Topics in Stat. Mech. (PHY 521-MAT 597)

Supplemental Lecture Notes

The following Table of Content will be dynamically adjusted as we progress through the material.

PART I. Stat-Mech and Thermo

Laws: imposed or emergent?

1

Theory emerging from Chaos

1.1 The puzzle of thermodynamics

Statistical Mechanics broke on the scene with Boltzmann's explanation of the major puzzle of **thermodyamics**. While the laws of mechanics are given by equations, the main principle of the phenomenological theory of Thermodynamics is expressed in an inequality:

$$\Delta S \ \geq \ 0\,. \tag{1.1}$$

It quantifies the observable processes' irreversibility in time in terms of an **entropy** function $S = S(V, N, E, ...)$. The big puzzle which Boltzmann successfully tackled was the reconciliation of the observed irreversibility of physical processes with the time reversibility of its the basic laws. In the process he presented an intrinsic formulation of entropy.

Boltzmann's insightful formula is

$$\boxed{S = k_B \log W} \tag{1.2}$$

where W is the number, or measure (in the continuous case), of microstates corresponding to a thermodynamic macrostate, the latter being described in terms of the few relevant extensive parameters, e.g. the volume (V), energy (E), number of particles (N), magnetization, and k_B is a constant (whose dimension is that of a ratio of energy over temperature).

1.2 An instructive example

For a quick grasp of the key observation which underlines the principles of statistical mechanics it may be instructive to consider the simple example of the adsorption process.

Adsorption occurs when particles (atoms, molecules or ions) of a gas or liquid get attached to sites on the surface of solid. In a simplified model the surface is represented by an array of V sites and it is assumed that for any N all configurations with that number of adsorbed particles and no more than one particle per site are equally likely.

The overall density of adsorbed particles is $n = N/V \in [0, 1]$. Two simple questions are worth considering.

1) Splitting the adsorption surface into two roughly equal parts, estimate the probability that the empirical densities in the two are visibly different, say $n_1 - n_2 = \Delta n$ excedes 10^{-4}. For concreteness

sake, consider a surface of size $1cm \times 1cm$ on which the vacancies are spaced $1nm$ apart, in which case $V \approx 10^{14}$.
2) For a specified number N of adsorbed particles, what is the probability distribution of the configuration within a relatively small patch on the adsorbing surface?

For the moment we postpone the second question. It leads to the principle of equivalence of ensembles that is discussed further below.

To address the first question one may proceed as follows. The number of possible configurations of $N = nV$ indistinguishable particles on V sites is given by:

$$W(V,N) \;=\; \binom{V}{N} \;=\; \frac{V!}{N!(V-N)!}\,. \tag{1.3}$$

This number is exponentially large in N. Its order of magnitude can be conveyed by writing it as

$$\boxed{W(V,N) \;\approx\; e^{s(n)V}} \tag{1.4}$$

where $s(n)$ would turn to be a function of the density. Its values are neither negligible nor divergent as long as $n = N/V$ is not very close to either 0 or 1.

In fact, $s(n)$ can be computed through Stirling's approximation:

$$N! \;= N[\log(N) - 1] + \log(2\pi N) + O(\frac{1}{N})\,, \tag{1.5}$$

from which one readily finds:

$$\boxed{s(n) \;=\; -\left[n\log n + (1-n)\log(1-n)\right]\,.} \tag{1.6}$$

This function is smooth and strictly concave over $[0,1]$, with $\max_n s(n) = s(1/2) = \log 2$.

Thus, assuming the probably is equidistributed among all the different configurations of the given number N of adsorbed particles, the probability that the densities (n_1, n_2) in the two half of the systems differ by Δn is

$$\Pr(n_1, n_2) \approx \exp\{\Delta s \cdot V\} \tag{1.7}$$

with

$$\Delta s = s(1/2 + \Delta n/2) - s(1/2 - \Delta n/2) \approx \frac{s''(1/2)}{4}(\Delta n)^2 = -(\Delta n)^2 < 0\,. \tag{1.8}$$

In situations where $V \approx 10^{14}$ even for $\Delta n = 10^{-4}$ the above is a truly negligible probability ($\approx \exp\{-10^6\}$).

The above calculation is an example of the predictably orderly behavior emerging from an underlying chaos. The detailed study of such phenomena form a core theme of statistical mechanics. The numbers of degrees of freedom which are of relevance for estimates of discrepancies in thermodynamic calculations for gases and fluids are estimable in terms of the Avogadro number $N_A = 6.0 \cdot 10^{23}$ (the number of particles per mole). In that range, probabilities of the order of e^{-N} are mind-bogglingly small.

1.3 The Stat-Mech Setup

Statistical mechanics offers an approach to the physics of a broad range of system. A salient feature is that the discussion involves two widely disparate scales, one referred to as the **macroscopic** and the other as the **microscopic** scale. In between, one may also talk about a range of **mesoscopic** scales.

On the suitably **small scale** the systems may be described in terms of a multitude of agents, e.g. molecules of the gas or liquid, electrons in a solid, or bits of information in a stream by which messages are being transmitted. Such system's "microstate" is parametrized through a **very large number of degrees of freedom**. Their nature may vary:

- Classical systems: the configuration of N particles in a region $V \subset \mathbb{R}^3$ is described by a point in the phase space $(V \times \mathbb{R}^3)^N$. For the liquid in a cup of tea N may be of the order of the Avogadro number, i.e. $\approx 10^{23}$.
- Quantum continuum systems: the microscopic state is described by a vector, or a density matrix, in a Hilbert space of dimension comparable with the number of states of the systems' classical analogs.
- Lattice systems: these may be of either quantum nature, such as large arrays of Q-bits, or arrays of variables describable in terms of random variables.

A condition of fundamental importance is the existence of a natural measure of micro-states at which macroscopically constrained state of a finite systems can be realized. Of fundamental importance is that this measure be one for which one may expect equidistribution for systems in thermodynamic equilibrium, constrained by a narrow range of values of the listed extensive parameters.

- For classical systems, a natural microstate measure is given by the Liouville measure $\prod_j (dq_j \, dp_j)$ integrated over the corresponding region in the classical phase space. E.g., in case the constraining variables are $(V, N, E, ...)$, with E specified to within ΔE the measure is

$$W(V, N, E\,;\, \Delta E) \;:=\; \int_{V^N} \int_{\mathbb{R}^{3N}} \mathbb{1}[H_N(\underline{q}, \underline{p}) \in (E, E + \Delta E)] \prod_{j=1}^{N} dq_j \, dp_j \tag{1.9}$$

- For quantum systems the natural counting is given by the dimension of the projection onto the corresponding subspace of states of the finite system. Thus for a quantum system of N particles in a volume V

$$W(V, N, E; \Delta E) \;:=\; \mathrm{Tr}_{\mathcal{H}_{N,V}} \, P_{H \in (E, E+\Delta E)} \,. \tag{1.10}$$

  where $\mathcal{H}_{N,V} = L^2_{stat}(V^N)$ is the appropriate Hilbert space of functions satisfying the suitable symmetry conditions. In each of the above cases there is room for adding additional constraints of the values of other extensive quantities, for instance magnetization.
- For discrete stochastic systems, such as the above gas adsorption model, the measure counts the number of microscopic configurations which are consistent with the macroscopic constraints.

$$W(V, N, E\,;\, \Delta E) \;:=\; \sum_{\omega \in \Omega_{\Lambda,N}} \mathbb{1}[H(\omega) \in (E, E + \Delta E)] \,. \tag{1.11}$$

In particular, the microstate counting measure should be robustly invariant under the relevant time evolution under which the constrained qualities are, by large, preserved (see comment below). This condition is satisfied in both the classical and quantum examples mentioned above.

The situation of particular interest here is described by the so called **thermodynamic limit**, which is when N and other extensive quantities V, E diverge (when measured on the microscopic scale) but their ratios converge to corresponding limits, i.e.

$$N \to \infty\,, \quad N/V \to n\,, \quad E/V \to u\,, \quad \text{etc}\ldots \tag{1.12}$$

1.4 Boltzmann's equidistribution hypothesis

Boltzmann's resolution of the entropy puzzle rests on the bold, yet physically arguable assumption, that the equilibrium state of a large system which is subject to macroscopic constraints, e.g. on the values of $(V, N, E, ...)$, is well described by an equidistribution among all the microscopic states of the system, which are consistent with the macroscopic constraints. In such a state, the mean values of physical quantities, e.g. functions $F : \Omega \mapsto \mathbb{R}$ (in reference to the last example), is given by the **microcanonical ensemble** average

$$\langle F \rangle \;=\; \sum_{\omega \in \Omega_{\Lambda,N}} F(\omega) \frac{\mathbb{1}[H(\omega) \in (E, E + \Delta E)]}{W(V, N, E\,;\, \Delta E)}\,. \tag{1.13}$$

Under the above assumption, and the order of magnitude estimate expressed in (**??**), the entropy of the state which is reached after the relaxation of thermodynamic constraints (once the system has settled into a thermodynamic equilibrium state) will be no less than that of the initial state of the multi-component system. The reasoning is similar to that which we carried explicitly in the simple example of the adsorption process.

The size of ΔE is of little relevance in the above discussion, provided it is large on the microscopic scale yet negligible on the macroscopic scale, and thus not affecting u.

1.5 Entropy's additivity and order of magnitude

From the natural multiplicativity of the micro-state count in any composite system

$$W(V_1 + V_2, E_1 + E_2, N_1 + N_2, ...) = W_1(V_1, E_1, N_1, ...) \cdot W_2(V_2, E_2, N_2, ...) \tag{1.14}$$

It follows that $\log W$ is additive over macroscopic subsystems. Thus the entropy $S(V, E, N, ...)$ is also an extensive quantity, whose density (per volume, or per the number of particles) is a function of the densities of the constrained extensive quantities.

It also follows that in terms of orders of magnitude,

$$W(V, N, E\,;\, \Delta E) \approx \exp\left\{ \frac{s(u, n)}{K_B} V \right\} \tag{1.15}$$

with $u = \frac{E}{V}$, $n = \frac{N}{V}$, etc.

Furthermore, thermodynamic stability combined with the above assumptions requires the entropy function $s(u,n)$ to be concave, and thus somewhat regular. More will be said on these points below.

1.6 Notes

- It is often asserted that Boltzmann's equidistribution hypothesis rests on an assumed **ergodicity** of the system's time evolution (described by the Hamiltonian flow on the system's phase space). We view that to be an oversimplification.

  The microstate counting measure which underlies the microcanonical ensemble (the Liouville measure over the phase space $\pi_j dx_j dp_j$) is invariant under **any** Hamiltonian dynamics. Thus the Boltzmann hypothesis is stable under the possible presence of minor deviations from strict stationarity of the Hamiltonian, as long as these preserve the macroscopic constrains within tolerable fluctuations ($|\Delta E| \ll E$). It would be realistic to say that Boltzmann's hypothesis even implicitly assumes such to occur. In contrast, for ergodicity to be even formulated a strict stationarity of the Hamiltonian (or at least periodicity in time) is essential, and is achievable only in perfectly insulated systems.

- In the absence of a naturally rational basis for the choice of an a-priori measure, the microstate counting function W requires some closer analysis. For example, in building the statistic theory of dice games it may seem a-priori natural to assign equal weight to all sequences outcomes. However, that would not be correct for games with a "loaded die". The question is of relevance in assigning an a-priori state counting measure W for models which lack the dynamical structure of the classical or quantum models.

  In case there is no sufficient information on the statistical or dynamical underpinning of the model, considerations of the above question may take one to the Bayesian inference theory, c.f.
  "Ten Great Ideas about Chance", by Persi Diaconis and Brian Skyrms, Princeton Univ. Press (2017).

- A brief yet informative summary of Boltzmann's seminal contributions to physics, and the world in which they were presented and debated, can be found on the Wikipedia page:

  https://en.wikipedia.org/wiki/Ludwig_Boltzmann

  The subject is of course also discussed in many other texts.

2

Gibbs ensembles

2.1 The partition function and the Legendre transform relations

The direct computation of the entropy function is a daunting task, which can be completed in only few simple examples. However much can learned about it through the partition function, which often is easier to approach.

The partition function is defined through the suitably *tilted* integral over the microcanonical ensemble:

$$\boxed{Z_\Lambda(\beta, N) \;=\; \int_{V^N}\int_{\mathbb{R}^{3N}} e^{-\beta H_N(\underline{q},\underline{p})} \prod_{j=1}^{N} dq_j\, dp_j} \tag{2.1}$$

or, in case of the discrete models,

$$\boxed{Z_\Lambda(\beta) \;=\; \sum_{\omega\in\Omega_{\Lambda,N}} e^{-\beta H(\omega)}\,.} \tag{2.2}$$

Rewritten in terms of an integral over the energy, this takes the form

$$\begin{aligned} Z_\Lambda(\beta, ...) &= \int_{\mathbb{R}} e^{-\beta E} e^{S(\Lambda,E,\dots)} dE \\ &= |\Lambda| \int_{\mathbb{R}} e^{|\Lambda|\left[-\beta u + s_\lambda(u,\dots)\right]} du\,. \end{aligned} \tag{2.3}$$

The winner takes all principle:

Due to the disparity in scales, i.e. the large size of the factor V in the exponent, the value of the integral in (2.3) is essentially determined by $\max_u\left[-\beta u + s(u,\dots)\right]$ (as we shall see the supremum is typically attained). Consequently, in the thermodynamic limit, the quantity

$$\Psi(\beta) \;:=\; \lim_{L\to\infty} \frac{1}{|\Lambda(L)|} \log Z_\Lambda(\beta, ...) \tag{2.4}$$

is related to the entropy through:

$$\boxed{\Psi(\beta) \;=\; \sup_u \left[-\beta u + s(u,\dots)\right]\,.} \tag{2.5}$$

As will be explained below, $\Psi(\beta)$ corresponds to the pressure at temperature $T = (k\beta)^{-1}$. The expression on the right is a particular case of the **Legendre transform**, on which we shall expand below.

2.2 Gibbs canonical ensembles

Naturally associated with the tilted integral is the state in which the probability weight of any microscopic configuration is proportional to $e^{-\beta H(\omega)}$ - which would be referred to as the Gibbs factor. That is, the microcanonical ensemble average (1.13) is replaced by

$$\boxed{\langle F\rangle_{\beta,\Lambda,N} \;=\; \sum_{\omega\in\Omega_{\Lambda,N}} F(\omega)\frac{e^{-\beta H(\omega)}}{Z_\Lambda(\beta,N)}} \tag{2.6}$$

which is referred to as the **canonical ensemble average**.

The concentration argument which leads to (2.5) also allows to conclude that for β such the function $[-\beta u + s(u,\dots]$ is maximized at a single value of u, in the thermodynamic limit the canonical canonical ensemble average at β **coincides**, assymptotically, with the microcanonical ensemble average at the corresponding energy density $E/|\Lambda| = u(\beta)$.

A similar replacement of a hard constraint by the seemingly softer tilting of the measure can be performed with respect to any of the other macroscopic variables. E.g., instead of constraining the particle number N, one may allow it to take all values but weight the configuration as follows:

$$\langle F\rangle_{\Lambda,\beta,\tilde{\mu}} \;=\; \frac{1}{Z_\Lambda(\beta,\tilde{\mu})}\sum_{\omega\in\Omega_\Lambda} F(\omega)e^{-\beta H(\omega)+\tilde{\mu}N(\omega)}\,, \tag{2.7}$$

where the normalizing factor is the **grand-canonical partition function**

$$\boxed{Z_\Lambda(\beta,\tilde{\mu}) \;:=\; \sum_{\omega\in\Omega_\Lambda} e^{-\beta H(\omega)+\tilde{\mu}N(\omega)}} \tag{2.8}$$

With all macroscopic constraints relaxed, that is replaced by the Gibbs factor in which they are weighted with their conjugate parameters ($E \mapsto \beta$, $N \mapsto \tilde{\mu}$, etc.) one obtains what is called the **grand-canonical ensemble**. Again, under the condition spelled above, the corresponding averages coincide in the thermodynamic limit.

A word about the notation: in the standard terminology $\boxed{\tilde{\mu} = \mu\beta}$ with μ the chemical potential.

