanishes on the boundaries $m = \pm 1$. Its maximum, $s(0) = \ln 2$, is reached at zero magnetization.

Let us stress that the energy and the entropy must have the same orders of magnitude ($=O(N)$) to allow for such a compromise and thus for the existence of a phase transition at finite strictly positive temperature. This is why the coupling J has be chosen to scale as $1/N$.

The calculation of the partition function relies on the following remark. The energy function (3.1) depends on the configuration $\mathcal{C}$ only through its magnetization $m(\mathcal{C})$ given by eqns (1.28) and (1.31),

$$E(\mathcal{C}) = -N \left(\frac{J}{2}\, m(\mathcal{C})^2 + h\, m(\mathcal{C}) \right) + \frac{1}{2} \quad . \tag{3.4}$$

This property leads to a drastic simplification: the sum over the 2^N configurations in the partition function Z (1.25) can be replaced with a sum over the $N+1$ values of the magnetisation, properly weighted by the multiplicity of each value.

Let us thus count the number $D(m)$ of configurations having intensive magnetisation m. These have N_+ spins up and N_- spins down with $N_\pm = N(1 \pm m)/2$. The number of such configurations is therefore given by the binomial coefficient

$$D(m) = \frac{N!}{N_+! N_-!} \quad . \tag{3.5}$$

In the large N limit, Stirling's formula gives access to the asymptotic expression of the entropy density, $s(m) = \ln D(m)/N$, at fixed magnetization,

$$s(m) = -\left(\frac{1-m}{2}\right) \ln\left(\frac{1-m}{2}\right) - \left(\frac{1+m}{2}\right) \ln\left(\frac{1+m}{2}\right) \quad , \tag{3.6}$$

Figure 3.1 displays $s(m)$ as a function of m.

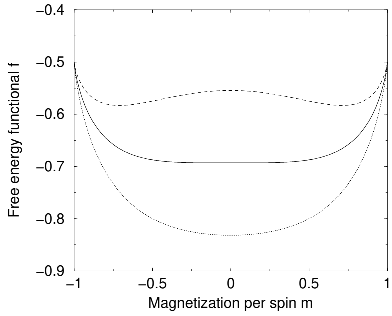

FIG. 3.2. Free-energy functional $\hat{f}(m)$ of the Ising model on the complete graph as a function of the magnetization m in zero magnetic field h and for three different temperatures ($J = 1$). From bottom to top, $T = 1.2$ (dotted curve), $T = T_c = 1$ (full curve), $T = 0.8$ (dashed curve). At criticality, the curvature of the $m = 0$ saddle-point vanishes, signaling the onset of a second order phase transition.

The partition function (1.25) reads

$$Z(T) = \sum_{m=-1,-1+\frac{2}{N},\ldots,1-\frac{2}{N},1} \exp\left[-N\,\hat{f}(m)/T\right] \qquad , \tag{3.7}$$

where the magnetization–dependent free energy functional is defined through

$$\hat{f}(m) = -\frac{J}{2}\,m^2 - h\,m - T\,s(m) \qquad , \tag{3.8}$$

up to $O(1/N)$ terms. For the moment, we shall restrict to the case of zero magnetic field, $h = 0$.

In the limit of an infinite number N of spins, the free-energy may be computed by means of the saddle-point (Laplace) method. We look for the magnetization m^* (that depends upon temperature T) minimizing $\hat{f}(m)$. The latter is plotted in Fig. 3.2 for three different temperatures. It can be seen graphically that the minimum of $\hat{f}$ is located at $m^* = 0$ when the temperature is larger than $T_c = J$ while there exist two opposite minima, $m = -m^*(T) < 0$, $m = m^*(T) > 0$ below this critical temperature. The optimum magnetization is solution of the saddle-point equation,

$$m^* = \tanh\left(J\,m^*/T\right) \qquad , \tag{3.9}$$

while the free-energy density is given by $f(T) = \hat{f}(m^*)$. The intensive energy and entropy per spin are easily obtained from the knowledge of m^*: $e^* = -\frac{J}{2}\,(m^*)^2$, $s^* = s(m^*)$.

Not only the minimum of $\hat{f}$ but the whole function has a deep statistical significance. Let us consider the probability that the magnetisation takes value m,

$$\text{Prob}[m] = \frac{1}{Z(T)} \sum_{\mathcal{C}/m(\mathcal{C})=m} \exp\left[-N\ \hat{f}(m)/T\right] \quad . \tag{3.10}$$

For very large sizes N, we expect this probability to be highly concentrated around the average magnetisation m^{*}[54]. Magnetisations m differing from m^* by some amount of the order of unity have positive but exponentially small-in-N values,

$$\text{Prob}[m] = e^{N\hat{\omega}(m)+o(N)} \tag{3.12}$$

where the rate function $\hat{\omega}$ takes negative values. Comparing equations (3.10) and (3.12) yields

$$\hat{\omega}(m) = -\frac{1}{T}\left[\hat{f}(m) - f(m^*)\right] \quad . \tag{3.13}$$

In other words, the free energy functional $\hat{f}$ gives access to the large deviations of the magnetisation. This point has important dynamical consequences which will be investigated in Section 3.2.3.

3.1.2 *Order parameter and symmetry breaking.*

In the absence of a magnetic field, the energy (3.1) is an even function of the spins: two opposite configurations $\{\sigma_1, \ldots, \sigma_N\}$ and $\{-\sigma_1, \ldots, -\sigma_N\}$ have equal Gibbs probabilities. As a consequence, the average $m(h=0,T)\langle\sigma\rangle$ of any spin vanishes. This result is true for any N and so, in the large N limit,

$$\lim_{N\to\infty} \lim_{h\to 0} m(h,T) = 0 \quad . \tag{3.14}$$

It is thus necessary to unveil the meaning of the saddle-point magnetization m^* arising in the computation of the partition function.

To do so, we repeat the previous calculation of the free-energy in presence of a magnetic field $h > 0$. The magnetization is now different from zero. At high temperature $T > T_c$, this magnetization decreases as the magnetic field h is lowered and vanishes when $h = 0$,

$$\lim_{h\to 0^+} \lim_{N\to\infty} m(h,T) = 0 \qquad (T > T_c) \quad . \tag{3.15}$$

Therefore, at high temperature, the inversion of limits between (3.14) and (3.15) has no effect on the final result.

[54] According to Section 1.3.3, small deviations of the order of $N^{-1/2}$ have finite probabilities. Setting $m = m^* + x/\sqrt{N}$ in eqn (3.10) and expanding $\hat{f}$ around its minimum, we obtain

$$\text{Prob}[x] \propto \exp\left[-\frac{1}{2T}\ \frac{d^2\hat{f}}{dm^2}(m^*)\ x^2\right] \quad . \tag{3.11}$$

Small fluctuations thus follow a normal law with a variance related to the inverse curvature of the free energy around its minimum.