2.3 An explicit example

Let us calculate explicitly the pressure function for the simple case of the adsorption model which was presented in section 1.2.

This system can also be viewed as a lattice gas model, in which there is no interaction beyond the on-site exclusion principle. Other than that, energy does not play a role, and in the microcanonical ensemble it is just the number of particles which is constrained.

For this models's canonical partition function the sum over microscopic configurations factorizes into independent sums:

$$Z_\Lambda(\tilde{\mu}) \;=\; \sum_{\omega\in\Omega_{\Lambda,N}} e^{\tilde{\mu}N(\omega)} \;=\; \prod_{x\in\Lambda}\left[\sum_{\tau_x=0,1} e^{\tilde{\mu}\tau_x}\right] \;=\; [1+e^{\tilde{\mu}}]^{|\Lambda|}\,. \tag{2.9}$$

This yields for the pressure function:

$$\Psi(\tilde{\mu}) \;=\; \lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|}\log Z_\Lambda(\tilde{\mu}) \;=\; \log(1+e^{\tilde{\mu}}) \tag{2.10}$$

(where the equality holds even at finite volumes).

Substituting (2.10) in (2.5) we learn that the system's entropy function $s(n)$ has as its Legendre transform

$$\sup_n\,[\,\tilde{\mu}u + s(n)] \;=\; \log(1+e^{\tilde{\mu}}) \tag{2.11}$$

It is worth noting that the passage to the Gibbs-tilted measures has its advantages:

i) The pressure can be evaluated without the assistance of Stirling's approximation (see exercises below).

ii) The canonical ensemble is also simpler than the canonical one. Even before the passage to thermodynamic limit the joint probability distribution of the variables τ_x is just the product measure in which for each finite collection $\tau_A = (\tau_x)_{x\in A}$

$$\Pr(\tau_A) \;=\; \frac{e^{\tilde{\mu}\sum_{x\in A}\tau_x}}{[1+e^{\tilde{\mu}}]^A}\,. \tag{2.12}$$

The value of $\tilde{\mu}$ at which the canonical ensemble approximates the microcanonical one is determined by the condition that the two agree on the particle density $n = N/|\Lambda|$. Since $\langle\tau\rangle_{\tilde{\mu}} = \Pr([\tau = 1])$ one may conclude that in this non-interacting model the relation is given by

$$\left(\langle\tau\rangle_{\tilde{\mu}} = \right)\frac{e^{\tilde{\mu}}}{1+e^{\tilde{\mu}}} \;=\; n\,. \tag{2.13}$$

Exploring the principle of **equivalence of ensembles** in this example, one find that for large systems the microcanonical ensemble and the "more relaxed" canonical ensemble locally converge to the same measure (in the thermodynamic limit), provided the parameter $\tilde{\mu}$ is set at a value which reproduces the global density of the constrained quantity (here $n = N/V$).

The two ensembles differ a bit on the global scale, since in the canonical ensemble the global value of N is not constrained. However by the well know central limit theorem, which is applicable in the above example, the typical deviations in the values of $N(\omega)/V = [\sum_{x\in\Lambda}\tau_x(\omega)]/V$ are only of order $O(1/\sqrt{N})$.

One should however be warned that fluctuations get to be significantly larger at phase transitions, which this simple model is lacking.

Exercises

2.1 Show that the Legendre transform of the entropy function which was computed in (1.6) (using Stirling's approximation) is consistent with (2.11).

3

Convexity and the Legendre transform

In this section we focus on the theory of convex functions, some of its basic notions and relevant theorems. Convexity plays a role in optimization problems and in particular its concepts appears naturally in Thermodynamics, as we saw in the previous chapter. The basic results of the general theory would continue to play a helpful role in the discussion which follows.

3.1 Convexity

Definition 3.1. 1) A set $D \subset \mathbb{R}^\nu$ is said to be convex if for any $x_0, x_1 \in D$ it includes all points of the form

$$x(t) = (1-t)x_0 + tx_1 \quad 0 \le t \le 1\,. \tag{3.1}$$

2) A real valued function defined over a convex set $D \subset \mathbb{R}^\nu$ is said to be **convex** if for any $x_0, x_1 \in D$

$$\boxed{F((1-t)x_0 + tx_1) \ \le\ (1-t)F(x_0) + tF(x_1)\,.} \tag{3.2}$$

The function is **concave** if it obeys the reversed inequality (i.e. if $(-F)$ is convex)[1].

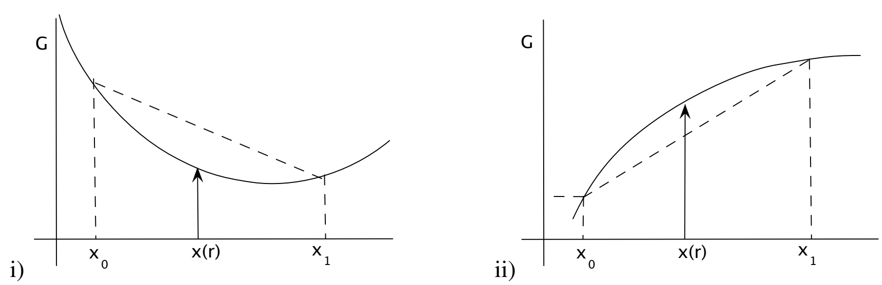

Figure 3.1 A convex function (i) and a concave one (ii). The properties are defined through the relation of the function's graph to its cords.

It may be noted that the defining property (3.2) has a natural extension to functions with values in $(-\infty, +\infty]$, i.e. for which $+\infty$ is allowed by not $-\infty$. We shall adapt this convention.

[1] Actually, it would suffice to restrict the values of t in (3.2) to $t = 1/2$. We skip here the infinitesimal proof of the two conditions' equivalence. The stated one offers a simpler starting point for some elementary arguments.

Theorem 3.2. *Let $G_\alpha(x)$ be a family, indexed by α, of linear [or more generally convex] functions over a common convex domain $D \in \mathbb{R}^\nu$. Then the function*

$$F(x) \ := \ \sup_\alpha G_\alpha(x) \tag{3.3}$$

is convex over D.

Proof The condition defining convexity is equivalent to the statement that for each pair of points in $\mathbb{R} \times D$ which lie above the graph of F the entire cord linking the two also lies entirely above the graph (see Fig. 3.1). Under the stated assumption this cord condition holds for all α. Hence at each point it also holds for the supremum over α. In other words, this condition is stable under the supremum in (3.3). □

The argument used in the above proof implies also the following useful statement.

Theorem 3.3. *Let F_n be a sequence of convex functions which converges pointwise to F. Then F is convex.*

The notion of convexity has a natural extension to functions defined over **affine spaces**, i.e. spaces over which the linear interpolation (3.1) makes sense. A relevant example is the space of **states**, which are defined as the mappings associating expectation values $\langle F \rangle$ to a given system's observables F, which are linear, normalized ($\langle \mathbb{1} \rangle \ = \ 1$), and positivity preserving.

It may however be good to first familiarize oneself first with the implications of convexity in one real variable.

3.2 Implications with regards to the continuity and differentiability

A local manifestation of convexity is monotonicity of the fist derivative (properly defined). Thus, for a twice differentiable function on an open interval convexity is equivalent to the condition:

$$\frac{d^2}{dx^2} F(x) \ \geq \ 0\,. \tag{3.4}$$

Without assuming differentiability, convexity implies (and is equivalent to) monotonicity of the cord slopes:

$$\frac{F(x_2) - F(x_1)}{x_2 - x_1} \ \geq \ \frac{F(x_2') - F(x_1')}{x_2' - x_1'} \tag{3.5}$$

for each two pairs of sites with $x_j' \ \geq \ x_j$, $j \ = \ 1, 2$, and $x_1 \ \neq \ x_2$, $x_1' \ \neq \ x_2'$. Following are some implications of this observation.

Over any open interval over which $f(x)$ is defined and takes finite values convexity implies continuity. At the boundary, the functions may only jumps upwards – as seen from the interior of the set (though of course this would still appear as a jump down from the side where the function takes the value $+\infty$). More explicitly:

Theorem 3.4 (Continuity). *A convex function defined over an interval $I \subset \mathbb{R}$ is continuous in the interval's interior and upper semicontinuous at boundary points, i.e. for any $x \in \partial I$*

$$F(x) \geq \lim_{y \to x\,; y \in I} F(y)\ . \tag{3.6}$$

The proof is left as an exercise. (A short argument can be based on (3.5).)

Theorem 3.5 (Differentiability). *Let F be a convex function defined over an open interval $I \subset \mathbb{R}$. Then*

i. The function is differentiable at almost every x, the exceptional points forming an enumerable set.
ii. On the set of points on which it exists, the derivative $F'(x)$ is monotone increasing in x.
iii. At all $x \in I$ the directional derivatives

$$F'_{\substack{+\\(-)}}(x) = \lim_{\substack{\Delta x \to 0\,, \Delta x > 0 \\ (\Delta x < 0)}} \frac{F(x + \Delta x) - F(x)}{\Delta x} \tag{3.7}$$

exist, and satisfy

$$F'(x-0) \ = \ F'_{-}(x) \ \leq \ F'_{+}(x) \ = \ F'(x+0)\,. \tag{3.8}$$

where $F'(x+0)$ and $F'(x-0)$ are the left and right limits of $F'(x)$.

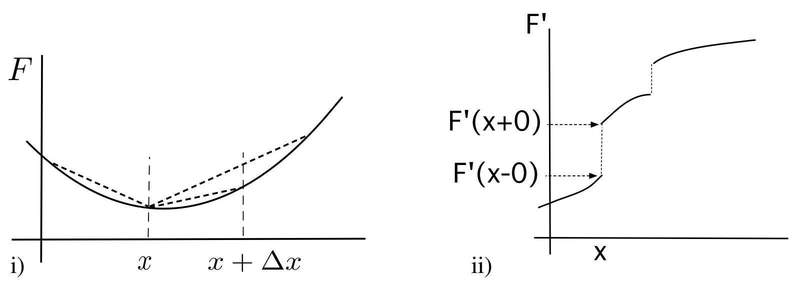

Figure 3.2 i) For any convex F the one sided derivatives exist since the slopes of the cords between x and $x + \varepsilon$ are monotone in ε. ii) The one sided derivatives are non-decreasing and may have jump discontinuities. At those $F'_{-}(x)$ is continuous from the left and $F'_{+}(x)$ is continuous from the right.

Proof One may start by considering the directional derivatives, say $F'_{+}(x)$. The existence of the corresponding limit in (3.7) can be deduced by noting that for a convex F the ratio there is monotone decreasing as $\Delta x \searrow 0$, and monotone increasing as $\Delta x \nearrow 0$.

The cord slopes relation (3.5) implies that $F'_{+}(x)$ is increasing in x. Monotonicity implies that the right and left limits $F'_{+}(x \pm 0)$ exist at all x, and this function may have only positive jump discontinuities, $F'_{+}(u+0) \ - \ F'_{+}(u-0) \geq 0$. Furthermore, these are summable over any strict subinterval $[x, y] \subset I$ since

$$\sum_{u \in (x,y)} [F'_{+}(u+0) \ - \ F'_{+}(u-0)] \ \leq \ F'_{+}(y) \ - \ F'_{+}(x) \ < \ \infty\,. \tag{3.9}$$

The sum here is over **all** sites in (x, y) but it is well defined since it involves only non-negative terms. The collection of non-zero terms in this sum can only be countable, since the sum of any uncountable collection of strictly positive terms is infinite (prove that!),

In conclusion, there is at most a countable collection of points at which $F'_+(x)$ fails to be continuous, and at those it has positive jump discontinuities. The cord slopes relation (3.5) allows also to conclude the relation (3.8). It implies, in particular, that at points of continuity of $F'_+(x)$ the right and left derivatives coincide ($F'_-(x) = F_+(x)$) and hence that $F(x)$ is differentiable there. □

Remark: The above discussion also implies that for any convex function the left and right limits of the directional derivatives agree and therefore may be written as just left or right limits of the derivative, i.e. $F'(x \pm 0)$, which satisfy

$$F'(x-0) \;=\; F'_-(0)\,, \quad F'(x+0) \;=\; F'_+(0)\,. \tag{3.10}$$

(A statement which it may be confusing to parse, but it is convenient to have.)

3.3 Convergence properties of convex functions

As we saw in Theorem 3.3 convexity is stable under pointwise limits. This will be regularly invoked in discussions of thermodynamic potentials, which are defined through a limiting procedure. The following will be particularly useful in that context.

Theorem 3.6. *Let F_n be a sequence of convex functions over a common open interval $I \subset \mathbb{R}$ which are differentiable and converge pointwise as $n \to \infty$. Then for every $x \in I$ at which $F(x) = \lim_{n\to\infty} F_n(x)$ is differentiable*

$$\boxed{F'(x) \;=\; \lim_{n\to\infty} F'_n(x)\,.} \tag{3.11}$$

Furthermore, regardless of the existence of $F'(x)$ the following relation holds

$$\boxed{F'_-(x) \;\le\; \liminf_{n\to\infty} F'_n(x) \;\le \limsup_{n\to\infty} F'_n(x) \;\le\; F'_+(x)\,.} \tag{3.12}$$

The proof is left as an exercise (see Ex. 3.1, and the hint given there).

3.4 The Legendre transform

Definition 3.7. Let G be a real valued measurable function defined over a set $B \in \mathbb{R}^\nu$. Its **Legendre transform** TG is defined over $\mathbb{R}^\nu$ by

$$\boxed{TG(y) \;=\; \sup_{x\in B}\{y\cdot x \;-G(x)\}} \tag{3.13}$$

Let us note that this formulation of the transform allows $TG(y)$ to take the value $+\infty$, but not $-\infty$. Aalso the defining property of convexity, stated in (3.2), admits a natural extension to functions with values in $(-\infty, +\infty]$. Hence it is natural to Hence it is natural to allow TG to the set over which the function is finite.

When the transform is applied to physical quantities, the variables x and y in (3.13) carry inversely related units. This corresponds to the observation that TG is defined over the dual space to that over which G is defined.

Theorem 3.8. *For any function G, the transform TG is a convex function over the domain B^*, which itself is a convex set.*

The statement is readily implied by Theorem 3.2. A version of the Legendre transform which automatically yields concave, rather than convex, functions is obtained by replacing supremum in (3.13) by infimum.

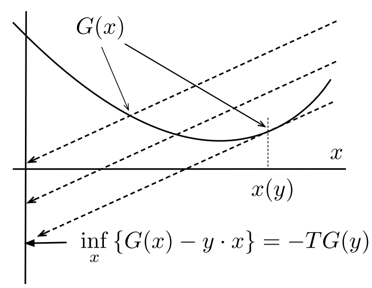

Figure 3.3 The Legendre transform: $-TG(y)$ corresponds to the lowest reach of the projection of the graph of G onto the vertical axis, at slope y. It is reached from the point(s) x at which $G'(x) = y$.

For convex functions G, and y strictly within the domain B^*, the supremum in (3.13) is attained in one of two ways: a point $x(y)$ where

$$G'(x-0) \ \le \ y \ \le \ G'(x+0)\,, \tag{3.14}$$

which in case $G(x)$ is differentiable at x means

$$\boxed{G'(x) \ = \ y\,,} \tag{3.15}$$

or over an interval along which $G'(x)$ is constant. With such $x(y)$:

$$\boxed{TG(y) \ = \ y \cdot x(y) - G(x(y))\,.} \tag{3.16}$$

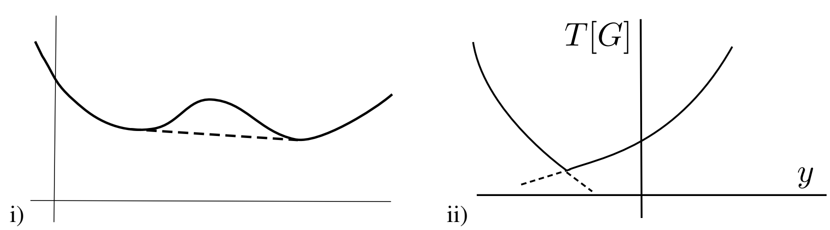

Figure 3.4 i) the “convex hull” of a non-convex function, and ii) a sketch of the resulting function’s Legendre transform.

It is of interest to note that if G is not **strictly convex**, i.e. its slope is constant over an interval, then TG has a **kink** singularity, i.e. a point at which $G'(y)$ is discontinuous. An example of such situation is depicted in Figure 3.4(i). And conversely, a kink singularity of G results in the graph of TG having a flat segment.

For functions which are not convex there is **loss of information** in passing from G to TG. That is so since the Legendre transform of G coincides with that of the convex hull function, $G_{hull} : \mathbb{R}^\nu \mapsto \mathbb{R}$. The latter is defined as the minimal convex function which is bounded above by G (as depicted in Fig. 3.4). There is also loss of information about the values of the function at the boundary of the domain where the function is finite, as the transform TG coincide with that of the function's lower-semicontinuous version (defined so the two agree on any open set over which G takes only finite values).

However, except for the last caveat, a convex function can be fully recovered from its transform:

Theorem 3.9 (Legendre transform's involutive property)**.** *For any convex function $G : \mathbb{R}^\nu \mapsto \mathbb{R} \cup \{+\infty\}$ which is lower-semicontinuous:*

$$\boxed{T\,[TG] \;=\; G\,.} \tag{3.17}$$

The proof is left as an exercise.

Remarks: 1) An argument which is quick and of added value can be made under the assumption that G is differentiable and strictly convex, in which case also TG is differentiable.
2) The assumption of lower semi-continuity is of relevance only for the function's behavior at the boundary of the region $D[G] = \{x \in \mathbb{R}^\nu \;:\; |G(x)| < \infty\}$.

Corollary 3.10. *For any differentiable convex function $F : \mathbb{R} \mapsto \mathbb{R}$ there is a single function G with values in $\mathbb{R} \cup \{+\infty\}$ for which $F = TG$. For F which is convex but not everywhere differentiable there are different functions G with which $F = TG$, all sharing a common convex hull.*

It may be added (though from our perspective mainly as just a curiosity) that the relation of G with its Legendre transform TG can be cast in a symmetric form by noting that for any pair of values of x and y

$$G(x) \;+\; TG(y) \;\leq\; y \cdot x \tag{3.18}$$

and, furthermore: for each y in the interior of the domain B^* the relation holds as equality at some x. Likewise for each x in the interior of B there is y at which the inequality is saturated (statement whose proof yields Theorem 3.17), thereby permitting to recover G from TG.

3.5 The corresponding differentials

For functions of k variables, $G(x_1, ..., x_k)$, one may consider a succession of Legendre transforms under which a number of the variables x_i are replaced by their conjugate pressures y_i:

$$[T_{(1,...,j)}G](\mathbf{y}, \mathbf{x}) \;=\; \sup_{x_1,...,x_j} \left[\sum_{i=1}^{j} x_i y_i \;-\; G(x_1, ..., x_k) \right] \tag{3.19}$$

where $(\mathbf{y}, \mathbf{x}) = (y_1, ..., y_j, x_{j+1}, ..., x_k)$. The corresponding extension of (3.15), stated in differential form, is:

$$d\,[T_{(1,...,j)}G] = \sum_{i=1}^{j} x_i(\mathbf{y}, \mathbf{x})\, dy_i \;+\; \sum_{i=j+1}^{k} y_i(\mathbf{y}, \mathbf{x})\, dx_i\,. \tag{3.20}$$

3.6 Jensen's inequality

No discussion of convexity is complete if it omits the following beautiful and useful principle.

Theorem 3.11 (Jensen's inequality)**.** *Let $\rho(dx)$ be a probability measure on $\mathbb{R}$ (or $\mathbb{R}^\nu$) with a finite moment: $\int |x|\rho(dx) < \infty$. Then for any convex function $F : \mathbb{R} \to \mathbb{R}$*

$$\int F(X)\rho(dx) \;\geq\; F\left(\int X\rho(dx) \right). \tag{3.21}$$

To quickly recover the direction of the inequality (which is reversed for F concave) it suffices to consider measures μ which are concentrated on two points. The inequality then reduces to the definition of convexity.

Proof The function's convexity implies that its graph lies above any of the graphs tangents. In particular, for any $x \in \mathbb{R}$:

$$F(x) \;\geq\; F(\langle x\rangle) + (x - \langle x\rangle)\, F'(\langle x\rangle + 0)\,. \tag{3.22}$$

Integrating over x with the probability measure $\mu(dx)$, and noting that

$$\int (x - \langle x\rangle)\, \mu(dx) = 0$$

one is left with the claimed (3.21). □

The above argument has a natural extension to the multidimensional case. While the statement's proof is elementary, it offers a versatile principle with many useful applications. Among those we shall encounter an entropy based variational characterization of the Gibbs equilibrium states.

Exercises

3.1 Prove Theorem 3.6, which concerns the convergence of derivatives of convex functions.
Hint: while pointwise convergence of $F_n(x)$ does not usually imply convergence of the

derivatives, it does imply convergence of the ratios $\frac{F_n(y)-F_n(x)}{y-x}$ for all pairs of sites $x < y$ in I. This combines well with the observation that for convex functions $\frac{F_n(y)-F_n(x)}{y-x} \in [F_n'(x), F_n'(y)]$.

3.2 Sketch a function $G : \mathbb{R} \mapsto \mathbb{R}$ with a discontinuous derivative. How is this singularity expressed in the function's Legendre transform? Sketch, and prove.

3.3 Describe the Legendre transform of a function which fails to be convex in a strict subset of its domain of definition, as depicted in Fig. 3.4.

3.4 Prove Theorem 3.9, which asserts the Legendre transform's involutive property: $T[TG] = G$ on suitable domain.
For partial credit prove the assertion under the assumption that both G and TG are strictly convex and differentiable.

3.5 Review exercise (2.1) and prove that the entropy of the adsorption model can be determined without invoking Stirling's approximation or other combinatorial calculation.

4

Thermodynamic Potentials

Before one turns deeper into Statistical Mechanics, it may be good to remind oneself of the basic tenents of Thermodynamics. This theory is a remarkable achievement of the data-driven approach to engineering and science. Its pinnacle was the introduction of the concept of entropy whose significance, key properties, and applications were grasped and formalized well before the emergence of a coherent explanation of its roots. The latter can be viewed as the first achievement of Boltzmann's statistical mechanics.

4.1 Entropy as a quantifier of irreversibility

The key postulate of Thermodynamics concerns realizable transitions between states of thermodynamic equilibrium:

The "2nd law" of Thermodynamics: *In processes which are realizable in an isolated system through the relaxation of macroscopic constraints the overall entropy can only increase*

$$\boxed{\Delta S(V, E, N, ...) \ \geq \ 0\,.} \tag{4.1}$$

More explicitly, the theory refers to systems composed of macroscopically distinct parts whose extensive conserved quantities (such as volume, energy and number of particles) are controllable through walls, some of which may be permeable to exchanges of selected quantities. Examples of the latter include walls which are permeable to heat flow but not particle exchange, and movable pistons through which the volume change in a process which generates work.

The dynamics taking place through such processes can be quite involved, ranging from adiabatic to turbulent. However the basic observation of thermodynamics is the irreversibility of the transitions which are realizable through guided releases of constraints. E.g., a drop of ink squirted into a cup of water will dissipate, and a scoop of ice cream dropped into a cup of hot coffee will melt. And there is no point waiting for the reversal of these dynamics to occur, even though the laws underlying the microscopic dynamics are invariant under time reversal.

Irreversibility is quantified in thermodynamics through the notion of *entropy* (denoted here by S). It is assumed, or asserted, that such a quantity exists, i.e. allows to express the realizable tradition by the above stated law, and furthermore that it can be quantified as a function of the system's extensive quantities by which the equilibrium states are characterized.

It is also often taken as an implicit assumption that states whose entropy is not conditionally maximal under a specified set of thermodynamic constraints would not persist, and would either spontaneously, or under the nudge of some random minuscule force, evolve and asymptotically converge into a state of higher entropy[1]

The resulting theory's highlights include:

- Temperature: the common notion of *temperature* of an equilibrium state is explained, and defined through the relation

$$\boxed{\frac{1}{k_B T} = \frac{\partial S}{\partial E}} . \tag{4.2}$$

  A remarkable aspect of this relation is that it implies the existence of *absolute scale*, with states of zero temperature generically (though with some notable exceptions) having zero entropy. This statement is known as the Third Law of thermodynamics.

- Heat: this initially elusive concept was recognized to be the energy transferred by other than mechanical means (work, etc.) ,cf. [1].

- Limits on the efficiency of engines: engines involve devices by which work is extracted through energy transfers between two energy reservoirs at different temperatures (and conversely of refrigerators which are devices by which heat can be extracted from a system and dumped into a hotter one, in a process in which inevitably also work is transformed into entropy-increasing heat).

- Free energy: a concept which expresses the amount of energy which can be extracted and used for work when the system's elements transition between states of specified temperature.

These, and many other applications of the theory can be found in numerous texts on the subject[2]

While the irreversibility of observed processes is an easily visible aspect of everyday's experience, the quantification of entropy seems to be initially less intuitive than that of conserved quantities such as energy (not to mention volume). Not surprisingly, this notion has been the subject of epistemological discussions. These have centered on the question to what extent is the concept derivable and quantifiable from a minimal set of observation about the physical processes. Among the contributions on the subject is Carathódory's axiomatic presentation of thermodynamics. A more recent discussion in this vein can be found in [2].

[1] The point is not always taken for granted, and manifestations of metastability form an interesting topic. Debatable examples range from an ingenious *piston problem* C.f. Herbert Callan **Thermodynamics** [1][1st edition], to the so-called *spin glasses*.

[2] Ibid (with preference for its first edition), where the theory is presented starting from the fundamental concept of entropy.

4.2 Extensivity and concavity of the entropy

In our haste to emphasize the main points, in the above summary we skipped over the proper presentation of the thermodynamics of equilibrium states. The more complete presentation should start by noting that the discussion refers to macroscopic systems which are **divisible** (i.e. can be partitioned, mentally and/or physically), **scalable** (i.e. can be increased in size), and whose equilibrium states are **homogeneous**.

In what is sometimes referred to as *Thermodynamic's Zeroth law* it is postulated that the relation of equilibrium among states of different subsystems, with respect to the exchange of energy, or any other specified extensive quantity, is transitive.

In particular, equilibrium exists also between different part of a given system. Correspondingly, the entropy function $S(V, E, N, ...)$ is also extensive, and is homogeneous of degree 1 in the other extensive parameters.

The next important observation is that the above postulates of thermodynamics require the entropy function $S(V, E, N, ...)$ to be concave. For if not, and there is a value of $(V, E, N, ...)$ and $(\Delta V, \Delta E, \Delta N, ...)$ for which

$$\begin{aligned} S(V, E, N, ...) &\geq \frac{1}{2}\left[S(V - \Delta V, E - \Delta E, N - \Delta N, ...) + S(V + \Delta V, E + \Delta E, N + \Delta N, ...)\right] \\ &= S\left(\frac{V}{2} - \frac{\Delta V}{2}, \frac{E}{2} - \frac{\Delta E}{2}, \frac{N}{2} - \frac{\Delta N}{2}, ...\right) + S\left(\frac{V}{2} + \frac{\Delta V}{2}, \frac{E}{2} + \frac{\Delta E}{2}, \frac{N}{2} + \frac{\Delta N}{2}, ...\right). \end{aligned} \tag{4.3}$$

then the system would be unstable with respect to a spontaneous decomposition into domains of different densities of the extensive parameters.

Concavity carries important and very useful implications. One of these is that the function is almost everywhere differentiable (c.f. previous section). The derivatives of the entropy function play a fundamental role in thermodynamics, as we shall next.

4.3 Thermal equilibrium and heat baths

When two thermodynamic systems at initial energies E_1 and E_2 are brought into "diathermal contact", i.e. one allowing heat flow without the transfer of matter, the state of equilibrium into which the pair will asymptotically relax, is one maximizing the total entropy subject to the constraint of constant $E_{Tot} = E_1 + E_2$. Assuming differentiability of the entropy functions (a condition which by the concavity of the entropy function is satisfied at almost every set of values of the controlling quantities) the equilibrium would be reached at a value of E_1 at which

$$\frac{\partial}{\partial E_1}\left[S_1(V_1, E_1, N_1, ...) + S_2(V_2, E_{Tot} - E_1, N_1, ...)\right] = 0\,. \tag{4.4}$$

Under this conditions the two systems are at equal values of the derivative. This leads to the following being a natural definition of thermodynamic temperature T and its inverse β

$$\frac{\partial}{\partial E} S(V, E, N, ...) = \beta \equiv \frac{1}{kT}\,. \tag{4.5}$$

with k determined by the choice of units for the quantities mentioned here.

Furthermore, in case the second system is much larger than the first one, its temperature will not be much affected by the exchange with the smaller systems. In the asymptotic version of such a situation the large system serves as a *heat bath*. The term refers to an idealized system which serves as a potential source or depository of energy, at constant temperature.

Concerning the question of units, it may be noted that the above mentioned laws of thermodynamics leave only linear mappings in the freedom in entropy's quantification. I.e. since the entropy is additive over subsystems, physics does not leave one with the choice of non-linear stretching in its scale. Furthermore, the so-called third law of thermodynamics, despite its occasional exceptions identifies a value which may be regarded as zero entropy. This limits the freedom in the quantification of entropy to just the choice of scale (a discussion of related questions can be found in [2].)

4.4 The Helmholtz free energy

When energy ΔE is drawn from a heat bath, its entropy decreases by $\beta\Delta E$, at constant $\beta = \frac{1}{kT}$. In processes for which the relevant entropy is the sum of that of the system and that of the heat bath by which its state is thermalized, the sum takes the form $S_{Tot} = S(V, E, N) + [\text{Const.} - \beta \text{E}]$.

Hence, the amount of energy which can be extracted from a system through gradual adjustment in its temperature, which defines the so-called **Helmholtz free energy**, is the quantity F which as a function of β is related to the system's entropy function through the relation

$$\boxed{F(T, N, V, ...) \ := \ \inf_E \left[E - T\, S(V, E, N, ...)\right]} \tag{4.6}$$

or, equivalently, as as $F(T, N, V, ...) = \widetilde{F}(\beta, N, V, ...)$ with

$$-\beta \widetilde{F}(\beta, N, V, ...) := \sup_E \left[S(V, E, N) \ - \ \beta E\right] \ . \tag{4.7}$$

Remark: While $F(T, ...)$ and $\widetilde{F}(\beta, ...)$ are different as mathematical functions of their stated arguments, the two represent the same physical quantity (with β identified as $(kT)^{-1}$). Hence, where the functional dependence should be clear from the context, we may omit the tilde in our notation.

The last two relations may be recognized as versions of the Legendre transform in E of the concave function $S(., E, ..)$. The general rule which was presented below as Theorem 3.8) allows to conclude that $F(T, N, V)$ is concave in T and $\beta\, F(\beta)$ is concave in β.

4.5 Other thermodynamic potentials

Like the energy also other extended variables can be controlled through reversible exchanges with the corresponding "baths", rather than by means of impregnable walls.

This makes relevant a host of thermodynamic functions which are obtained through suitable applications of the Legendre transform. In such transformations control parameters of *extensive* nature (i.e. conserved quantities which are additive over subsystems) are individually replaced by conjugate *intensive* control parameters.

Another example of this principle is the **Gibbs free energy**[3]:

$$\boxed{G(p,T,N_1,...N_r) \;=\; \inf_{E,V}\left[E + pV - TS(V,E,N_1,...N_r)\right]\ .} \tag{4.8}$$

It is often referred to as a state function (as function of the intensive control parameters (T,p)).

It is also useful to note the change in the change in the differential forms which accompany the transformation. In physics literature the primality relation between S and E is reversed, and the starting functional relation is expressed as $E(V,S,N,...)$. The corresponding differential is

$$\mathrm{d}E = T\mathrm{d}S - p\mathrm{d}V + \sum_J \mu_j \mathrm{d}N_j + ... \tag{4.9}$$

where p is the pressure (related to the work required to reduce the system's volume), and μ_j the chemical potential for the j-th species of particles.