The situation drastically changes at low temperature. When $T < T_c$, the degeneracy between the two minima of f is lifted by the magnetic field. Due to the field, a contribution $-h\ m$ must be added to the free-energy (3.8) and favours the minimum in m^* over that in $-m^*$. The contribution to the partition function (3.7) coming from the second minimum is exponentially smaller than the contribution due to the global minimum in m^* by a factor $\exp(-2Nhm^*/T)$. The probability measure on spins configurations is therefore fully concentrated around the global minimum with positive magnetization and

$$\lim_{h\to 0^+} \lim_{N\to\infty} m(h,T) = m^*(T) \qquad (T < T_c) \quad . \tag{3.16}$$

From (3.14) and (3.16), the meaning of the phase transition is now clear. Above the critical temperature, a small perturbation of the system (e.g. a term in the energy function pushing spins to take value $+1$ rather than -1), is irrelevant: as the perturbation disappears ($h \to 0$), so do its effects ($m^* \to 0$), see eqn (3.15). Conversely, below the critical temperature, a small perturbation is enough to trigger strong effects: spins have a non zero average $m^* > 0$ even after the perturbation has disappeared ($h = 0$), see eqn (3.16), a phenomenon called spontaneous magnetization. At low temperature, two phases with opposite magnetizations m^* and $-m^*$ coexist. Adding an infinitesimal field h favours and selects one of them. In more mathematical terms, the magnetization m is a non-analytic and discontinuous function of h at $h = 0$.

To sum up, the average magnetization $m(T)$ vanishes in the high temperature phase and acquires a finite (non zero) value in the low temperature phase. It is an order parameter: its value (zero or non-zero) gives some quantitative statistical information on the configuration variables, and indicates the phase the system is in.

The phase transition appears here to be intimately related to the notion of symmetry breaking. In the case of the Ising model, the probability distribution over configurations is symmetrical, that is, left unchanged under the reversal of spins $\sigma \to -\sigma$. A high temperature, this symmetry also holds for average quantities: $\langle\sigma\rangle = 0$. At low temperature, the reversal symmetry is broken since, in presence of an infinitesimal perturbation, $\langle\sigma\rangle = m^* \neq 0$. The initial symmetry of the system implies only that the two possible phases of the system have opposite magnetizations m^* and $-m^*$. In the present case, the symmetry of the system was easy to identify, and to break! We shall see in the next Chapters that more abstract and complex symmetries may arise in other models. The understanding of phase transitions very often will rely on the breaking of associated symmetries.

We end up with a comment about the mean-field nature of the Ising model on the complete graph. The correlation function between any two spins e.g. σ_1 and σ_2 can be easily accessed from the knowledge of the free energy as a function of the coupling for

$$\langle \sigma_1\, \sigma_2 \rangle = \frac{2T}{N-1}\, \frac{\partial}{\partial J} \ln Z(T) \tag{3.17}$$

from eqn (3.1). In the large N limit, we obtain from the expression (3.8) for the free energy,

$$\langle \sigma_1 \, \sigma_2 \rangle = \big(m^*(T) \big)^2 \quad . \tag{3.18}$$

Therefore, the correlation function of two spins is simply equal to the product of the average values of the spins. We conclude that, in the thermodynamic limit, spins decorrelate: the joint distribution of the values of the spins is the product of the single spin distributions[55]

$$\mathrm{Prob}[\sigma_1, \sigma_2] = \mathrm{Prob}[\sigma_1] \; \mathrm{Prob}[\sigma_2] \qquad (N \to \infty) \tag{3.19}$$

This identity extends higher numbers of spins: the joint probability of a any k-uplet of spins factorises when $N \to \infty$ (and k is kept fixed). Obviously factorisation does not hold when k is of the order of N, see the Gibbs measure itself corresponding to the $k = N$ case. The factorisation property is a direct consequence of the underlying interaction graph we have chosen (Fig. 1.10B), where the coupling between every two spins is weak. It would not hold for the Ising model on a planar graph (Fig. 1.10A) for which neighbouring spins are clearly strongly correlated.

That joint spin probability distributions can be expressed as the product of single spin probability distributions is a drastic simplication at the origin of the analytical resolution of our model. In fact, a consequence of the factorisation property is that only the single spin probability distribution matters. As this probability can be entirely described through a unique parameter e.g. the magnetisation, solving the model amounts to find a self-consistent equation for this parameter, namely eqn (3.9). For this reason models enjoying the factorisation property are called mean field models in statistical mechanics.

3.1.3 *Vicinity of the transition and critical exponents.*

To complete the present analysis, we now investigate the properties of the Ising model close to the critical temperature $T_c = J$ and define $T/T_c = 1 + \tau$ with $|\tau| \ll 1$. The spontaneous magnetization reads from (3.9),

$$m^*(\tau) = \begin{cases} 0 & \text{if } \tau \geq 0 \quad , \\ \sqrt{-3\tau} & \text{if } \tau \leq 0 \quad . \end{cases} \tag{3.20}$$

Thus the magnetization grows as a power of the shifted temperature τ: $m^*(\tau) \sim (-\tau)^\beta$ with $\beta = 1/2$. β, not to be confused with the inverse temperature, is called a critical exponent since it characterizes the power law behaviour of a physical quantity, here the magnetization, close to criticality. Such exponents are universal in that they are largely independent of the "details" of the definition of the model.

[55]Let $p_{++}, p_{-+}, p_{+-}, p_{--}$ be the four joint probabilities. We have: $p_{+-} = p_{-+}$ since spins can be interchanged, $(p_{++} + p_{+-}) - (p_{-+} + p_{--}) = m^*(T)$ by definition of the average magnetisation, $(p_{++} + p_{--}) - (p_{-+} + p_{+-}) = m^*(T)^2$ from eqn (3.18), and $p_{++} + p_{+-} + p_{-+} + p_{--} = 1$ for normalisation. We deduce that $p_{\sigma_1,\sigma_2} = p_{\sigma_1} \times p_{\sigma_2}$ where $p_\sigma = \frac{1}{2}(1 + \sigma m^*(T))$ is the single spin probability.

Another exponent of interest is related to the finite size effect at the transition. So far, we have calculated the average values of various quantities in the infinite size limit $N \to \infty$. We have in particular shown the existence of a critical temperature separating a phase where the sum of the spins is on average zero ($\tau > 0$) from a phase where the sum of the spins acquires an $O(N)$ mean ($\tau < 0$). At the transition point ($\tau = 0$), we know that the sum of spins cannot be of order N; instead we have a scaling in N^δ with $\delta < 1$.

What is the value of δ? From expression (3.7), let us expand the free-energy function $\hat{f}(m)$ (3.8) in powers of the magnetization $m = O(N^{\delta-1})$,

$$\hat{f}(m) - \hat{f}(0) = \frac{\tau}{2}\, m^2 + \frac{1}{12}\, m^4 + O(m^6, \tau\, m^4) \qquad , \tag{3.21}$$

with $f(0) = -T \ln 2$. Above the critical temperature, $\tau > 0$, the average magnetization is expected to vanish. Due to the presence of the quadratic leading term in (3.21), the fluctuations of m are of the order of $N^{-1/2}$. The sum of the spins, $N\, m$, has a distribution whose width grows as $N^{1/2}$, giving $\delta = 1/2$.

At the critical temperature, the partition function reads from (3.7),

$$Z \simeq 2^N \int dm\; e^{-N\, m^4/12} \qquad . \tag{3.22}$$

The average magnetization thus vanishes as expected and fluctuations are of the order of $N^{-1/4}$. The sum of the spins, $N\, m$, thus has a distribution whose width grows as $N^{3/4}$, giving $\delta = 3/4$.