The differential form of the Legendre - transformed function $G(p,T,N_1,...,N_r)$ is

$$\boxed{\mathrm{d}G \;=\; -S\ \mathrm{d}T + V\,\mathrm{d}p + \sum_{i=1}^{r}\mu_i \mathrm{d}N_i} \tag{4.10}$$

Another quantity we shall encounter is the **grand canonical potential** which is the thermodynamical variational function for the situation where all the extensive quantities but volume are controlled through equilibria with the corresponding reservoirs. In the entropy based notation, this function is given by the Legendre transform:

$$-\beta\ U(V,\beta,\mu_1,...\mu_r) \;=\; \sup_{E,V}\left[S(V,E,N_1,...N_r) - \beta E + \sum_{j=1}^{r}\tilde{\mu}_j N_j\right]. \tag{4.11}$$

We follow here the notational rule which is explained below (4.7), i.e. omit the tilde in what would more properly be written as $\widetilde{U}(V,\beta,\mu) = U(V,T,\mu)$.

4.6 First order phase transitions

The manipulation of the Legendre transforms may be confusing a bit, especially once one starts to switch between the transform's convex and concave version. Let us therefore note that assuming sufficient differentiability, including that of the minimizing value of (E,V) as function of (T,p), at given N, the simple rules of calculus permit to deduce from (4.8) the inverse relation:

$$\boxed{S\ (V,E,N,..) = -\frac{\partial G(T,p,N)}{\partial T}} \tag{4.12}$$

[3] For consistency with the standard usage, the free energy functions are expressed here in the energy-temperature centered notation, i.e. that of (4.6) rather than the entropy-β centered notation of (4.7).

where $(V, E) = (V(T, p), E(T, p))$ are values at which the infimum in (4.8) is realized (see Exercise 4.1). By the convexity arguments of Chapter 3 at all (T, p, N) (i.e. throughout the thermodynamics phase space) the function $G(T, p, N)$ has right and left derivatives in T, and these coincide at almost all (T, p, N) and in such case the relation does hold as stated.

However, the derivative of the concave function may exhibit discontinuities. Such discontinuities signal first order phase transitions[4].

A well known example of that phenomenon is the freezing point of H_2O, at which one finds liquid - solid coexistence. The two single-sided derivatives then yield the different entropy densities of the two phases.

Continuing with the last observation, if should be noted that $G(T, p, N) = E(T, p) + pV - T\,S(V(T, p), E(T, p), N)$, which being defined through a version of the Legendre transform (4.8), is continuous. Hence the discontinuity in the entropy is compensated by a discontinuity in the energy density. That difference is the latent heat associated with this phase transition.

4.7 The thermodynamic pressure

For functions like $S(V, E, \mathbf{N})$ which are homogeneous of the first degree, i.e. satisfy

$$S(\lambda V, \lambda E, \lambda \mathbf{N}) = \lambda S(V, E, \mathbf{N}) \tag{4.13}$$

the full Legendre transform is singular. By the definition used here it would yield 0 or $\pm\infty$, depending on the value of p). On the other hand, the homogeneity implies that $U(V, T, \mu)$ is linear in the volume. Thus, with the natural definition of the pressure $p(\beta, \mu)$ one has

$$-\,p(\beta,\mu) \;=\; \frac{\partial U(V,\beta,\mu)}{\partial V} = \frac{U(V,\beta,\mu)}{V}\,. \tag{4.14}$$

This observation, combined with the considerations presented in Section 6, would yield the following relation of the thermodynamic pressure with the statistic mechanical grand-canonical partition function (which is defined and discussed below):

$$\boxed{p(\beta,\mu) \;=\; \lim_{L\to\infty} \frac{\beta^{-1}}{|\Lambda(L)|} \log Z_{\Lambda(L)}(\beta,\mu)\,,} \tag{4.15}$$

The existence of this limit is one of the basic and general results of statistical mechanics.

4.8 Relation with Statistical Mechanics

A big question raised by Thermodynamics, and the challenge addressed by Boltzmann, was the intrinsic meaning and explanation of Entropy.

[4] By the function's homogeneity, at given (T, p) the number of particles N does not affects the location of singularities of $G(T, p, N)$.

Boltzmann's explanation, and the resolution of this puzzle, can be viewed as the beginning of Statistical Mechanics. The resulting theory allows to address many more questions, including the analysis of the phase structures and the phase transitions observed in systems which range from the experimentally accessible physics, to simplified mathematical models with similar behavior. A remarkable facts is that the similarity between the two realities extends to topics such as conditions for phase transitions, symmetry breaking, and the values of critical exponents.

And, as is the case with other successful mathematically abstractions of the physics around us the success of Thermodynamic in quantifying the possible, and analyzing what is not, has inspired surprising developments in other directions. Thus *entropy* appears now as a common term in theories of Information, Coding, Dynamical systems, and Large Deviation principles, and also in the mathematical field of Analysis.

Exercises

4.1 Assuming all the relevant differentiability, prove that for energy (or energies) $E = E(V, T, N)$ at which the infimum in (4.6) is realized

$$S\ (V, E, N, ..) = -\frac{\partial F(T, V, N)}{\partial T}\,. \tag{4.16}$$

(Hint: it helps to start by stating the differential relation that is implied by E being a minimizer at the specified values of (T, V, N).)

4.2 Give an expression for the specific heat of water's boiling transition, at constant pressure, in terms of water's Gibbs free energy function $G(p, T, N)$. (Explain your reasoning.)

References

[1] H. Callen **Thermodynamics and an Introduction to Thermostatistics** (Willey, 1985)

This classical reference on the subject offers an extended discussion of thermodynamics centered on the entropy principle (though the point seems to have been stressed more in its first edition).

[2] E. Lieb and J. Yingvason *The physics and mathematics of the second law of thermodynamics*. Phys. Rep. **310**, Issue 1, 1-96 (1999).

5

The pressure function in the thermodynamic limit

5.1 The basic setup, and notation

In their microscopic details statistic mechanical systems vary. However they typically share a number of key features. To capture the essence, we now turn to lattice models.

Finite (classical) systems may be described by arrays of elemental variables $\{\sigma_x\}$ labeled by sites of a graph with periodic structure. By default we shall take the substratum over which the variables are defined to be the integer lattice $\mathbb{Z}^d$.

Within this a setup we shall employ the following notation:

i) $\{\sigma_x\}_{x\in\mathbb{Z}^d}$ are the basic "microscopic" variables.
ii) Ω_0 is the measurable space in which the local variables take values.
Thus $\Omega_0 = \{-1, +1\}$ for the ±1 valued spin variables, as in the Ising model, and $\Omega_0 = \mathcal{S}^{N-1}$ (the unit sphere in $\mathbb{R}^N$ for the the continuous spin variables of $O(N)$ models.
iii) More generally we assume that Ω_0 is a measurable space equipped with a finite measure
iv) $\mu_0(d\sigma)$ is a finite measure on Ω_0, which serves as our "a-priori" measure (for systems with some natural symmetry, e.g. of rotations, this would be an invariant measure).
v) $\Omega = \Omega_0^{\mathbb{Z}^d}$, and $\Omega_\Lambda = \Omega_0^\Lambda$, are the spaces of the system's configurations over the full graph and, correspondingly, its subsets $\Lambda \subset \mathbb{Z}^d$.
vi) $\mu_\Lambda(d\sigma) = \prod_{x\in\Lambda} \mu_0(d\sigma_x)$ is the corresponding a priori (product) measure on Ω_0^Λ.
vii) $H_\Lambda(\sigma_\Lambda)$ would denote the configurations' energy function, $H_\Lambda : \Omega_\Lambda \mapsto \mathbb{R}$.
Borrowing a term from classical and quantum mechanics H is typically referred to as the system's **Hamiltonian**.

In many situations of interest the graph admits a sequence of tilings by finite blocks. In the case of $\mathbb{Z}^d$ a convenient choice would be to tile the lattice by translates of $\Lambda(L) = (L/2, L/2]^d$. Two desired features are:

i) for each L the tiles are graph-isomorphic to each other,
ii) the surface to volume ratio vanishes asymptotically:

$$\lim_{L\to\infty} \frac{|\partial\Lambda_L|}{|\Lambda_L|} = 0 \,. \tag{5.1}$$

Other choices for the graph may also be considered. However in order for our discussion to be of relevance one would still like to keep some degree of homogeneity, e.g. periodicity. Examples include the honeycomb lattice (in two dimensions), and the body centered lattice in d dimensions. Typically the differences in the graph's local structure affect the critical values of the parameters at which phase transitions occur, and in some cases also our ability to solve the model, but typically it does not fundamentally change the large scale phenomenology.

In contrast, changes in the surface to volume relation, e.g. when the dimension changes or when $\mathbb{Z}^d$ is replaced by a regular tree graph may also affect the phenomenology, possibly including the appearance of qualitatively new phases.

5.2 Extensive energy functions

A convenient representation/construction of a lattice model's extensive Hamiltonian is

$$\boxed{H_\Lambda(\sigma) \ = \ \sum_{A\subset\Lambda} J_A \Phi_A(\sigma)} \ = \ \sum_{x\in\Lambda}\left(\sum_{A\ni x}\frac{1}{|A|}J_A\Phi_A(\sigma)\right) \tag{5.2}$$

where $J_A\Phi_A(\sigma)$ is an interaction term associated within the set of variables in $A \subset \mathbb{Z}^d$, with $\Phi_A(\sigma)$ depending only on $\sigma_A := \{\sigma_x\}_{x\in A}$, i.e. the restriction of the configuration to A. These functions are taken to be normalized by the condition

$$\sup_\sigma |\Phi_A(\sigma)| \ = \ 1\,, \tag{5.3}$$

so that he strength of the corresponding interaction terms is controlled by the parameter J_A. The collection of coupling constants, at implicitly specified $\{\Phi_A(\sigma)\}_{A\subset\mathbb{Z}^d}$, will be denoted $\mathcal{J} = \{J_A\}_{A\subset\mathbb{Z}^d}$.

For example, the Ising model's Hamiltonian

$$H(\sigma) = -\sum_{\langle x,y\rangle} J_{x-y}\sigma_x\sigma_y \ - \ h\sum_x \sigma_x\,, \tag{5.4}$$

with $J_{x-y} = J_{y-x}$, is cast in the above form by letting

$$\Phi_A(\sigma) \ = \ \begin{cases} -\sigma_x\sigma_y & A=\{x,y\} \\ -\sigma_x & A=\{x\} \\ 0 & |A|>2 \end{cases} \quad , \quad J_A \ = \ \begin{cases} J_{x-y} & A=\{x,y\} \\ h & A=\{x\} \\ 0 & |A|>2 \end{cases} \quad . \tag{5.5}$$

A Hamiltonian (or interaction) of the form (5.2) is said to be **translation invariant** if for all $u\in\mathbb{Z}^d$ and $A\subset\mathbb{Z}^d$

$$\boxed{J_A = J_{A+u} \qquad \text{and} \quad \Phi_{A+u}(\sigma) \ = \ \Phi_A(S_u\sigma)} \tag{5.6}$$

with S_u the shift: $(S_u\sigma)_x \equiv \sigma_{x-u}$.

The interaction is said to be of a **finite range**, R, if

$$\Phi_A(\sigma)\equiv 0 \quad \text{for all } A\subset\mathbb{Z}^d \text{ of diameter larger than } R \tag{5.7}$$

The second expression in (5.2) is of help in bounding the energy per site for translation invariant interactions. For this purpose, D. Ruelle [1] introduced the norm:

$$\boxed{\|\mathcal{J}\| \ := \ \sum_{A \ni 0} \frac{1}{|A|} \, |J_A|} \tag{5.8}$$

where $|A|$ is the set's cardinality. It facilitates the following basic estimate.

Lemma 5.1. *Let H and H' be a pair of Hamiltonians with common interaction terms $\{\Phi'_A\} = \{\Phi_A\}$ but different coupling constants, $\mathcal{J}$ and $\mathcal{J}'$. Then for any for $\Lambda \subset \mathbb{Z}^d$ and $\sigma \in \Omega_\Lambda$*

$$|H_\Lambda(\sigma)| \ \leq \ \|\mathcal{J}\| \, |\Lambda| \tag{5.9}$$

and

$$|H_\Lambda(\sigma) \ - \ H'_\Lambda(\sigma)| \ \leq \ \|\mathcal{J} - \mathcal{J}'\| \, |\Lambda| \, . \tag{5.10}$$

The proof is left as Exercise 5.1. These bounds show that $\|\mathcal{J} - \mathcal{J}'\|$ provides a relevant metric on the linear space of interactions (expressed in terms of the coupling constants $\mathcal{J}$).

5.3 Pressure as a generating function(al)

The **partition function** of finite system with the free boundary conditions is the tilted integral/sum

$$\boxed{Z_\Lambda(\beta, \mathcal{J}) := \int_{\Omega_\Lambda} e^{-\beta H_\Lambda(\sigma)} \, \mu(d\sigma)} \tag{5.11}$$

which in the discrete case, with μ the counting measure, reduces to

$$Z_\Lambda(\beta, \mathcal{J}) = \sum_{\sigma \in \Omega_\Lambda} e^{-\beta H_\Lambda(\sigma)} \quad .$$

For thermodynamic reasons, which were presented in section 4.5, the following quantity is referred to as the finite volume **pressure** in $\Lambda \subset \mathbb{Z}^d$ (with β^{-1} absorbed in the notation $\Psi = \beta p$)

$$\boxed{\Psi_\Lambda(\beta, \mathcal{J}) := \frac{1}{|\Lambda|} \ln Z_\Lambda(\beta, \mathcal{J})} \tag{5.12}$$

with $\mathcal{J} = \{J_A\}$ denoting the interaction parameters, as in (5.2)).

In statistical mechanics the pressure serves also a generating function, in the sense that its derivatives provide information on the mean values and variances of the bulk averages of extensive quantities computed in the corresponding canonical ensemble:

$$\begin{aligned} \frac{\partial}{\partial \beta} \Psi_\Lambda(\beta, \mathcal{J}) &= -|\Lambda|^{-1} \langle H_\Lambda \rangle_{\beta, \Lambda} \\ \frac{\partial}{\partial J_A} \Psi_\Lambda(\beta, \mathcal{J}) &= -\beta |\Lambda|^{-1} \left\langle \frac{\partial}{\partial J} H_\Lambda \right\rangle_\beta^{(\Lambda)} , \end{aligned} \tag{5.13}$$

and

$$\frac{\partial^2}{\partial \beta^2} \Psi_\Lambda(\beta, J) = \frac{1}{|\Lambda|} \langle \left(H_\Lambda - \langle H_\Lambda \rangle_{\beta,\Lambda} \right)^2 \rangle_{\beta,\Lambda} \geq 0\,. \tag{5.14}$$

Two important consequences of these relations (in reverse order) are:

Convexity: For any finite volume, $\Psi_\Lambda(\beta, \mathcal{J})$ is convex in β and at given β it is jointly convex in $\{J_A\}_{A \subset \mathbb{Z}^d}$.

Lifshitz continuity: For interactions with translation invariant Hamiltonians

$$|\Psi_\Lambda(\beta, \mathcal{J}) - \Psi_\Lambda(\beta, \mathcal{J}')| \leq \beta \, \|\mathcal{J} - \mathcal{J}'\| \,. \tag{5.15}$$

The two play a key role in the proof of the next result, which forms the subject's cornerstone.

It is of interest to note that the pressure's convexity, which follows from (5.14), can be alternatively viewed in terms of the following principle.

Lemma 5.2. *For any real valued measurable function ϕ on a probability space $(\Omega, d\mu)$ (or just a positive measure space), the function*

$$\Psi(h) := \ln \int e^{h\phi(\omega)}\, d\mu(\omega) \tag{5.16}$$

is convex in h (on any convex domain over which the right side is finite).

Proof Let $h_t = (1-t)\, h_0 + t\, h_1$ with $t \in [0,1]$. Then

$$\begin{aligned} \int e^{h_t H(\omega)}\, \mu(d\omega) &= \int (e^{h_0 H(\omega)})^{1-t}\, (e^{h_t H(\omega)})^t\, \mu(d\omega) \\ &\leq \left(\int e^{h_0\, H(\omega)}\, \mu(d\omega) \right)^{1-t} \left(\int e^{h_1\, H(\omega)}\, \mu(d\omega) \right)^t , \end{aligned} \tag{5.17}$$

where the last step is Hölder's inequality, $\left|\int f g\, d\mu\right| \leq \left[\int |f|^p\, d\mu\right]^{\frac{1}{p}} \left[\int |g|^q\, d\mu\right]^{\frac{1}{q}}$ for $\frac{1}{p} + \frac{1}{q} = 1$. Hence $\Psi(h_t) \leq (1-t)\, \Psi(h_0) + t\Psi(h_1)$. □

5.4 Thermodynamic limit for the pressure function

In the following result, we make room for the possible specification for finite systems of boundary conditions, or more generally the addition to H_Λ of a term $\phi^\sharp_\Lambda(\sigma)$ which does not affect the limiting energy desnsity for which

$$\sup_\sigma |\phi^\sharp_\Lambda(\sigma)| = o(|\Lambda|)\,. \tag{5.18}$$

We shall denote the corresponding finite volume partition function by $Z^{(\sharp)}_{\Lambda(L)}(\beta, \mathcal{J})$, and the related pressure function as $\Psi^{(\sharp)}_{\Lambda(L)}(\beta, \mathcal{J}) = \frac{1}{|\Lambda|} \log Z_{\Lambda(L)}$.

Theorem 5.3 (The thermodynamic limit for cubes)**.** *For any translational invariant interaction with $\|\mathcal{J}\| < \infty$, and finite volume corrections satisfying* (5.18)*, the following limit exists*

$$\Psi(\beta, \mathcal{J}) \;:=\; \lim_{L\to\infty} \frac{1}{|\Lambda(L)|} \log Z^{(\sharp)}_{\Lambda(L)}(\beta, \mathcal{J})\,, \tag{5.19}$$

The limiting function does not depend on the boundary conditions, is convex in β and at given β it is jointly convex in $\{J_A\}_{A\subset\mathbb{Z}^d}$. Furthermore, as a functional over the linear space of interactions it satisfies

$$|\Psi(\beta, \mathcal{J}) - \Psi(\beta, \mathcal{J}')| \;\leq\; \beta\, \|\mathcal{J} - \mathcal{J}'\|\,. \tag{5.20}$$

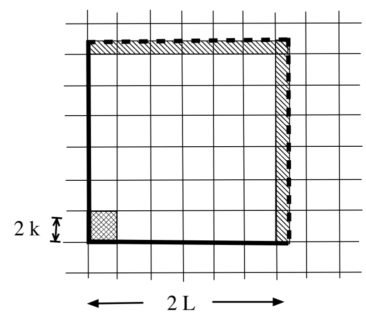

Figure 5.1 The tiling which is used in the proof of Theorem 5.5

Proof It is convenient to first establish the stated claims for interactions of finite range, $R < \infty$, and without the boundary terms Φ....

For a fixed k let us tile Λ_L by disjoint translates of Λ_k, as indicated in Fig. 5.1, labeling the tiles as C_j.

Splitting from $H_{\Lambda_L}(\sigma)$ the contribution of Φ_A for which A either includes sites in different tiles, or sites in tiles which are not fully contained in the larger box, one may decompose the Hamiltonian decomposes into a sum of non-overlapping terms and a remainder:

$$H_{\Lambda_L}(\sigma) = \sum_{j:\, C_j\in\Lambda_L} H_{C_j}(\sigma) + \; D_{\Lambda_L,k}(\sigma) \tag{5.21}$$

with $D_{\Lambda_L,k}(\sigma)$ the correction to

$$\frac{\sup_\sigma |D_{\Lambda_L,k}(\sigma)|}{|\Lambda_L|} \;\leq\; 2\,d\,\|\mathcal{J}\| \left[\frac{R}{2k} \;+\; \frac{2k}{2L}\right] =:\; \eta(L,k) \tag{5.22}$$

This yields the partition function bounds:

$$Z_{\Lambda_L}(\beta, \mathcal{J})\, e^{-\eta(L,k)|\Lambda_L|} \;\leq\; Z_{\Lambda_k}(\beta, \mathcal{J})^{\lfloor L/k\rfloor^d} \;\leq\; Z_{\Lambda_L}(\beta, \mathcal{J})\, e^{\eta(L,k)|\Lambda_L|} \tag{5.23}$$

with $\lfloor\cdot\rfloor$ denoting the integral part of x).

$$\Psi_{\Lambda_L}(\beta, \mathcal{J}) \;-\eta(L,k) \;\leq\; \left(\frac{k}{L}\left\lfloor\frac{L}{k}\right\rfloor\right)^d \Psi_{\Lambda_k}(\beta, \mathcal{J}) \;\leq\; \Psi_{\Lambda_L}(\beta, \mathcal{J}) \;+\eta(L,k)$$

that is

$$\left| \Psi_{\Lambda_L}(\beta, \mathcal{J}) \;-\; \left(\frac{k}{L} \left\lfloor \frac{L}{k} \right\rfloor \right)^d \Psi_{\Lambda_k}(\beta, \mathcal{J}) \right| \;\leq\; \eta(L, k) \tag{5.24}$$

Considering the implications for fixed but large $k \in \mathbb{N}$, and $L \to \infty$, one may conclude that $\Psi_{\Lambda_L}(\beta, \mathcal{J})$ forms a Cauchy sequence, and hence for any interaction of finite range the pressure function converges.

The convexity property of functions is stable under pointwise limits, and hence is inherited by the limiting function. Likewise, the Lifshitz bound (5.15) leads by continuity to (5.20) – at this point still limited to interactions of finite range.

To drop that restriction one may observe that any interaction with $\|\mathcal{J}\| < \infty$ can be approximated in norm by finite range interactions. More explicitly, for any $\varepsilon > 0$ there is a finite range interaction $\mathcal{J}_\varepsilon$ such that $\|\mathcal{J} - \mathcal{J}_\varepsilon\| \leq \varepsilon$. From the finite volume continuity condition (5.15) one inherits:

$$\left| \Psi(\beta, \mathcal{J}) - \Psi(\beta, \mathcal{J}_\varepsilon) \right| \;\leq\; \|\mathcal{J} - \mathcal{J}_\varepsilon\| \;\leq\; \varepsilon\,, \tag{5.25}$$

and similar bound for $\mathcal{J}'$. For the finite range approximations we already established the uniform bound

$$\left| \Psi(\beta, \mathcal{J}_\varepsilon) - \Psi(\beta, \mathcal{J}'_\varepsilon) \right| \;\leq\; \|\mathcal{J}_\varepsilon - \mathcal{J}'_\varepsilon\|\,. \tag{5.26}$$

Combining the last two estimates and taking $\varepsilon \to 0$ one learns that (5.20) is valid for all translation invariant interactions of finite norm.

Furthermore, under the assumption (5.31) the contribution of the ‘boundary terms’ to $|\Lambda|^{-1} \log Z_\Lambda$ vanishes in the limit.

□

Remark: Though this is not used in the proof, it may be of interest to note that by taking the limit $L \to \infty$ in (5.24) one may also learn about the rate of convergence. For an interaction of a finite range R this yields:

$$\left| \Psi(\beta, \mathcal{J}) - \Psi_{\Lambda(k)}(\beta, \mathcal{J}) \right| \;\leq\; 2d\, \|\mathcal{J}\|\, \frac{R}{k} \tag{5.27}$$

5.5 Extension to van Hove sequences of volume

From the convergence of the pressure for regular cubes one may conclude that the same holds true for other sequences of finite volumes. For a simple criterion under which the above argument extends quite naturally, let $\{\Lambda_{\alpha,k}\}_{\alpha \in \mathcal{J}}$ be a collection of translates of $\Lambda(k)$ which tiles (or partitions) the graph $\mathbb{Z}^d$, i.e. for which the vertex set of $\mathbb{Z}^d$ is the disjoint union

$$\mathbb{Z}^d \;=\; \sqcup_\alpha \Lambda_{\alpha,k} \tag{5.28}$$

(as depicted in figure 5.5). For any finite $\Lambda \subset \mathbb{Z}^d$ let $N_{+,k}$ and $N_{-,k}$ be the inner and outer packing numbers, i.e.

$$N_{+,k}(\Lambda) = \left| \{\alpha \in \mathcal{I} \mid \Lambda_{\alpha,k} \cap \Lambda \neq \emptyset \} \right|$$
$$N_{+,k}(\Lambda) = \left| \{\alpha \in \mathcal{I} \mid \Lambda_{\alpha,k} \subset \Lambda \} \right| \tag{5.29}$$

.

Definition 5.4. A sequence of finite subsets $\Lambda^{(n)} \subset \mathbb{Z}^d$ of divergent volumes is called a **van Hove sequence** if

$$\lim_{n\to\infty} \frac{N_{-,k}(\Lambda^{(n)})}{N_{+,k}(\Lambda^{(n)})} \ = \ 1\,. \tag{5.30}$$

Condition (5.30) is equivalent to the statement that for each $k < \infty$ the fraction of the (finite) volume of $\Lambda^{(n)}$ taken by points within distance k from the boundary (or from the set's complement) tends to zero ([**?**]).

Natural examples are obtained by intersecting the lattice $\mathbb{Z}^d$ with scaled up version of a fixed domain $D \subset \mathbb{R}^d$ of a piecewise smooth boundary.

Convergence in the van-Hove sense will be expressed by $\Lambda_n \Uparrow \mathbb{Z}^d$.

The arguments used in the proof of Theorem 5.5 yield also the following generalization.

Corollary 5.5 (The termodynamic limit)**.** *Let $\mathcal{J}$ be a translational invariant interaction of a system formulated over $\mathbb{Z}^d$. Then for any van Hove sequence of finite subsets $\Lambda^{(n)} \subset \mathbb{Z}^d$, and a sequence of boundary terms satisfying*

$$\sup_{\sigma} |\phi^{\sharp}_{\Lambda}(\sigma)| = o(|\Lambda|) \qquad (\textit{for } |\Lambda| \to \infty) \tag{5.31}$$

the pressure converges and has the same limit as in (5.32).

The above statement is conveyed somewhat less precisely by saying that the pressure converges in the van Hove limit, and writing symbolically:

$$\lim_{\Lambda \Uparrow \mathbb{Z}^d} \Psi^{\sharp}_{\Lambda}(\beta, \mathcal{J}) \ = \ \Psi(\beta, \mathcal{J})\,. \tag{5.32}$$

Notes

The existence of thermodynamic limit for the pressure is of fundamental significance for statistical mechanics. The corresponding results for models formulated in the continuum ($\mathbb{R}^d$) and for quantum systems are discussed in the classical text by D. Ruelle [**?**].

The presentation of pressure as a Lifshitz continuous functional over the space of translation invariant Hamiltonians in the metric induced by the norm $\|\mathcal{J}\|$, is due to David Ruelle. It is of help in the proof of convergence for interactions of unbounded range. In addition, through the relations (5.13) this perspective also allows to identify the infinite volume Gibbs states as tangent functionals to the pressure $\Psi(\beta, \mathcal{J})$, regarded as a functional over the linear space of interactions (a Banach space under the norm (5.8)).

The above was also seen as a step which could facilitate the formulation of the renormalization group flow on mathematically firm grounds. However, it was found that in the vicinity of phase transitions the decimation transformation tend to produce probability measures (on the space of configurations) which are not presentable as Gibbs states for interactions of finite norm $\|\mathcal{J}\|$. Thus the above goal is still unaccomplished. It remains the subject of ongoing studies (c.f [**?**]).

Exercises

5.1 Prove the pair of energy estimates (5.9) and (5.10).

5.2 Consider the d-dimensional Ising Hamiltonian with translation invariant interaction

$$H(\sigma) \; = \; -\sum_{\{x,y\}} J_{|x-y|}\sigma_x\sigma_y - h\sum \sigma_x$$

in which J_n are not limited to finite range.

i. Under what condition on the coupling constants $\{J_n\}$ would the energy of a given spin's interaction with the rest be bounded uniformly in the system's size?

ii. In the one-dimensional version of the model under what condition on $\{J_n\}$ would the total interaction of spins in $\Lambda(L) = [-L, L]$ with the rest of the system (i.e. the complement of $\Lambda(L)$ in $\mathbb{Z}$) be bounded uniformly in L?

iii. Which of the above pair of conditions suffice for the convergence of this models's pressure function $\Psi_\Lambda(\beta, \mathcal{J}) := \frac{1}{|\Lambda|} \ln Z_\Lambda(\beta,)$ in the thermodynamic limit (i.e. for the sequence of finite volumes $\Lambda(L) = [-L, L]^d$ in the limit $L \to \infty$) ?

5.3 Given a translation invariant interaction with $\|\mathcal{J}\| < \infty$ explain how can it be approximated by a finite range interaction $\mathcal{J}^{(R)}$ such that for every finite subset $\Lambda \subset \mathbb{Z}^d$ the corresponding energy functions satisfy

$$|H_\Lambda(\sigma) \; - \; H_\Lambda^{(R)}(\sigma)| \; \le \; \varepsilon|\Lambda| \tag{5.33}$$

for all configurations σ (where H and H' are related to $\mathcal{J}$ and $\mathcal{J}^{(R)}$ through (5.2)).

By how much would the thermodynamic pressure $\Psi(\beta, \mathcal{J})$ differ?
(That is: state an upper bound on $|\Psi(\beta, \mathcal{J}) - \Psi(\beta, \mathcal{J}^{(R)})|$.)

References

[1] David Ruelle *Statistical Mechanic; Rigorous Results* (Benjamin 1969; reprinted by World Scientific 1999).
[2] Barry Simon *"The Statistical Mechanics of Lattice Gases, Vol. I"* (Princeton Univ. Press, 2014).
[3] Sacha Friedli and Yvan Velenik *"Statistical Mechanics of Lattice Systems: a Concrete Mathematical Introduction"* (Cambridge University Press, 2017).
(It may still be downloadable from the authors' web site:
`http://www.unige.ch/math/folks/velenik/smbook/index.html`.)

6

Gibbs Equilibrium States

6.1 States formulated as expectation value functionals

Let us start with a clarification of the notion of **states** in statistical mechanics.

In the setup described in Section 5, we consider a system of a multitude of degrees of freedom. Their values parametrize the system's **microstates**, ω, whose collection forms the **space of configurations** Ω_Λ. The number, or measure, of microstates satisfying macroscopic constraints gives rise to Boltzmann's entropy function $S(V, E, N, ...)$.

In contrast, the macroscopic notion of a state, as used here, is based on the **expectation value functionals** which are mappings associating expectation values to the system's observables.

For classical systems **observables** correspond to real (or complex)-valued functions

$$f : \Omega \to \mathbb{R} \quad (\text{or } \mathbb{C}) .$$

States are presentable in terms of probability measures $\rho(d\omega)$ on the probability space $(\Omega, \mathcal{B})$ with the natural sigma algebra $\mathcal{B}$, on which more will be said in the next section. The corresponding expectation value functional is the mapping

$$f \mapsto \int_\Omega f(\omega)\, \rho(d\omega) =: \langle f \rangle_\rho ,$$

with $\langle f \rangle_\rho$ a convenient shorthand notation for the expectation value of f in a specified state ρ.

The formulation of states as expectation-value functionals defined over the system's observables is applicable also to quantum systems. As we shall recall below, in that case the system's observables are described by self adjoint operators, and the closest analogs to microstates (of finite systems) are vectors, or more precisely rays, in the relevant Hilbert space.

6.2 Gibbs states

Gibbs states, of finite systems of the type presented in the previous section, are probability measures of the form

$$\boxed{\rho_{\Lambda,\beta}(d\omega_\Lambda) = \frac{e^{-\beta H_\Lambda(\omega)} \mu_\Lambda(d\omega)}{Z_\Lambda(\beta, N)}} \tag{6.1}$$

where $\mu_\Lambda(d\omega)$ is the a-priori measure on Ω_Λ, $H_\Lambda(\omega)$ is the energy function (referred to as the **Hamiltonian**), and the normalizing factor is the partition function

$$Z_\Lambda(\beta) := \int_{\Omega_\Lambda} e^{-\beta H_\Lambda(\omega)} \mu(d\omega) \tag{6.2}$$

which was discussed in the previous section.

In the terminology of Section 2, expectation value with respect to such "'tilted" probability measures $\rho_{\Lambda,\beta}$ are referred to as a canonical ensemble average (at constant temperature), in contrast with Boltzmann's microcanonical ensemble (at prescribed energy).