The *size* of the critical region (in temperature) is defined as the largest value τ_{max} of the shifted temperature τ leaving unchanged the order of magnitude of the fluctuations of the magnetization m. A new critical exponent ν that monitors this shift is introduced: $\tau_{max} \sim N^{-1/\nu}$. Demanding that terms on the r.h.s. of (3.21) be of the same order in N, we find $\nu = 2$.

3.2 Dynamical properties.

3.2.1 *Master equation and dynamical rate function*

Let us turn now to the dynamical formulation of Section 1.3.4. The transition matrix W (1.53) is a $2^N \times 2^N$ matrix, most entries of which are null since the rate between two configurations differing by more than one spin vanishes. As the energy function E depends on configurations $\mathcal{C}$ through their magnetisation $M(\mathcal{C})$ (1.28) only, so do the transition rates. In the following we will denote $M(\mathcal{C}'), M(\mathcal{C})$ by M', M respectively to lighten notations. Magnetisations M and M' each take $N+1$ possible values ranging from $-N, -N+2, \ldots, N-2, N$. Flipping a spin from value $-\sigma$ to σ gives rise a change of magnetisation equal to $M' - M = 2\sigma$, and of energy, from eqn (3.4),

$$\Delta E = -\big(M' - M\big) \left(\frac{J(M+M')}{2\,N} + h\right) = -2\,\sigma\,(J\,m + h) + \frac{2}{N} \tag{3.23}$$

where m is the intensive magnetisation, $m \equiv M/N$. This, together with special choices of the rate function w (1.54) satisfying detailed balance e.g. Metropolis

(1.55), Glauber (1.56), or Exponential (1.57) rates, entirely defines the $N \times (N+1)$ off-diagonal transition rates

$$W[\mathcal{C}', \mathcal{C}] = \begin{cases} w\big(-2\,\sigma\,(J\,m + h) + \frac{2}{N}\big) & \text{if} \mathcal{C}' \text{is obtained from} \mathcal{C} \text{by flipping a spin from} -\sigma \text{to} \sigma \\ 0 & \text{otherwise} \end{cases} \tag{3.24}$$

We now have to solve master equation (1.43). A simplification occurs if we suppose that the initial probability over configurations, $P(\mathcal{C}, t = 0)$, is uniform over configurations with equal magnetisations. Examples of probabilities satisfying this assumption are $P(\mathcal{C}, 0) = 1$ if $\mathcal{C} = (+, +, \ldots, +, +)$ and 0 otherwise, and $P(\mathcal{C}, 0) = \frac{1}{2^N}$, which, respectively, correspond to probabilities centered on the all–spin–up configuration, and uniform over all configurations. Then, as transition rates between configurations depend on their magnetisations only, the probability $P(\mathcal{C}, t)$ keeps its uniformity over configurations with the same magnetisation at all times,

$$M = M' \longrightarrow P(\mathcal{C}, t) = P(\mathcal{C}', t) \ , \quad \forall\ t\ . \tag{3.25}$$

Uniformity is a precious property in that it allows us to write probabilities over configurations in terms of probabilities over magnetisations[56],

$$P(\mathcal{C}, t) = P_R\big(M, t\big) / \binom{N}{\frac{N+M}{2}} \quad . \tag{3.27}$$

This represents a drastic simplification of the problem. Rather than having to study the dynamics of the set of configurations $\mathcal{C}$, of cardinality equal to 2^N, we are left with the evolution of the magnetisations M, which take $N + 1$ distinct values only.

Insertion of definition (3.27) into eqn (1.43) yields a master equation for the dynamics of magnetisations,

$$\frac{d}{dt} P_R(M', t) = \sum_M W_R[M', M]\ P_R(M, t) \tag{3.28}$$

where the diagonal elements of the transition matrix are defined through, see eqn (1.45),

$$W_R[M, M] = - \sum_{M'(\neq M)} W_R[M', M] \tag{3.29}$$

and the off-diagonal entries read

[56]The combinatorial factor dividing the r.h.s. of eqn (3.27) is equal to the number of ways of chosing $\frac{N+M}{2}$ spins up among N spins, that is, to the number of configurations having magnetisation M. Its presence ensures that the new probability P_R is properly normalised,

$$\sum_{M=-N,-N+2,\ldots,N-2,N} P_R(M, t) = 1 \quad . \tag{3.26}$$

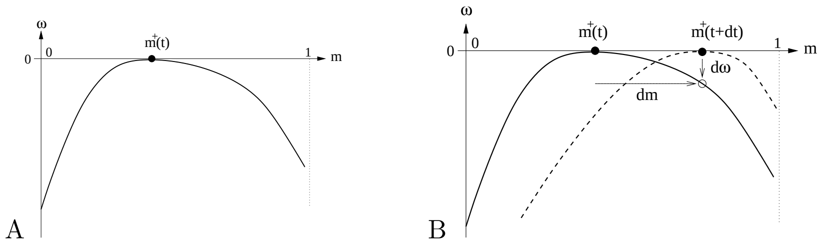

FIG. 3.3. Rate function $\omega(m,t)$ as a function of the magnetisation m at a given time t. **A**. ω is negative for all magnetisations, but vanishes for the most likely magnetisation, $m^+(t)$ (full dot). **B**. Rate functions at time t (full curve) and $t+\delta t$ (dashed curve). The empty dot indicate the point of coordinates $(m^+(t)+\delta m, \delta\omega)$, see text.

$$W_R[M', M] = \sum_{\mathcal{C}/M(\mathcal{C})=M} W[\mathcal{C}', \mathcal{C}] \times \binom{N}{\frac{N+M'}{2}} \Big/ \binom{N}{\frac{N+M}{2}} \tag{3.30}$$

where $\mathcal{C}'$ is any configuration with magnetisation M'. Obviously the transition elements vanishes when $M' \neq M \pm 2$. When $M' = M + 2\sigma$, $\mathcal{C}'$ can be obtained through a transition from any of the $\frac{N+\sigma\, M'}{2}$ configurations $\mathcal{C}$ having one more spin equal to $-\sigma$ (and one less spin equal to σ). Using expression (3.24) for the rates, we obtain from eqn (3.30)[57],

$$W_R[M+2\sigma, M] = N\left(\frac{1-\sigma\, m}{2}\right)\, w\left(-2\,\sigma\,(J\,m+h) - \frac{2}{N}\right) \quad . \tag{3.31}$$

We are now capable of analysing evolution equation (3.29) in the large N limit. From the general results of Section 1.3.4 $P_R(m,t)$ converges, at large times, to the Gibbs measure (3.10). Inspired by the large N scaling (3.12) of the Gibbs measure, we look for a solution of master equation (3.29) of the form

$$P_R(M = N\,m, t) = \exp\left[N\,\omega\,(m,t) + o(N)\right] \tag{3.32}$$

for large N. The rate function ω describes, as in the Gibbs limit (3.12), the large deviations of the magnetisation m; it is a negative function of m over the range $0 \leq m \leq 1$ which vanishes for the most likely magnetisation, $m^+(t)$, as sketched in Fig. 3.3A. The new feature is that these deviations, and the representative curve of ω change with time t.