Gibbs equilibrium states provide a natural description of the states of finite system which are in thermal contact (i.e. free to exchange energy) with a heat bath of the specified temperature $T = (k_B\beta)-1$.

Although the system's energy is not constrained, by the "winner takes all" argument which leads to (2.5) for β such the function $[-\beta u + s(u, \dots)]$ is maximized at a single value of u, in the thermodynamic limit the probability measure $\rho_{\Lambda,\beta}$ concentrates on configurations of energy density approaching that value. Hence the different ensembles are generically asymptotically equivalent. Exceptions occur at phase transitions in case the energy is discontinuous if β.

6.3 Gibbs states' variational characterization

Gibbs states admit a variational characterization which offers a useful perspective. Instrumental for that is the following notion of entropy of measures.

Definition 6.1. (The entropy of a state) Let $\rho(dx)$ be a probability measure on a measurable space $(X, \mathcal{B})$, and $\mu(dx)$ a positive "reference measure" with respect to which ρ is absolutely continuous. The following is referred to as the entropy of ρ relative to μ

$$S(\rho\,|\,\mu) := -\int_X \log\left(\frac{\delta\rho}{\delta\mu}(\omega)\right)\frac{\delta\rho}{\delta\mu}(\omega)\mu(d\omega) \quad \Big(= \int_X \log\left(\frac{\delta\rho}{\delta\mu}(\omega)\right)\rho(d\omega)\Big), \tag{6.3}$$

where $\frac{\delta\rho}{\delta\mu}(\omega)$ is the density (the "Radon-Nikodym derivative") of ρ with respect to μ.

Through the Jensen inequality one has the following upper bound.

Theorem 6.2. *In the above setup, for a given reference measure μ the mapping $\rho \mapsto S(\rho\,|\,\mu)$ is concave in ρ. Furthermore,*

$$S(\rho\,|\,\mu) \;\leq\; \log\mu(\Omega_\Lambda) \tag{6.4}$$

Furthermore, in case $\mu(\Omega_\Lambda) < \infty$ the above inequality is saturated (i.e. holds as equality) only on case ρ is the normalized multiple of μ (i.e. $\rho(d\omega) = \mu(d\omega)/\mu(\Omega)$).

Before presenting its proof let us present this statement's relevant implication.

Theorem 6.3. *(Gibbs states' variational characterization) For any finite system of the structure described above, with an a-priori reference distribution $\mu(d\omega)$ and energy function $H_\Lambda(\omega)$, the Gibbs measure* (6.1) *minimizes the following state function*

$$\mathcal{F}_\beta(\rho) := \int_{\Omega_\Lambda} H_\Lambda(\omega)\,\rho(d\omega) - \beta^{-1} S(\rho\,|\mu_\Lambda) \tag{6.5}$$

Proof of Thoeorm 6.3 A clearly equivalent of the statement is that the Gibbs state ρ_β **maximizes** is the probability measure ρ which maximizes the following functional

$$\rho \quad \mapsto \quad S(\rho\,|\,\mu_\Lambda) - \beta \int_{\Omega_\Lambda} H_\Lambda(\omega)\,\rho(d\omega) \tag{6.6}$$

A simple calculation shows that the above difference can be presented in terms of the relative entropy of ρ with respect to the Gibbs state as:

$$S(\rho\,|\,\mu_\Lambda) - \beta \int_{\Omega_\Lambda} H_\Lambda(\omega)\,\rho(d\omega) = S(\rho\,|\,\rho_\Lambda(d\omega)) + \log Z_\Lambda(\beta) \tag{6.7}$$

Hence the claim readily follows from Theorem 6.2 □

To prove the bound stated in Theorem 6.4 let us start with the following version of the Jensen inequality.

Theorem 6.4. *For any measure space $(X, \mathcal{B}, d\mu)$, of positive measure, any integrable $g : X \to \mathbb{R}$, and any concave function $F : R \to \mathbb{R}$*

$$\int F(g(x))\,\mu(dx) \;\leq\; F(\langle g\rangle_\mu)\;\mu(X), \tag{6.8}$$

where $\langle g\rangle_\mu$ (the normalized mean of g) is defined by the condition

$$\int_X [g(x) - \langle g\rangle_\mu]\;\mu(dx) = 0\,. \tag{6.9}$$

Proof The statement can be deduced from its normalized version, or just directly from the following tangent bound, which applies to any concave function F (regardless of the definition of $\langle x\rangle$)

$$F(\,g(x)\,) \;\leq\; F(\,g(\langle x\rangle)\,) \;+\; [g(x) - g(\langle x\rangle)]\;F'(\,g(\langle x\rangle) + 0\,)\,. \tag{6.10}$$

Combining that with (6.9) one finds that upon integration over $\mu(dx)$ the contribution of the last term to the integral vanishes, leaving one with the claimed (6.8). □

Using (6.8) we now complete the postponed task:

Proof of Thm 6.2 The dependence of the entropy on the probability measure ρ can be presented as

$$S(\rho\,|\,\mu) := \int_X F\left(\frac{\delta\rho}{\delta\mu}(\omega)\right)\mu(d\omega) \tag{6.11}$$

with $F(x) = -x\log x$ which is strictly concave over $[0,\infty)$. To apply the corresponding Jensen inequality let us first note that

$$\int \left[\frac{\delta\rho}{\delta\mu}(x) - \frac{1}{\mu(X)}\right]\mu(dx) = 0\,. \tag{6.12}$$

Thus, by Theorem 6.4

$$\int_X F\left(\frac{\delta\rho}{\delta\mu}(\omega)\right)\mu(d\omega) \ \leq \ F\left(\frac{1}{\mu(X)}\right)\cdot\mu(X) = \log\mu(X) \tag{6.13}$$

Furthermore, from the strict concavity of F one may conclude that the inequality is sharp unless $\frac{\delta\rho}{\delta\mu}(\omega)$ is constant, which requires ρ to be a normalized version of μ. □

The variational characterization of the Gibbs measure as the maximizer of the functional in (6.6) indicates that the states provide a compromise between two different pulls: to keep the mean energy low higher weight is given to configurations of low energy, yet to gain entropy the measure is not supported exclusively on the ground states, but spread more extensively. At low temperatures (high β) the energy considerations dominate. At high temperature (low β) the energy considerations are less relevant and entropy considerations dominate.

A simple example of the above will be seen in our discussion of ferromagnetic spin models, for which the above perspective yields an intuitive grasp of the model's phase transition. (Still, the above loose description does not suffice since the phase transitions occurs only in high enough dimensions; $d > 1$ for the discrete valued spins with short range interaction, and $d > 2$ for such systems with continuous symmetry.)

6.4 The pressure as the Gibbs measure's generating function

As we saw in the previous section, the pressure function $\Psi_\Lambda(\beta,\mathcal{J}) := \frac{1}{\Lambda}\log Z_\Lambda(\beta,\mathcal{J})$ provides Gibbs states' generating function, through relations such a:

$$\begin{aligned} \frac{\partial}{\partial\beta}\Psi_\Lambda(\beta,\mathcal{J}) &= -|\Lambda|^{-1}\langle H_\Lambda\rangle_{\beta,\Lambda} \\ \frac{\partial^2}{\partial\beta^2}\Psi_\Lambda(\beta,J) &= \ \frac{1}{|\Lambda|}\langle\left(H_\Lambda - \langle H_\Lambda\rangle_{\beta,\Lambda}\right)^2\rangle_{\beta,\Lambda} \ \geq \ 0\,. \end{aligned} \tag{6.14}$$

More generally, regarding $\Psi_\Lambda(\beta,\mathcal{J})$ as function of the collection of the coupling constants $\mathcal{J} = \{J_A\}$ which appear in (5.2) one has

$$\frac{\partial}{\partial J_A}\Psi_\Lambda(\beta,\mathcal{J}) = -\frac{\beta}{|\Lambda|}\left\langle\frac{\partial}{\partial J_A}H_\Lambda\right\rangle_{\beta,\Lambda}\,, \quad \text{etc.} \tag{6.15}$$

Furthermore, from the convexity arguments mentioned above we learn that at inverse temperatures β at which the infinite volume function is differentiable in β the finite volume energy density converges to its thermodynamic value:

$$\lim_{\Lambda\Uparrow\mathbb{Z}^d}|\Lambda_L|^{-1}\langle H_\Lambda\rangle_{\beta,\Lambda} = -\frac{\partial}{\partial\beta}\Psi(\beta,\mathcal{J})\,. \tag{6.16}$$

Furthermore, that holds true **regardless of the choice of the finite volume boundary conditions**.

For β at which the derivative of $\Psi(\beta, ...)$ is discontinuous, the values of $|\Lambda_L|^{-1}\langle H_\Lambda\rangle_{\beta,\Lambda}$ do depend on the boundary conditions (manifesting in this manner a first-order phase transition). In that case, the range of observable energy density values asymptotically collapses onto the interval $-[\frac{\partial}{\partial\beta}\Psi(\beta+0, ...),\ \frac{\partial}{\partial\beta}\Psi(\beta-0, ...)]$.

Similar statements apply to the relation of the densities of all other extensive quantities in relation to the derivatives of the pressure with respect to the coefficients of the corresponding collection of terms in the Hamiltonian. For instance, such a conjugacy is found in the relation between the Ising model's magnetization per volume and the the derivative of Ψ in the magnetic field h, of (5.4).

6.5 Concentration of measure and large deviation bounds

The asymptotic concentration of the densities of thermodynamic extensive quantities, such as the energy or magnetization, is further quantified by the following large deviation estimate. In particular: the probability that in a large rectangular (squarish) domain the energy density deviates by ϵ, either up or down from its thermodynamic value, or range in case of discontinuity, is exponentially small in the volume.

Theorem 6.5. *For an extensive system of Hamiltonian of the form* (5.2)*, for each finite β there are functions $\delta_{\beta,\pm}$ such that for any $\varepsilon > 0$, at large enough L:*

$$\begin{aligned}\mathbb{P}^{\#}_{\beta,\Lambda_n}\left(\frac{1}{|\Lambda|}H^{\#}_{\Lambda} \le -\frac{\partial\Psi}{\partial\beta}(\beta+0,\mathcal{J})-\varepsilon\right) &\le e^{-\delta_{\beta,+}(\varepsilon)\,|\Lambda|}\\ \mathbb{P}^{\#}_{\beta,\Lambda_n}\left(\frac{1}{|\Lambda|}H^{\#}_{\Lambda} \ge -\frac{\partial\Psi}{\partial\beta}(\beta-0,\mathcal{J})+\varepsilon\right) &\le e^{-\delta_{\beta,-}(\varepsilon)\,|\Lambda|}\end{aligned} \tag{6.17}$$

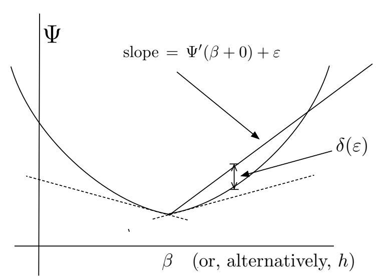

Figure 6.1 The gap construction which produces a lower bound on the large deviation rate function $\delta(\varepsilon)$ for the ε-deviations in the energy density.

Proof As can be read from (6.14), the typical order of fluctuations of extensive quantities' is $O(\sqrt{|\Lambda|})$. Hence shifts of the density by even a small ε in the limit $L \to \infty$ represent a **large deviation**.

To bound the probability of deviations down let start with the observation that, for all $t > 0$

$$\mathbb{1}[H \leq (E-\varepsilon)\,|\Lambda|] \;\leq\; e^{-tH} e^{t\,(E-\varepsilon)\,|\Lambda|}\,. \tag{6.18}$$

(since since $\mathbb{1}[Q \;\leq\; 0] \;\leq\; e^{-tQ}$). We shall apply this to

$$E = -\,\Psi\,'(\beta+0). \tag{6.19}$$

Averaging (6.18) over the Gibbs probability measure one concludes that for any $t > 0$:

$$\begin{aligned}
\mathbb{P}^{\sharp}_{\beta,\Lambda}\Big(H^{\sharp}_{\Lambda} \leq (E-\varepsilon)\,|\Lambda|\Big) &\leq \left[\int_{\Omega_\Lambda} e^{-(t+\beta) H^{\sharp}_{\Lambda}(\sigma)} \frac{\mu(d\sigma)}{Z^{\sharp}_{\Lambda}(\beta)}\right] e^{t\,(E-\varepsilon)|\Lambda|} \\
&= \frac{Z^{\sharp}_{\Lambda}(\beta+t)}{Z^{\sharp}_{\Lambda}(\beta)} e^{t\,(E-\varepsilon)\,|\Lambda|} = \\
&= \exp\Big\{\Big[\Psi^{\sharp}_{\Lambda}(\beta+t) - \Big(\Psi^{\sharp}_{\Lambda}(\beta) + t(\Psi\,'(\beta+0)+\varepsilon)\Big)\Big]\,|\Lambda|\Big\}
\end{aligned} \tag{6.20}$$

where we see the partition function at shifted to $(\beta + t)$.

The next step is to optimize this bound over t, in a manner explained in Figure 6.1. Due to the convexity of the limiting function Ψ, for small enough $t > 0$ this function satisfies:

$$\Psi(\beta+t) \leq \Psi(\beta) + t\,(\Psi\,'(\beta+0)+\varepsilon) \;<\; 0\,. \tag{6.21}$$

Consequently, there is $t(\varepsilon) > 0$ for which

$$\Psi(\beta+t) - \Psi(\beta) + t(E-\varepsilon) \;\leq\; -2\delta_{\beta,+}(\varepsilon) \tag{6.22}$$

at some $\delta(\varepsilon) > 0$ (the factor 2 is for the convenience of ensuing expressions). The pointwise convergence of the finite volume pressures allows to conclude that for large enough L also

$$\boxed{\Psi^{\#}_{\Lambda(L)}(\beta+t) - \Psi^{\#}_{\Lambda(L)}(\beta) + t(E-\varepsilon) \;\leq\; -\,\delta_{\beta,+}(\varepsilon)} \tag{6.23}$$

(for arbitrary boundary conditions).

Upon substitution in (6.20) this yields

$$\mathbb{P}^{\sharp}_{\beta,\Lambda}\Big(H^{\sharp}_{\Lambda} \leq (-\Psi\,'(\beta-0)-\varepsilon)\,|\Lambda|\Big) \;\leq\; e^{-\delta_{\beta,+}(\varepsilon)\,|\Lambda|} \tag{6.24}$$

for L large enough.

To bound the probabilities of fluctuations in the other direction, similar reasoning (or a reflection $H \to -H$) yields:

$$\mathbb{P}^{\sharp}_{\beta,\Lambda}\Big(H^{\sharp}_{\Lambda} \geq (-\Psi\,'(\beta-0)+\varepsilon)\,|\Lambda|\Big) \;\leq\; e^{-\delta_{\beta,-}(\varepsilon)\,|\Lambda|} \tag{6.25}$$

□

Notes

The derivation of the large deviation bound given here is an extension to interacting systems of the strategy which was used early on by Bernstein for a large deviation result for iid random variables. The method has seen many extensions, including Cramér large deviation expansions for martingales, and culminating in the more general, and multilevel, Donsker-Varadhan theory of large deviations.

Exercises

6.1 Boundary conditions of interest for the d-dimensional Ising model include the following choices for the boundary terms in the finite-volume Hamiltonian for the Ising spin system in $\Lambda(L) = \Big(-\lfloor L/2 \rfloor, \lfloor L/2 \rfloor \Big]^d$:

$$H^{(\tau)}_{\Lambda(L)}(\sigma) = -J \sum_{\substack{\{x,y\}\subset\Lambda \\ |x-y|=1}} \sigma_x\sigma_y \; - \; J \sum_{\substack{x\in\Lambda, y\in\mathbb{Z}^d\setminus\Lambda \\ |x-y|=1}} \sigma_x\tau_y \; - \; h\sum_{x\in\Lambda}\sigma_x \tag{6.26}$$

with

$$\tau_y \;=\; \begin{cases} 0 & \text{free b.c.} \\ +1 & + \text{ b.c.} \\ -1 & - \text{ b.c.} \end{cases} \;, \quad \text{and} \quad \tau_y \;=\; \sigma_{\mathrm{p}er(x)}/2 \quad \text{for the periodic b.c.} \tag{6.27}$$

where $\mathrm{p}er(x)$ is to be summed over the sites $u \in \Lambda(L) \setminus \{x\}$ which are the neighbors of x under he periodic boundary conditions.

i. Prove that $\Psi(\beta, J, h)$ (the system's pressure in the infinite volume limit) is convex in h.
ii. Summarize the arguments proving that at (β, h) for which $\Psi(\beta, h)$ is differentiable with respect to h, for all boundary condition:

$$\lim_{L\to\infty} \frac{1}{|\Lambda(L)|} \langle M_{\Lambda(L)} \rangle^{\sharp}_{\beta,\Lambda} \;=\; -\frac{1}{\beta}\frac{\partial}{\partial h}\Psi(\beta, h)\,, \tag{6.28}$$

where $M_\Lambda := \sum_{x\in\Lambda}\sigma_x$ (the finite system's bulk magnetization).

Remark: The ongoing interest in the Ising model owes much to the fact that (6.28) fails for the $2D$ Ising model at $h = 0$ and low temperatures, i.e. $\beta > \beta_c$. We shall next turn to its proof by Rudolf Peierls (who was later knighted for his contributions to science and technology).

References

Gibbs equilibrium states are discussed extensively in the bibliography listed in the previous Chapter. More will be said on the subject below, and references will be added accordingly.

General formulation of the theory of large deviations, and results of interest for stat mech and other probabilistic settings, can be found in the following references (among many others).

- S.R.S. Varadhan , “Large deviations”, The Annals of Probability, Vol. 36, No. 2, 397-419 (2008).
- R.S. Ellis, “Entropy, Large Deviations and Statistical Mechanics”, (Springer 1985).
- A. Dembo and O. Zeitouni, “Large Deviations Techniques and Applications”. (Springer 2010).

PART II. Phase transitions and symmetry breaking

7

Phase transition: the Peierls proof of symmetry breaking in the $2D$ Ising model

The Ising model was formulated by Wilhelm Lenz in 1920, in an attempt to improve upon the Curie-Weiss (mean-field) model of ferromagnetism. Ferromagnets which exhibit permanent magnetization at room temperatures loose it when the temperature is raised above a critical value, their "Curie temperature". The mean-field model of the transition does not account for some of the phase transition's characteristics, such as the observed divergence of the specific heat as $T \uparrow T_c$ and other details of the critical behavior.

The problem was presented by Lenz to his student Ernst Ising, who in his 1924 PhD thesis showed the negative result that in its one dimensional version the model's relevant thermodynamic functions are analytic in the magnetic field at all temperatures $T > 0$, i.e. the model does not exhibit any phase transition. The situation was rescued by Rudolf Peierls who in 1936 showed that in higher dimensions the short range model does undergo a phase transition, and exhibits spontaneous magnetization.

Following that, the Ising model has been the arena for a sequence of consequential insights. These include the Kramers-Wannier [2] duality, through which the exact value of the critical temperature can be determined, and Onsager's exact solution of the two dimensional model in 1944, which showed a logarithmic divergence in the specific heat. A plethora of methods and insights concerning phase transitions and critical phenomena has followed. The model's role for Statistical Mechanics has been compared to that of the Drosophila fly [1] for molecular biology.

7.1 The setup and the main result

The Ising spin model on $\Lambda \subset \mathbb{Z}^d$ has as its basic variables a collection of ± 1 valued variables $\{\sigma_x\}_{x\in\Lambda}$ and a Hamiltonian (the energy function) of the form

$$\boxed{H_{\Lambda,J,h}(\sigma) := -\sum_{\{x,y\}\subset\Lambda} J_{x,y}\,\sigma_x\sigma_y \;-\; \sum_{x\in\Lambda} h\,\sigma_x\,.} \tag{7.1}$$

In this section we focus on the *nearest neighbor ferromagnetic* (n.n.f.) interaction, at $J > 0$:

$$J_{x,y} = \begin{cases} J & \|x-y\| = 1 \\ 0 & \text{otherwise} \end{cases} \tag{7.2}$$

[1] A 3mm long fruit fly, in which one purportedly finds 75% of the genes which are know to cause disease in humans.

The corresponding finite volume Gibbs equilibrium state $\langle\cdot\rangle_{\Lambda,J,h,\beta}$ at *inverse temperature* $\beta \geq 0$ is the probability measure under which the expectation value of any function $F : \{\pm 1\}^\Lambda \to \mathbb{R}$ is given by

$$\boxed{\langle F\rangle^\sharp_{\beta,h,\Lambda} \; = \sum_{\omega\in\Omega_{\Lambda,N}} F(\omega)\frac{e^{-\beta H^\sharp_\Lambda(\omega)}}{Z^\sharp_\Lambda(\beta,h)}} \tag{7.3}$$

where $\sharp$ represents the boundary conditions. A natural pair of boundary conditions ($\sharp = \pm$) corresponds to fixing the spins along the boundary as all + (or alternatively all $-$).

Infinite volume Gibbs states on $\mathbb{Z}^d$, which we shall denote by $\langle\cdot\rangle_{J,h,\beta}$, are defined through suitable limits of the above ($\Lambda_L = [-L, L]^2 \cup \mathbb{Z}^d$, $L \to \infty$).

In contrast to the model's behavior in one dimension, whose discussion we omit at the moment, for higher dimension one has the following basic result .

Theorem 7.1 (Peierls [1])**.** *For the 2D Ising model there exists $\beta_P < \infty$ such that at $h = 0$ the finite volume magnetization satisfies, for all $x \in \Lambda$*

$$\begin{aligned} \langle\sigma_x\rangle^+_{\Lambda,\beta,0} \;&\geq m(\beta) \\ \langle\sigma_x\rangle^-_{\Lambda,\beta,0} &\leq -m(\beta)\,, \end{aligned} \tag{7.4}$$

with $\boxed{m(\beta) > 0}$ *for all $\beta > \beta_P$.*

Before presenting the proof let us briefly recall some of this statement's implications.

Thermodynamics:

In thermodynamic terms the bounds (7.4) imply the existence of a line of **first order phase transitions**. It is expressed in the discontinuity of the magnetization as a function of the external field, at $h = 0$ and $\beta > \beta_P$. This is manifested in a cusp singularity for the pressure along the line $\{(\beta, h) : \beta \geq \beta_P, h = 0, \}$ in the model's parameter space. More explicitly:

Corollary 7.2. *For any $\beta > \beta_P$ at $h = 0$ the pressure fails to be differentiable with respect to h, satisfying:*

$$\frac{\partial}{\partial h}\Psi(\beta, 0-) \;\leq\; -m(\beta) \;<\; m(\beta) \;\leq\; \frac{\partial}{\partial h}\Psi(\beta, 0+) \tag{7.5}$$

(The deduction is by the relations discussed in Section 6, cf. Theorem 6.5.)

Statistical Mechanics:

At the stat mech level, (7.4) demonstrates that at high enough β the Gibbs equilibrium states are **sensitive to the boundary conditions**. That is, the difference in the expectation values of the local observable σ_x does not vanish in the limit $L \to \infty$, even as the boundary recedes away.

For a more explicit formulation of this statement it is natural to take the infinite volume limits of the finite volume states. Viewing states as expectation value functionals of functions $f(\sigma)$ there are two natural limiting states to consider:

$$\langle f \rangle_\beta^+ = \lim_{L\to\infty} \langle f \rangle^+_{\Lambda_L,\beta,0}\,, \quad \text{and} \quad \langle f \rangle^- = \lim_{L\to\infty} \langle f \rangle^-_{\Lambda_L,\beta,0}\,. \tag{7.6}$$

More is said on that in the Notes below.

The limit are initially considered only for local functions, i.e. functions for which $f(\sigma)$ depends only spins within a finite subset of the limiting graph $\mathbb{Z}^2$.

In the present case, the mere convergence in (7.6) for all local f can be deduced through monotonicity arguments (the FKG inequality) which would be discussed elsewhere. Taking that for granted (or temporarily avoiding the issue by restricting the discussion to convergent subsequences), the Peierls Theorem implies for $\beta > \beta_P$ the two limiting states are distinct, with

$$\langle \sigma_x \rangle_\beta^+ = -\langle \sigma_x \rangle_\beta^- \geq m(\beta) > 0 \tag{7.7}$$

Symmetry breaking:

The non-vanishing of the magnetization in the above limiting states is a phenomenon of **symmetry breaking**. At zero external field the both the Hamiltonian (7.1) and the a-priori measure are invariant under the global spin flip

$$\sigma_x \longmapsto -\sigma_x \quad \forall x\,. \tag{7.8}$$

The non-vanishing of the mean magnetization means that the limiting states, $\langle - \rangle_\beta^+$ and its flipped image $\langle - \rangle_\beta^-$, do not have that symmetry.

7.2 The Peierls argument

To prove (7.4) let us translate it to a bound on the probability that σ_x takes the opposite value to that of the boundary spins. Since $\mathbb{1}[\sigma_x = -1] = (1 - \sigma_x)/2$, it suffices to show that at high enough β the probability of this event satisfies

$$\boxed{\langle \mathbb{1}[\sigma_x = -1] \rangle^+_{\Lambda,\beta,0} \leq 1/2 - m(\beta)/2} \tag{7.9}$$

at some $m(\beta) > 0$.

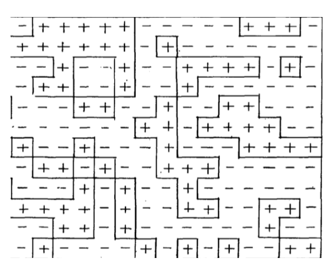

Figure 7.1 Peierls contours, as drawn in his original paper.

To bound this probability, Peierls associates with each spin configuration a collection of closed contours, built of the dual graph's edges, passing between sites of opposite spin values. A loop γ within Λ is said to occur as **a contour of the configuration** σ if the configuration's spins take constantly one value on γ's inside and the opposite value on its outside (defined by the natural algorithm).

Noting that under the $+$, or $-$, boundary conditions the event that σ_x differs from the bounday value requires the site x to be encircled by at least one contour, the proof proceed by bounding the probability of such an event. There are two steps in Peierls argument:

i. an energy-driven bound on the probability that a contour of length n is realized
ii. an entropy estimate, bounding the number of loops of length n encircling x.

At low enough temperature energy considerations prevail.

More explicitly: noting that

$$\sigma_x \sigma_y = 2 \cdot \mathbb{1}[\sigma_x = \sigma_y] - 1$$

the Ising Hamiltonian at $h = 0$ and the +boundary conditions can be rewritten as

$$H_\Lambda^{(+)}(\sigma) = 2 \sum_\gamma |\gamma| \; \mathbb{1}[\gamma \text{ occurs as a contour of } \sigma] - J|\mathcal{E}(\Lambda)| \,, \tag{7.10}$$

where $|\gamma|$ denotes the contour's length, and $|\mathcal{E}|$ is the number of edges of Λ.

In the following discussion we restrict the attention to contours along which the value inside is the opposite of the boundary spins, and denote the indicator function of this event as:

$$\mathbb{1}_\gamma[\sigma] := \mathbb{1}[\gamma \text{ occurs as a contour of } \sigma, \text{ flipped on the inside}] \tag{7.11}$$

Lemma 7.3 (The Peierls contour estimate)**.** *For the Ising model on $\mathbb{Z}^2$ with the Hamiltonian* (7.1) *at $h = 0$ and $\beta \geq 0$, the probability that any given simple closed path on the dual graph occurs as a contour satisfies*

$$\boxed{\mathbf{Pr}_\Lambda^+ \left(\{\sigma \textit{ has } \gamma \textit{ as one of its contours}\}\right) \;=\; \langle \mathbb{1}_\gamma[\sigma] \rangle_{\Lambda,\beta,0}^+ \;\leq\; e^{-2\beta J |\gamma|}} \tag{7.12}$$

Proof For each specified closed loop γ, let $T\gamma : \Omega(\Lambda) \to \Omega(\Lambda)$ be the involutive mapping under which the spins are flipped within γ and left unchanged on its outer side. This mapping associates in a $1-1$ fashion to each configuration in which the contour occurs one in which it does not, whose energy is lower by exactly the length of γ. Hence:

$$\begin{aligned} \langle \mathbb{1}_\gamma[\sigma] \rangle_{\Lambda,\beta,0}^+ &= \frac{\sum_{\sigma \in \Omega(\Lambda)} \mathbb{1}_\gamma[\sigma] e^{-\beta H_\Lambda^+(\sigma)}}{\sum_{\sigma \in \Omega(\Lambda)} e^{-\beta H_\Lambda^+(\sigma)}} \\ &\leq \frac{\sum_{\sigma \in \Omega(\Lambda)} \mathbb{1}_\gamma[\sigma] e^{-\beta H_\Lambda^+(\sigma)}}{\sum_{\sigma \in \Omega(\Lambda)} \mathbb{1}_\gamma[\sigma] e^{-\beta H_\Lambda^+(T_\gamma \sigma)}} = e^{-2\beta J |\gamma|} \end{aligned} \tag{7.13}$$

where the bound holds since this is exactly the ratio of the corresponding terms in the numerator and denominator. □

Next, for an estimate on the number of contours of length n encircling a given site x, note that each such contours can be drawn by starting with an edge which pierces in the upward direction the line drawn "to the right of x", for which there are not more than $n/2$ choices, and at each of the subsequent steps moving in one of at most 3 possible directions. The number of such paths is bounded by $\boxed{\frac{n}{2}3^n}$.

Proof of Theorem 7.1 To bound the probability that $\sigma_x = -1$, let $C_x(\sigma)$ be the connected cluster (in the $\mathbb{Z}^2$ nearest neighbor, or the diagonally next-nearest-neighbour sense) of sites on which the spins take that value. The outer boundary of this cluster is a contour of σ with $-$ on its inner side.

Hence under the + boundary conditions $\sigma_x = -1$ requires x to be encircles by at last one contour of inner sign $-$. Applying the union bound, one gets

$$\boxed{\langle \mathbb{1}[\sigma_x = -1]\rangle^+_{\Lambda,\beta,0}} \leq \langle \mathbb{1}_\gamma[\sigma]\rangle^+_{\Lambda,\beta,0} \leq \sum_{\gamma \text{ encircling } x} e^{-2\beta J|\gamma|} \leq \tag{7.14}$$
$$= \sum_{n\geq 4} \mathrm{card}\{\gamma|\gamma \text{ encircles } x,\, |\gamma| = n\,\} \cdot e^{-2\beta J n} \leq \boxed{\sum_{n\geq 4} \frac{n}{2}\,(3e^{-2\beta J})^n}$$

where we combined (7.12) with the above entropy bound.

The last sum converges for $\beta > \widehat{\beta}$, the latter defined by

$$3\; e^{-2\widehat{\beta}\, J} = 1\,. \tag{7.15}$$

The claimed bound (7.4), in the form of (7.9), holds for $\beta > \beta_P$ with β_P defined by the slightly more demanding condition:

$$\sum_{n\geq 4} \frac{n}{2}\,(3e^{-2\beta_P J})^n = 1/2\,. \tag{7.16}$$

□

7.2.1 A stochastic geometric manifestation of the phase transition

The pair of infinite volume states $\langle - \rangle^{\pm}_{\beta}$ defined through (7.6) allow to add to our vocabulary terms which are simpler to state in the context of infinite systems. The proper formulation of probability measures over the configurations of infinity systems will be the subject of the next section. For a hint of what that enables let us consider the following notion.

Definition 7.4. An infinite spin system's configuration is said to exhibit **"(+) percolation"** if the set of sites where $\sigma_x = +1$ includes an infinite connected component. The **"(−) percolation"** event is obtained by replacing (+) by (−).

The Peierls contour analysis presented above allows to prove:

Theorem 7.5. *For $\beta > \beta_P$ (the latter defined by* (7.16)*) the infinite system's probability distribution, which corresponds to the states $\langle - \rangle^{\pm}_{\beta}$ satisfy*

$$\begin{aligned} &\langle \mathbb{1}[\textit{the spin configuration exhibits} - \textit{percolation}]\rangle^+_\beta = 0 \\ &\langle \mathbb{1}[\textit{the spin configuration exhibits} + \textit{percolation}]\rangle^+_\beta = 1 \end{aligned} \tag{7.17}$$

while for $\langle - \rangle_\beta^-$ the opposite it true.