[57]Check that $\frac{N+\sigma(M+2\sigma)}{2} \times \binom{N}{\frac{N+M+2\sigma}{2}} \Big/ \binom{N}{\frac{N+M}{2}} = \frac{N-\sigma M}{2}$. Notice that expression (3.31) makes sense when both M and $M' = M+2\sigma$ are in the range $[-N;N]$ *i.e.* for authorized magnetisations. If, for instance, $M = N$, $\sigma = 1$, W_R is not defined, and expression (3.31) vanishes since the transition from magnetisation N to $N+2$ is not permitted.

Insertion of hypothesis (3.32) into master equation (3.29) leads, in the large N limit, to the following partial differential equation for the evolution of the rate function ω,[58]

$$\frac{\partial \omega}{\partial t}(m,t) = H\left(m, \frac{\partial \omega}{\partial m}(m,t)\right) \tag{3.33}$$

where the function H is defined through

$$H(m,\hat{m}) = \sum_{\sigma=\pm 1} \frac{1+\sigma\, m}{2}\; w\big(2\sigma(J\,m+h)\big)\; \left(e^{\,2\sigma\hat{m}} - 1\right) \quad . \tag{3.34}$$

Evolution equation (3.33) complemented with the initial condition over P_R *i.e.* the value of function $\omega(m,t=0)$[59] entirely defines the rate function ω for all magnetisation and times. Most properties of the rate function $\omega(m,t)$ can be guessed from simple arguments that we now expose; the detailed resolution of eqn (3.33) is intrisically related to the ideas of pathes and path integrals, and left to Section 3.3.1.

3.2.2 *Relaxation of the magnetisation*

Let us draw the representative curve of the rate function ω at some time t (Fig. 3.3A). Close to the top point with coordinates $(m^+(t),0)$, we consider the point P of coordinates $(m^+(t)+\delta m, \delta\omega)$ where δm and

$$\delta\omega = \frac{\partial \omega}{\partial m}\,\delta m + O(\delta m^2) \tag{3.35}$$

are both very small in modulus (empty dot in Fig. 3.3B). In P, the representative curve of ω is almost flat and we are allowed to linearise evolution equation (3.33),

$$\frac{\partial \omega}{\partial t} = R\big(m^+(t)\big)\,\frac{\partial \omega}{\partial m} + o\left(\frac{\partial \omega}{\partial m}, \delta m\right) \tag{3.36}$$

where

$$R(m) \equiv \frac{\partial H}{\partial \hat{m}}\big(m,0\big) = \sum_{\sigma=\pm 1} \big(m+\sigma\big)\; w\big(2\sigma(J\,m+h)\big)\;. \tag{3.37}$$

It turns out that the values of the two first order derivatives of ω in P appearing in eqn (3.36) are simply related. Call δt the delay at which the most likely

[58] The transition matrix relates magnetisations m, m' at times $t, t' = t+\delta t$ for vanishing δt. Transitions are possible for $m' - m = 2\frac{\sigma}{N}$ only, with $\sigma = 0, \pm 1$. Thus $N\,\omega(m' - 2\frac{\sigma}{N}, t) = N\,\omega(m',t) - 2\sigma\frac{\partial \omega}{\partial m} + o(1)$. Hence expression (3.34) for H (note the change $\sigma \to -\sigma$). It is important to notice here that the variation of $N\,\omega$ is of the order of one, much smaller than the $o(N)$ term in the logarithm of the probability P_R (3.32). However this term is a function of the magnetisation m, and will change by $o(N)/N = o(1)$ during the transition. The same scaling is found for its derivative with respect to time t. This justifies eqn (3.33).

[59] For instance, $\omega(m,0) = s(m) - \ln 2$ for the above mentioned choice $P(\mathcal{C},0) = \frac{1}{2^N}$ where function s is defined in eqn (3.6)

magnetisation will lie right above P. From the condition $m^+(t+\delta t) = m^+(t)+\delta m$ we deduce an identity relating the delay and the relative abscissa of P,

$$\delta m = \frac{dm^+(t)}{dt}\,\delta t + O(\delta t^2) \quad . \tag{3.38}$$

During this time delay, the value of the rate function has increased from $\delta\omega$ to 0, giving

$$0 - \delta\omega = \frac{\partial \omega}{\partial t}\,\delta t + O(\delta t^2, \delta m\,\delta t) \quad . \tag{3.39}$$

Combination of eqns (3.35), (3.36), (3.38), and (3.39) leads to the equation for the evolution of the most likely magnetisation,

$$\frac{d}{dt} m^+(t) = -\,R\big(m^+(t)\big) \quad . \tag{3.40}$$

Expression (3.37) for R has now a simple interpretation. The spin which is chosen by the dynamics at time t has probability $\frac{1+\sigma m}{2}$ to be equal to $\sigma(=\pm 1)$. It will be flipped with transition rate $w(2\sigma(m+h))$ and change the overall magnetisation by -2σ, in agreement with (3.40).

While function R quantitatively depends on the choice for the rate function w, its main qualitative features do not, and are related to the free-energy functional $\hat{f}$ (3.8) only. Indeed, using detailed balance condition (1.54), definition (3.37) may be rewritten as

$$R(m) = (1-m)\, w\big(-2(J\,m+h)\big)\,\left[\exp\left(\frac{2}{T}\frac{d\hat{f}}{dm}(m)\right) - 1\right] \quad . \tag{3.41}$$

We deduce that R has the same sign as the derivative of $\hat{f}$; in particular the zeroes of the two functions coincide. This general statement is illustrated for a specific choice of parameters (temperature, field, transition rate) in Fig. 3.4A. As clearly appears from the figure, under evolution equation (3.40), the magnetisation $m^+(t)$ will converge at long times towards a local minimum of $\hat{f}$. This outcome is not ambiguous when $\hat{f}$ admits a unique minimum *i.e.* above the critical temperature. Conversely, at low temperature, which one of the two existing minima will eventually be reached depends on the initial condition. If the magnetisation at time $t=0$ is smaller (respectively larger) than the abscissa m_0 of the local maximum of $\hat{f}$, $m^+(t)$ will converge to m_- (resp. m_+). This phenomenon is reminiscent of the symmetry breaking phenomenon studied in Section 3.1.2, and is called dynamical symmetry breaking. Notice that dynamical symmetry breaking is apparently incompatible with the general result of Section 1.3.4 asserting that the long time solution of the master equation should coincide with the Gibbs measure. Consider the specific case of Fig. 3.4A. The Gibbs magnetisation is the position of the lowest minimum of $\hat{f}$, and thus equal to m_+. Nevertheless, starting from an initial condition $m(0) < m_0$ e.g. all spins down, the system will quickly relax towards the 'wrong' minimum m_-. The

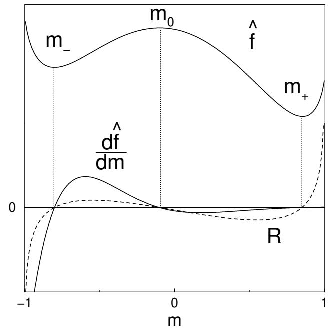

FIG. 3.4. Free energy functional $\hat{f}$ (top full curve) as a function of the magnetisation m for the Ising model at temperature $T = 0.7$ with $J = 1$, $h = 0.03$. The dashed curve represents the function R monitoring magnetisation relaxation (3.40) in the case of Glauber dynamics (1.56); R and the derivative of $\hat{f}$ (bottom full curve) have the same sign all over the magnetisation range. The extrema of $\hat{f}$ *i.e* the local minima m_-, m_+ and the local maximum m_0 coindice with the zeroes of R.

solution of this paradox is that our study of the dynamics assumes the thermodynamic limit $N \to \infty$ is taken first, prior to sending time to infinity while the Gibbs measure is certainly reached when we sent the time to infinity for a finite system size.

3.2.3 *Barriers, metastability and states*

As said above, for finite size N, we expect the rate function ω to converge towards the Gibbs rate function $\hat{\omega}(m)$ (3.12). It is a simple check that the latter is indeed a stationary solution of eqn (3.33). Using the relationship (3.13) between the rate function $\hat{\omega}$ and the free-energy function $\hat{f}$ (3.8), we obtain with definition (3.34) for function H,

$$H\left(m, \frac{\partial \hat{\omega}}{\partial m}(m)\right) = \frac{1}{2}\big[1 - m - e^{-2(J\,m+h)/T}(1+m)\big] \times \big[w\big(2(J\,m+h)\big)\,e^{2(J\,m+h)/T} - w\big(-2(J\,m+h)\big)\big] = 0 \quad . \tag{3.42}$$

for any transition rate w that fulfills detailed balance (1.54). The rate function $\hat{\omega}$ is plotted in Fig. 3.5 for the same parameters as Fig. 3.4.

So far, we have considered the dynamics of the Ising model for times t kept finite as $N \to \infty$. In this regime, we have found that, starting with a configuration of magnetisation smaller than m_0, the magnetisation relaxes to the 'wrong' value m_-. What happens next, that is, on time scales diverging exponentially with N can be inferred from the shape of the rate function in Fig. 3.5. At times increasing exponentially with N, $t \sim e^{N\tau}$, we expect configurations of magnetisation m

close to m_- to be visited by the dynamics with their expected exponentially small-in-N probabilities

$$\text{Prob}[m] = C_N \times e^{N\,\hat{\omega}(m)+o(N)} \tag{3.43}$$

where the normalisation constant C_N ensures that $\text{Prob}[m_-] = 1$ in the large N limit: $C_N = e^{-N\,\hat{\omega}(m_-)+o(N)}$. The larger the time scale τ, the further away from m_- magnetisations m are visited. More precisely, at time $t \sim e^{N\tau}$, accessible magnetisations m are those for which the probability (3.43) is not much smaller than $1/t \sim e^{-N\tau}$ *i.e.* such that [60]

$$\hat{\omega}(m) \geq \hat{\omega}(m_-) - \tau \quad . \tag{3.45}$$

Let us stress that statement (3.45) does not disagree with with eqn (3.40) for the dynamics of the most likely magnetisation. If at some time $t \sim e^{N\tau}$ a magnetisation $m \neq m_-$ is reached, this magnetisation will almost surely relax to the value m_- in a finite time, and it will take roughly the same exponential time for the system to reach magnetisation m again[61]. Relationship (3.45) between time scales τ and accessible magnetisations m is illustrated in Fig. 3.5, and holds as long as τ is smaller than the time scale

$$\tau_- = \hat{\omega}(m_-) - \hat{\omega}(m_0) \tag{3.46}$$

associated to the configurations located in the local minimum of $\hat{\omega}$. Magnetisations $m_0 + \epsilon$, however small $\epsilon > 0$, indeed relax in a finite time towards the Gibbs value m_+. The exploration process of less and less likely magnetisation then resumes in the local minimum of $\hat{f}$ centered around m^+. When the time reaches $t \sim e^{N\tau_+}$ where

$$\tau_+ = \hat{\omega}(m_+) - \hat{\omega}(m_0) \quad , \tag{3.47}$$

the configurations of magnetisation m_0, and consequently the whole metastable state centered around m_- can be reached again. Finally, for even larger times $t \sim e^{N\tau_{therm}}$ with

[60] This statement can be understood as follows. Let $\mathcal{I} = [m_1; m_2]$ be the set of magnetisations fulfilling eqn (3.43) at some time t. We have $m_1 < m_- < m_2$, $\omega(m_1) = \omega(m_2) = \omega(m_-) - \Omega$, where Ω has to be determined. Magnetisations smaller than m_1 or larger than m_2 have not been visited yet and have essentially null probabilities. The probability $q(t')$ that the magnetisation has never left interval $\mathcal{I}$ up to time $t + t'$ fulfills $q(0) = 1$ and $\frac{dq}{dt'}(t') = -w\,q(t')$, where

$$w = W_R\big[N\,m_1 - 2, N\,m_1\big]\ \text{Prob}[m_1] + W_R\big[N\,m_2 + 2, N\,m_2\big]\ \text{Prob}[m_2] \tag{3.44}$$

since magnetisations leak out from $\mathcal{I}$ through the boundaries only. As rates W_R (3.31) are of the order of N, we have $w \sim \text{Prob}[m_1] = \text{Prob}[m_2] \sim e^{-N\Omega}$ from (3.45). Thus the probability that no magnetisation outside $\mathcal{I}$ has been visited after delay $t' = e^{N\tau'}$ is $q(t') = e^{-w\,t'} \sim \exp\{-e^{N(\tau'-\Omega)}\}$. We have $q = 1$ if $\Omega > \tau'$, $q = 0$ if $\Omega < \tau'$ (Griffiths, Weng, Langer 1966). Hence eqn (3.45).

[61] In few words, while it takes a finite time to go down in the free energy landscape, going up requires exponentially long times.

$$\tau_{therm} = \hat{\omega}(m_+) - \min_m \hat{\omega}(m) \quad , \tag{3.48}$$

all configurations can be visited by the dynamics with a frequence equal to their Gibbs probability. τ_{therm} is called thermalisation time scale: it is the time scale necessary for a complete sampling of the Gibbs measure.

We conclude that, starting from an initial condition $m < m_0$, the magnetisation almost surely sticks to the value m_- at all times $t < e^{N\tau_- + o(N)}$, with large deviations described by eqn (3.45). Consequently, an observer carrying out a numerical experiment on a computer running may find this time practically infinite and wrongly conclude that the average magnetisation is m_- (rather than m_+)[62]. This phenomenon is called metastability, and the set of configurations defining the local minimum of $\hat{f}$ around m_-, metastable state. A metastable state is a region of the space of configurations in which the system remains trapped from a huge time before escaping to another region[63]. This trapping time, $t \sim e^{N\tau_{metastable}}$, is called life time of the metastable state. Going back to the Ising model case, the life time associated to the metastable state around magnetisation m_- is given by the height of the barrier separating this state from the Gibbs state,

$$\tau_{metastable} = \tau_- = \frac{1}{T}\big(\hat{f}(m_0) - \hat{f}(m_-)\big) \tag{3.49}$$

from eqns (3.46) and (3.13). We shall come back to these notions in Section 3.3.1.

3.3 Complements

3.3.1 *Pathes and path-integral.*

In this section, we propose an alternative expression for the probability for the magnetisation based on the concept of path-integral. As a byproduct, this approach will allow us to solve eqn (3.33) for the dynamical rate function. Our starting point is a new expression for the transition matrix W_R based on the following trigonometric identity holding for integer-valued Δ

$$\int_0^{2\pi} \frac{d\theta}{2\pi}\, e^{i\theta\Delta} = \begin{cases} 1 \text{ if } \ \Delta = 0 \\ 0 \text{ otherwise} \end{cases} . \tag{3.50}$$

Introducing $\hat{m} = i\theta$ instead of the angle, we rewrite the transition rate

$$W_R[M', M] = \sum_{M''} \int_0^{2\pi i} \frac{d\hat{m}}{2\pi i}\, e^{\hat{m}\,(M''-M)}\, W_R[M', M'']$$

[62]For the parameters of Fig. 3.5, $\tau_- \simeq 0.066$, and $e^{N\tau_-} \simeq 5\ 10^{28}$ with $N = 1000$ spins. A sensible order of magnitude for the flipping time of a spin *in silico* is about 10^{-9} second. Thus, neglecting non exponential contribution to the barrier crossing time, it would take on the average about 100 hundreds time the age of the universe (10 billions years) to reach the correct Gibbs magnetisation m_+...

[63]The vocable metastable underlines the discrepancy with the true stability of the Gibbs measure which holds forever.

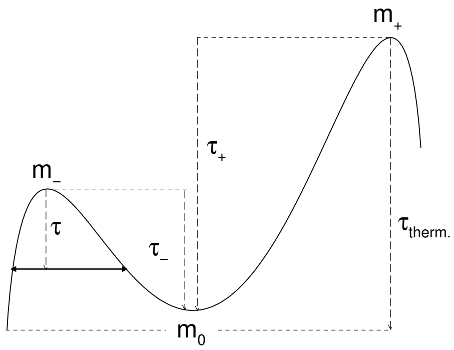

FIG. 3.5. Time scales and barriers for the dynamics of magnetisation for the Ising model with $T = 0.7$, $J = 1$, $h = 0.03$. The full curve is the rate function $\hat{\omega}$. After the initial relaxation the magnetisation is equal to the metastable value m_-. The range of magnetisations accessible to the dynamics at time $t \sim e^{N\tau}$ is symbolised by the plain line with double arrow. At time $t \sim e^{N\tau_-}$, the bottleneck in m_0 can be passed, and the magnetisation jumps to its most likely value m_+. Magnetisations smaller than m_0 are accessible again for $t \sim e^{N\tau_+}$, and the thermalisation process is complete for $t \sim e^{N\tau_{therm}}$.

$$= \int_0^{2\pi i} \frac{d\hat{m}}{2\pi i}\, e^{\hat{m}\,(M'-M)} \times N\; H\left[\frac{M'}{N}, \hat{m}\right] \tag{3.51}$$

where H is defined in eqn (3.34).

Let us now integrate master equation (3.29) over a small time interval δ,

$$\begin{aligned} P(M', t+\delta) &= P(M',t) + \delta \sum_M W_R[M',M]\; P(M,t) + O(\delta^2) \qquad (3.52)\\ &= \sum_M \int_0^{2\pi i} \frac{d\hat{m}}{2\pi i}\, e^{\hat{m}\,(M'-M)+\delta\, N\, H[M'/N,\hat{m}]+O(\delta^2)}\; P(M,t) \end{aligned}$$

where we have made used of eqn (3.51). Iterations of eqn (3.52) permits us to express the probability of magnetisation at time τ in terms of the one at time 0, and of $J = \tau/\delta$ sums and J integrals over intermediary magnetisations M_j and 'angular' variables $\hat{m}_j$ respectively,

$$P(M_J, \tau) = \sum_{M_0} \dots \sum_{M_{J-1}} \int \frac{d\hat{m}_0}{2\pi i} \dots \int \frac{d\hat{m}_{J-1}}{2\pi i}\; e^{N\,\mathcal{S}_J[\{M_j,\hat{m}_j\}]}\; P(M_0, 0)\ . \tag{3.53}$$

The integration bounds are the same as in eqn (3.52) and are omitted for the sake of conciseness. The exponential weigth reads, up to $O(\delta^2)$ additive terms,

$$\mathcal{S}_J[\{M_j, \hat{m}_j\}] = \delta \sum_{j=0}^{J-1} \left\{ \hat{m}_j\, \left(\frac{M_{j+1}-M_j}{N\,\delta}\right) + H\left[\frac{M_{j+1}}{N}, \hat{m}_j\right]\right\}\ . \tag{3.54}$$

One of the sequences of magnetisations $\{M_0, M_1, \ldots, M_J\}$ contributing to (3.53) is shown in Fig. 3.6. Allowed sequences are continuous due to $|M_{j+1} - M_j| \le 2$. As δ is chosen smaller and smaller, the number J of intermediary time steps increases. In the continuous time limit $\delta \to 0$, we assume that the magnetisation sequences can be expressed from a single differentiable function: $M_j = N\, m(j \times \delta)$ (Fig. 3.6). The J-dimensional sum over magnetisation becomes a functional integral over the magnetisation function $m(t)$ with $t \in [0;\tau]$, with a measure denoted by $\mathcal{D}m(t)$. The same assumption is made for the 'angular' variables, $\hat{m}_j = \hat{m}(j \times \delta)$, and leads to the following concept of path-integral.

A path, or trajectory over the time range $[0;\tau]$, is a set of two differentiable functions $\{m(t), \hat{m}(t)\}$ over this time interval, $0 < t < \tau$. The action $\mathcal{S}$ is a function from the set of possible pathes to real numbers defined as the continuous time limit of $\mathcal{S}_J$ (3.54),

$$\mathcal{S}(\{m, \hat{m}\}) = \int_0^\tau dt \left[\hat{m}(t)\, \frac{dm}{dt}(t) + H\big(m(t), \hat{m}(t)\big)\right] \tag{3.55}$$

The probability that the magnetisation is equal to m_τ at time τ given its value m_0 at time 0 is given by the integral of $e^{N\mathcal{S}}$ over all pathes constrained to the desired initial and final values for the magnetisation,

$$\text{Proba}[m_\tau, \tau | m_0, 0] = \int_{m(0)=m_0}^{m(\tau)=m_\tau} \mathcal{D}m(t) \int \mathcal{D}\hat{m}(t)\; e^{N\,\mathcal{S}(\{m,\hat{m}\})}\ . \tag{3.56}$$

The integration measure over pathes $\{m(t), \hat{m}(t)\}$ is not easily defined for continuous time, and should be thought as the $\delta \to 0$ limit of the measures associated to the finite J sums and integrals in eqn (3.53).

In the large N limit, the path integral (3.56) is dominated by the path $\{m^*(t), \hat{m}^*(t)\}$ maximising the action $\mathcal{S}$, that is, the solution of the functional extremisation equations[64]

$$\frac{\delta \mathcal{S}}{\delta \hat{m}(t)}(\{m^*, \hat{m}^*\}) = 0 \to \frac{dm^*}{dt}(t) = -\frac{\partial H}{\partial \hat{m}}\big(m^*(t), \hat{m}^*(t)\big) \tag{3.57}$$

$$\frac{\delta \mathcal{S}}{\delta m(t)}(\{m^*, \hat{m}^*\}) = 0 \to \frac{d\hat{m}^*}{dt}(t) = \frac{\partial H}{\partial m}\big(m^*(t), \hat{m}^*(t)\big) \tag{3.58}$$

These two ordinary first order differential equations, once completed by the boundary conditions $m(0) = m_0, m(\tau) = m_\tau$, generally guarantee the existence

[64] Functional differentiation is an extension of usual differentiation to functionals. Let $L(x)$ be a functional over the set of functions $x(t)$, $0 < t < \tau$. Some examples are $L_1(x) = \int_0^\tau dt\, x(t)^2$, $L_2(x) = x(\tau/2)$, $L_3(x) = \int_0^\tau dt\, y(t)\, \frac{dx}{dt}(t)$. The functional derivate of L with respect to x in t is the kernel $K(t)$, if it exists, characterizing the change in L under small functional variations $\epsilon(t)$, $L(x+\epsilon) = L(x) + \int_0^\tau dt\ K(t)\ \epsilon(t) + O(\epsilon^2)$. The usual notation for K is $\frac{\delta L}{\delta x(t)}$. Coming back to the above examples, we obtain $\frac{\delta L_1}{\delta x(t)} = 2\, x(t)$, $\frac{\delta L_2}{\delta x(t)} = \delta(t - \tau/2)$ where δ denotes the Dirac distribution, and $\frac{\delta L_3}{\delta x(t)} = -\frac{dy}{dt}(t)$. The latter result is obtained through an integration by part.

FIG. 3.6.

and uniqueness of the optimal (also called classical) path. The optimal action is interpreted as the dynamical rate function, compare eqns (3.56) and (3.32),

$$\omega(m_\tau, \tau) = \mathcal{S}(\{m^*, \hat{m}^*\}) \ , \tag{3.59}$$

when all magnetisations but m_0 have zero probabilities at initial time. The same conclusion can be reached when applying the characteristic method to solve partial differential equation (3.33)[65].

Expression (3.34) for H shows that $\hat{m}^*(t) = 0$ is a solution of eqn (3.58). The corresponding action vanished from (3.55), and so does the rate function ω. Equation (3.57) for $m^*(t)$ reduces to the relaxation equation (3.40) for the most likely magnetisation $m^+(t)$ as expected.

Generally speaking, imposing a final value for the magnetisation different from the local minima m_-, m_+ will compell us to look for a solution with $\hat{m}^* \neq 0$. The corresponding optimal path has a simple statistical interpretation. The value of the magnetisation $m^*(t)$ is the best possible one *i.e.* the one with highest probability allowing one to reach magnetisation m_τ at time τ starting from m_0. The associated variable, $\hat{m}^*(t)$, corresponds to the partial derivative of ω at as function of time.

3.3.2 *On small dynamical fluctuations*

So far, our dynamical analysis has led to the conclusion that all magnetisations but the location m^* of the minimum of the free energy $\hat{f}$ have vanishingly small

[65] These results are found back from the observation that partial differential equation (3.33) involves first derivatives only, and can be solved with the characteristic method. To do so, we proceed in two steps. First, we define the function $\hat{m} = \dfrac{\partial \omega}{\partial m}$ and differentiate eqn (3.33) with respect to m to obtain

$$\frac{\partial \hat{m}}{\partial t} = \frac{\partial H}{\partial m}(m, \hat{m}) + \frac{\partial H}{\partial \hat{m}}(m, \hat{m}) \frac{\partial \hat{m}}{\partial m} \tag{3.60}$$

Equation (3.60) is now linear in the partial derivatives and the application of the characteristic method is immediate. $z = \hat{m}(m, t)$ defines a bidimensional surface $\hat{\mathcal{M}}$ in the space (m, t, z); we look for unidimensional trajectories $m(t), t, z(t)$ constrained to lie on $\hat{\mathcal{M}}$. The constraint reads $z(t) = \hat{m}\big(m(t), t\big)$; differentiating with respect to time, we obtain

$$\frac{dz}{dt} = \frac{\partial \hat{m}}{\partial m}\frac{dm}{dt} + \frac{\partial \hat{m}}{\partial t} = \frac{\partial \hat{m}}{\partial m}\left[\frac{dm}{dt} + \frac{\partial H}{\partial \hat{m}}(m, z)\right] + \frac{\partial H}{\partial m}(m, z) \tag{3.61}$$

where we have used eqn (3.60). We conclude that the trajectories defined by eqns (**??**) (with the change of notation $z \to \hat{m}$) do lie on surface $\hat{\mathcal{M}}$. Varying the initial conditions for $m, \hat{m}$ allows us to span the whole surface, and obtain the solution of eqn (3.33). The idea of trajectory intrinsic to the characteristic method is equivalent to the one of optimal (classical) path in the path-integral formalism. The reader with a background in mechanics (Goldstein ..). will have recognized the equivalence between eqns (3.57,3.58) and the Hamilton equations associated to 'Hamiltonian' H, and between the action $\mathcal{S}$ and the Hamilton-Jacobi functional.

probabilities at long time. This result holds for the intensive magnetisation, that is, the magnetisation per spin, but does not prevent small fluctuations to exist. Drawing our inspiration from Section 1.3.3, we expect magnetisations deviating from m^* by $O(1/\sqrt{N})$ to have a substantial probability. This guess can be quantitatively supported as follows. Let us denote by $\rho(x,t)$ the probability that the amplitude of the fluctuation equals x at time t,

$$P_R(M = m^* N + x\sqrt{N}, t) \propto \rho(x,t) \tag{3.62}$$

up to some (x-independent) normalisation constant. Inserting expression (3.62) for the probability into eqn (3.29) and expanding in powers of $N^{-1/2}$, we obtain in the large N limit the diffusion equation[66]

$$\frac{\partial \rho}{\partial t}(x,t) = \left(\frac{D^*}{2} \frac{\partial^2}{\partial x^2} + V^*\, x\, \frac{\partial}{\partial x} + V^* \right) \rho(x,t) \tag{3.64}$$

up to $o(1)$ additive terms. The coefficients read

$$\begin{aligned} V^* &= \sum_{\sigma=\pm 1} \Big[w\big(2\sigma(J\, m^* + h)\big) + 2J(1+\sigma\, m^*)\; w'\big(2\sigma(J\, m^* + h)\big) \Big] \\ D^* &= \sum_{\sigma=\pm 1} 2\left(1+\sigma\, m^*\right)\; w\big(2\sigma(J\, m^* + h)\big) \quad , \end{aligned} \tag{3.65}$$

where w' denotes the first derivative of w. While V^* andD^* depend on the specific choice for the transition rate w, their ratio[67]

$$\omega = \frac{V^*}{D^*} = \frac{1}{2T}\, \frac{d^2 \hat{f}}{dm^2}(m^*) \tag{3.66}$$

is a purely Gibbsian quantity in that ω depends on the free energy $\hat{f}$ and the temperature only. Notice that D^* is clearly positive from definition (3.65); V^* and

[66] Expansion of the transition rate (3.31) gives

$$\begin{aligned} W_R[M+2\sigma, M] &= N\left(\frac{1-\sigma\, m^*}{2} - \frac{\sigma\, x}{2\sqrt{N}}\right)\; w\left(-2\sigma\left(J\, m^* + h + \frac{J\, x}{\sqrt{N}}\right) - \frac{2J}{N}\right) \\ &= N\, W_0^*(\sigma) + \sqrt{N}\, W_1^*(\sigma) + W_2^*(\sigma) + o(1) \end{aligned} \tag{3.63}$$

with $W_0^*(\sigma) = (1-\sigma m^*)\, w(-2\sigma u)/2$, $W_1^*(\sigma) = -\sigma x\big(w(-2\sigma u) + 2J(1-\sigma m^*)\, w'(-2\sigma u)\big)/2$, $W_2^*(\sigma) = (J^2x^2 - (1-\sigma m^*))\, w'(-2\sigma u) + J^2 x^2\,(1-\sigma m^*)\, w''(-2\sigma u)$, and $u \equiv J\, m^* + h$. Similarly, we obtain $W[M, M+2\sigma] = N\, W_0^*(-\sigma) + \sqrt{N}\, W_1^*(-\sigma) + \hat{W}_2^*(\sigma) + o(1)$ with $\hat{W}_2^*(\sigma) = w(2\sigma u) + (J^2x^2 + 1 - \sigma m^*)\, w'(2\sigma u) + J^2 x^2\,(1+\sigma m^*)\, w''(2\sigma u)$. Finally we expand

$$P[M+2\sigma, t] \propto \rho\left(x + \frac{2\sigma}{\sqrt{N}}, t\right) = \rho(x,t) + \frac{2\sigma}{\sqrt{N}}\, \frac{\partial \rho}{\partial x}(x,t) + \frac{2}{N}\, \frac{\partial^2 \rho}{\partial x^2}(x,t) + o\left(\frac{1}{N}\right) \; .$$

Inserting the above expansions into eqn (3.29) and exploiting the condition $R(m^*) = 0$ with R defined in (3.37), we see that the contributions of order N and $\sqrt{N}$ vanish. The contribution of the order of unity yields partial differential equation (3.64).

[67] Using the stationary condition of $\hat{f}$ in m^*, $m^* = \tanh\big((m^*+h)/T\big)$, see (3.9), we obtain $D^* = 4\,(1-m^*)\, w(-2(Jm^*+h))$. From eqn (3.37), we remark that V^* is simply the derivative of R in m^*. Differentiating expression (3.41) for R yields $V^* = D^*/2/T \times d^2\hat{f}/dm^2(m^*)$.

ω are positive (respectively negative) if m^* is a local minimum (resp. maximum) of the free energy $\hat{f}$.

Let us look for the eigenfunctions of the linear operator acting on $\rho(x,t)$ on the r.h.s. of (3.64), that is, for distributions showing an exponential dependence upon time, $\rho(x,t) = \rho(x)\,\exp(\lambda t)$,

$$\lambda\,\rho(x) = \left(\frac{D^*}{2}\,\frac{\partial^2}{\partial x^2} + V^*\,x\,\frac{\partial}{\partial x} + V^*\right)\rho(x) \qquad (3.67)$$

Equation (3.67) bears a strong analogy with the well-studied quantum mechanical problem of the harmonic oscillator in one dimension. The connection is easily seen with the change of function

$$\psi(x) = \rho(x)\,\exp\left(\frac{\omega}{2}\,x^2\right) \qquad (3.68)$$

It is simple to check that ρ is a solution of eqn (3.64) with eigenvalue λ if ψ fulfills the stationary Schrödinger equation of the harmonic oscillator,

$$E\,\psi(x) = \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\,\omega^2\,x^2\right)\psi(x) \qquad (3.69)$$

where the energy is given by

$$E = \frac{\omega}{2} - \frac{\lambda}{D^*} \quad . \qquad (3.70)$$

The spectrum of the harmonic oscillator with frequency $|\omega|$ is discrete and each eigenvalue E_n labelled by an integer $n \geq 0$. The eigenvalues and corresponding eigenfunctions are

$$E_n = \left(n + \frac{1}{2}\right)|\omega| \quad , \qquad \psi_n(x) = H_n(x)\,e^{-|\omega|x^2/2} \qquad (3.71)$$

where H_n is the Hermitte polynomial of degree n (Cohen-Tannoudji mettre ref. exacte). We deduce from mapping (3.70) that the spectrum of our diffusion equation is discrete too, and that the eigenvalues and eigenfunctions are given by (Ruijgrok, Tjon 1973))

$$\lambda_n = D^*\left(\frac{\omega - |\omega|}{2} - n\,|\omega|\right) \quad , \qquad \rho_n(x) = H_n(x)\,e^{-(\omega+|\omega|)x^2/2} \quad . \qquad (3.72)$$

The general solution of (3.64) can be expressed as a linear combination,

$$\rho(x,t) = \sum_{n\geq 0} c_n\,\exp(\lambda_n\,t)\,\rho_n(x) \quad , \qquad (3.73)$$

where the coefficients c_n can be determined from the initial distribution $\rho(x,0)$. Two cases have to be considered:

- $\underline{m^* \text{ is a local minimum of } \hat{f}}$ (ω is positive): the smallest eigenvalue (in modulus) is $\lambda_0 = 0$; all other eigenvalues are negative, and the corresponding modes decrease over characteristic times $t_n = 1/|\lambda_n|$. At large times the only contribution to ρ in (3.73) is provided by the $n = 0$ mode: the eigenfunction $\rho_0(x)$ is a Gaussian measure with zero mean and inverse variance 2ω and coincides with the Gibbs distribution (3.11) for the fluctuations of the magnetisation.
- $\underline{m^* \text{ is a local maximum of } \hat{f}}$ (ω is negative): the spectrum is identical to the previous case except that the zero mode is absent; all eigenvalues are negative and ρ decays to zero with increasing time. Furthermore, the eigenfunctions $\rho_n(x)$ (3.72) are not bounded (in modulus) when fluctuations get larger and larger, $x \to \pm\infty$. These results unveil the nature of the fixed point solution $m^* = m_0$ for the dynamics of the magnetisation (3.40). Any small fluctuation around the initial magnetisation m_0 will get amplified and, depending on its sign, will push the magnetisation away towards m_- or m_+ (Fig. 3.4). The time required for this amplification is related to the eigenvalue λ_1 (Griffiths, Weng, Langer 1966; Langer 1969) and contributes to the finite N corrections to the barrier crossing time (3.49).

The above analysis[68] does not apply right at the critical temperature, where the second derivative of $\hat{f}$ vanish. From Section 3.1.3, we expect typical fluctuations to be of the order of $N^{-1/4}$ in that case. The evolution equation for the distribution of critical fluctuations can be mapped onto the Schrödinger equation for an anharmonic quantum oscillator with quartic potential.

3.4 Exercices

1. How does equation (3.9) get modified in presence of a non-zero magnetic field h? Calculate explicitely the free-energy for $h \neq 0$, and check the correctness of the statements in Section 3.1.2.
2. Consider the Blume-Emery-Griffiths model on the complete graph K_N with energy function

$$E(\sigma_1, \ldots, \sigma_N) = -\frac{1}{N}\sum_{i<j} \sigma_i \sigma_j - \Delta \sum_i \sigma_i^2 - h \sum_i \sigma_i \qquad , \qquad (3.74)$$

where the spins σ_i may take values $-1, 0, +1$. Compute the free-energy of the BEG model in the infinite size N limit as a function of temperature, magnetic field h and chemical potential Δ. What are the order parameters, and the different phases characterizing the BEG model?
See Blume, Emery, Griffiths (1971).

[68]The present case is an illustration of the general relationship existing between (the Fokker-Planck equation associated to) the stochastic motion of a classical particle in a potential and submitted to a random Gaussian force with (the Schödinger equation associated to) a quantum particle in the same potential (Zinn-Justin).