To outline the proof, let us denote by K^+ the (+) percolation event, and by $\mathcal{L}^+_{L_0,L_1}$ the event that Λ_{L_0} and $\Lambda^c_{L_1}$ are connected by a path along which $\sigma_u = +1$. The similarly defined events with + replaced by − will be denoted K^- and $\mathcal{L}^-_{L_0,L_1}$ correspondingly. As it is easy to see:

$$\mathbb{1}[K^-] = \lim_{L_0\to\infty} \lim_{L_1\to\infty} \mathbb{1}[\mathcal{L}^-_{L_0,L_1}](\sigma) \tag{7.18}$$

where the limits exist by monotonicity, as the function is monotone decreasing in L_1 and increasing in L_0. Theorem 7.5 can therefore be deduced from the following statement (combined with the bounded convergence theorem).

Lemma 7.6. *For the 2D Ising model with the nearest neighbor interaction* (7.1) *at* $h = 0$*, and* $\beta > \widehat{\beta}$ *(i.e. at which* $3\ e^{-2\widehat{\beta} J} < 1$*)*

$$\begin{aligned} \lim_{L_0\to\infty} \lim_{L_1\to\infty} \langle \mathbb{1}[\mathcal{L}^-_{L_0,L_1}]\rangle^+_\beta &= 0 \\ \lim_{L_0\to\infty} \lim_{L_1\to\infty} \langle \mathbb{1}[\mathcal{L}^+_{L_0,L_1}]\rangle^+_\beta &= 1 \end{aligned} \tag{7.19}$$

Sketch of the proof: The first equation in (7.19) follows by noting that with the + boundary conditions the event $\mathcal{L}^-_{L_0,L_1}$ requires the existence of a contour of length at least $2(L_1 - L_0)$ at distance L_0 to the origin. Its probability can therefore be bounded by a sum similar to that in (7.14). However in the present situation the sum starts at $2(L_1 - L_0)$ rather than $n = 4$.

The second equation in 7.19 is proven by first recognizing that for $\mathcal{L}^+_{L_0,L_1}$ to fail the configuration has to include a contour encircling Λ_{L_0} within Λ_{L_1}. The probability for that is bounded by the corresponding sum.

□

A point to appreciate here is that in the above argument the probability of percolation is approached through its quasi local manifestations. That is necessary since the convergence of finite volume to the infinite volume probabilities is guaranteed only for local events. The existence of an infinite connected cluster is not a local event. It can even be said that this event is "measurable at infinity". We shall clarify such concepts in a later section.

Remarks:

1) The above percolation considerations lead to the interesting observation that the model's symmetry breaking can be deduced for all β satisfying $3\, e^{-2\beta J} < 1$, which is a simpler condition than (7.16).

2) The Fortuin-Kasteleyn-Ginibre inequality, and the related coupling principle, allow to deduce that in this model symmetry breaking in any form can occur only if (7.4) holds with $m(\beta) \neq 0$. Thus the above produces a real improvement on the critical temperature, as defined by spontaneous magnetization.

3) A further improvements can be obtained by replacing the factor 3 by the connectivity constant of self avoiding walks on $\mathbb{Z}^2$. However, the critical point of the Ising model on this graph can be ascertained exactly by other means.

Notes

1) Peierls's original argument [1] was streamlined a bit by R. Griffiths [4] and, independently, by R.L. Dobrushin [5].
2) The exact value of the two dimensional model's phase transition temperature is given by

$$\sinh(2J\beta) = 1\,, \tag{7.20}$$

which is the self-dual point of the Kramer-Wanier duality relation [2]

$$\sinh(2J\beta)\ \sinh(2J\beta^*) = 1\,. \tag{7.21}$$

3) The model's self-duality relation at the point determined by (7.20) does not suffice to prove that the model has a phase transition at this point (rather than having an intermediate regime between two mutually dual points). There are different ways to arrive at this deduction, each providing a valuable lesson on other aspects of this model. These include:
   i. Onsager's exact solution of this very model [3].
   ii. A "sharpness of phase transition" result which implies that (in any dimension) Ising model's long range order sets in right after the loss of exponential decay of correlations [7], combined with a proof that the model and its dual cannot simultaneously exhibit the percolation described above. A similar issue arrises in a range of self-dual two-dimensional percolation problems, to some of which this tactic is also applicable. (The topic may be further discussed below.)
4) The Peierls argument can be viewed as a perturbative method for extending our understanding of the model's ground state configurations into analysis of its low temperature phases. As such, it has found its robust generalization in the Pirogov-Sinai theory [6]. Its application extend over a range of other statistic mechanical systems, and are not limited to two dimensions. (References to it will be expanded.)

Exercises

7.1 Complete the proof of Lemma 7.6.

7.2 *Optional, extra credit question.* Prove Theorem 7.5. That is: explain how from Lemma 7.6 one may deduce the existence of percolation in the model's infinite volume limit at $\beta > \widehat{\beta}$.

The two dimensional Ising model has been the subject of a particularly rich collection of works. These have in turn have been discussed in many reviews. The following short list is focused on the original works directly related to the points presented above.

References

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8

Continuous symmetry breaking ($d > 2$)

The Peierls argument proving symmetry breaking in the Ising model does not extend to systems which admit continuous spin deformations of arbitrarily low energy cost. A prototypical example of such is provided by the vectorized version of the Ising model of N components spin vectors $\underline{\sigma}_x = (\sigma_{x,1}, ..., \sigma_{x,N})$, of unit length, and the translation invariant Hamiltonian

$$H(\underline{\sigma}) = -\frac{1}{2} \sum_{x,y \in \mathbb{Z}^d} J_{x-y} \, \underline{\sigma}_x \cdot \underline{\sigma}_y \; - \; \sum_{x \in \Lambda} \underline{h} \cdot \underline{\sigma}_x \tag{8.1}$$

and the a-priori single spin measure $\mu(d\underline{\sigma})$ being the spherically symmetric distribution of the unit sphere.

Unlike the case of discrete symmetry, in such models (with finite-range bounded interaction) continuous symmetry breaking at $\underline{h} = \underline{0}$ does not occur in two dimensions[1] However, a spin-wave argument which will be recalled below indicates that continuous symmetry breaking may occur in dimensions $d > 2$.

The objective on this section is to present a remarkable argument, due to Fröhlich, Simon and Spencer [1], which enables to carry the spin wave analysis to its desired conclusion, at least for systems meeting a stringent reflection symmetry condition. The method developed in the process has also many other applications, many of which were presented by J. Fröhlich, R. Israel, E. Lieb, and B. Simon in [2]. These two works ought to be viewed as part of our subject's canon. Yet, as is also explained there, the task is not finished and there is still need for a more broadly applicable analysis.

8.1 The spin wave perspective

The spin-wave expressions and relations which are presented next apply to N component unit spins just as they do to single component σs. Thus, to un-encumber the presentation, we shall present their theory in the context of single component spins. Its vectorized version is obtained by underscoing each σ, and where appropriate replacing single multiplication by dot product.

When discussing the finite volume Gibbs states, whose infinite volume is expected to be

[1] The exact version of this statement is the Mermin-Wagner theorem, whose exact formulation and proof will be discussed later.

translation invariant it is natural to start with finite systems in

$$\Lambda(L) := (-L/2, -L/2+1, ..., L/2]^d \tag{8.2}$$

under the periodic boundary conditions. Furthermore, it is instructive to present the relevant quantities in spin-wave terms.

This is enabled by Fourier's representation of any function defined over Λ, which in our case is the spin configuration $\sigma = \{\sigma_x\}_{x\in\Lambda}$, as a superposition of "spin waves" of corresponding amplitudes $\widehat{\sigma}_p$:

$$\sigma_x := \frac{1}{\sqrt{L^d}} \sum_{p\in\Lambda_L^*} \widehat{\sigma}_p \, e^{-ip\cdot x} \tag{8.3}$$

with p for which the wave is periodic over $\Lambda(L)$ i.e. the sum ranges over the lattice points in the Brillouin zone

$$\Lambda_L^* := (-\pi, \pi]^d \cap \tfrac{\pi}{L}\mathbb{Z}^d \,. \tag{8.4}$$

The inverse relation, by which $\{\widehat{\sigma}_p\}$ can be computed for a given spin configuration is

$$\widehat{\sigma}_p := \frac{1}{\sqrt{L^d}} \sum_{x\in\Lambda_L} e^{ip\cdot x}\sigma_x \tag{8.5}$$

Under the normalization chosen here the Parseval-Plancherel relation between the ℓ^2 norms of a function and its Fourier transform takes the form of the sum rule

$$\sum_{p\in\Lambda^*} \|\widehat{\sigma}_p\|^2 \;=\; \sum_{x\in\Lambda} \|\sigma_x\|^2 \;= |\Lambda| \,. \tag{8.6}$$

with the last equality holding for spins of constant magnitude $\|\sigma_x\| = 1$.

The decomposition into spin waves is especially convenient in case the Hamiltonian is taken with the periodic boundary conditions. In that case the Hamiltonian decouples into a **sum of single-mode contributions**.

For spins of unit length, $\|\sigma_x\| = 1$, and pair interactions it is convenient to shift the Hamiltonian by a constant term and symmetrize the couplings (none of which affects the Gibbs states) which allows to present it as:

$$H_\Lambda^{\mathrm{per}}(\sigma) = \boxed{\frac{1}{2} \sum_{\{x,y\}\subset\Lambda} J_{x-y} \, \|\sigma_x - \sigma_y\|^2} - h \sum_{x\in\Lambda} \sigma_x \;=\; -\frac{1}{2} \sum_{x,y\in\Lambda} J_{x-y}\sigma_x\sigma_y \; - h \sum_{x\in\Lambda} \sigma_x \tag{8.7}$$

with

$$J_u = J_{-u} \,, \qquad \text{and} \quad J_0 = -\sum_{\substack{n\in\mathbb{Z}^d \\ \|n\|=1}} J_n \,. \tag{8.8}$$

Formulated as such, the spin-spin interaction energy is given by a non-negative quadratic form, which is invariant under periodic shifts, and manifestly has a family of zero energy modes (in which the spins are constant).

In any such situation plane waves are of interest, as they form an orthonormal basis of functions in the Hilbert space $\ell^2(\Lambda)$, which are eigenfunctions of the shift operator, and thus also of the linear operator of matrix elements are given by J_{x-y}. Through either the quadratic form's spectral representation, or the explicit change of coordinates described by (8.5)

$$\boxed{H_{\Lambda_R}(\sigma) = \sum_{p\in\Lambda_L^*} \mathcal{E}(p)\,|\widehat{\sigma}_p|^2 \;-\; h\;\sqrt{|\Lambda|}\,\widehat{\sigma}_0} \quad \text{with} \quad \mathcal{E}(p) := \frac{1}{2}\sum_{u\in\Lambda_L} e^{ip\cdot u} J_u \tag{8.9}$$

In the case of the nearest neighbor interaction the corresponding expressions are

$$J_u^{(n.n.)} = \delta_{\|u\|=1} - 2d\delta_{\|u\|=0} \tag{8.10}$$

and

$$\mathcal{E}(p) := \sum_{j=1}^{d}[1-\cos(p_j)] = 2\sum_{j=1}^{d}\sin^2(p_j/2) \quad \left(\approx \frac{1}{2}\|p\|^2 \text{ for } p \text{ small}\right), \tag{8.11}$$

where one can recognize the coincidence with the matrix elements of the discrete Laplacian (aka the second difference operator) $\frac{1}{2}\Delta_{x,y}$.

The change of perspective, in which the spin configuration $\{\sigma_x\}$ is presented as a configuration of plane waves of amplitude $\{\widehat{\sigma}(p)\}$ is completed by noting that the Fourier transform of the spatial spin-spin correlation function of any shift-invariant state $\rho_{\Lambda_L} = \langle - \rangle_{\Lambda_L}$ reappears as the intensity of the p-th mode:

$$\boxed{\widehat{S}_\rho^{(L)}(p) := \sum_{x\in\Lambda_L} e^{ip\cdot x}\langle\sigma_0\sigma_x\rangle_{\Lambda_L} \;=\; \langle|\widehat{\sigma}(p)|^2\rangle_{\Lambda_L}\,.} \tag{8.12}$$

8.2 Symmetry breaking as a condensation phenomenon

A heuristic explanation of the possibility of continuous symmetry breaking in dimensions $d > 2$ is provided by the combination of:

- the **equipartion law**, which while not really a theorem is presented to students of physics as a thumb rule: the energy stored in each quadratic mode is expected to be about $\frac{1}{2}kT$ ($= \frac{1}{2\beta}$)
- the sum rule provided by (8.6).

The combination of the two leads to sufficient condition for symmetry breaking in which one may find an echo of the mechanism underlying the **Bose-Einstein phase transition** (condensation, in a systems of Bose particles, into a macroscopic occupation of the ground state).

Proposition 8.1 (Condition implying symmetry breaking)**.** *For* $d > 2$*, assume that in a systems of bounded spins on* $\mathbb{Z}^d$ *with the nearest neighbor interaction* (8.7)*, the following* **gaussian domination bound** *holds*

$$\boxed{\mathcal{E}(p)\widehat{S}_{\rho,\beta}^{(L)}(p) \le \frac{1}{2\beta}}\,, \tag{8.13}$$

and let

$$C_d := \frac{1}{(2\pi)^d}\int_{[-\pi/2,\pi/2]^d} \frac{1}{\mathcal{E}(p)}\mathrm{d}p\,. \tag{8.14}$$

Then for any $\beta > C_d/2$:
1)

$$\boxed{\liminf_{L\to\infty} \left\langle \Big\| \frac{1}{|\Lambda_L|} \sum_{x\in\Lambda_L} \sigma_x \Big\|^2 \right\rangle \geq 1 - C_d/(2\beta) \quad (>0)} . \tag{8.15}$$

2) the system's pressure has discontinuous derivative (cone singularity) at $h = (0, ..., 0)$
3) in the infinite volume limit the system has Gibbs states of non-zero magnetization, in which the spin-rotation symmetry is broken.

It should be noted that the dimension condition $d > 2$ (for finite range interactions) enters here through the requirement of the local integrability of $1/|p|^2$.

Proof of Proposition 8.1: 1) The Parseval-Plancherel identity (8.6) yield the following sum rule for spins of constant magnitude $\|\sigma_x\| = 1$:

$$\frac{1}{|\Lambda|}\|\hat{\sigma}_0\|^2 + \frac{1}{|\Lambda|}\sum_{p\in\Lambda^*\setminus\{0\}} \|\hat{\sigma}_p\|^2 \;=\; 1 \quad \Big(= \frac{1}{|\Lambda|}\sum_{p\in\Lambda^*}\|\hat{\sigma}_p\|^2\Big). \tag{8.16}$$

The case $p = 0$ was separated from the rest for two reasons: i) it is of special interest to us, as it encodes the bulk mean magnetization,

$$\frac{1}{|\Lambda|}\|\hat{\sigma}_0\|^2 = \Big\|\frac{1}{|\Lambda_L|}\sum_{x\in\Lambda_L}\sigma_x\Big\|^2 , \tag{8.17}$$

and ii) the gaussian domination bound does not provide any information on it since $\mathcal{E}(0) = 0$. Taking the mean value we learn that

$$\left\langle \Big\|\frac{1}{|\Lambda_L|}\sum_{x\in\Lambda_L}\sigma_x\Big\|^2 \right\rangle = 1 - \frac{1}{|\Lambda|}\sum_{p\in\Lambda^*\setminus\{0\}} \langle \|\hat{\sigma}_p\|^2\rangle = 1 - \frac{1}{|\Lambda|}\sum_{p\in\Lambda^*\setminus\{0\}} \widehat{S}^{(L)}_\beta(p) . \tag{8.18}$$

Now using (8.13) we find

$$\left\langle \Big\|\frac{1}{|\Lambda_L|}\sum_{x\in\Lambda_L}\sigma_x\Big\|^2 \right\rangle \geq 1 - \frac{1}{2\beta}\left[\frac{1}{|\Lambda|}\sum_{p\in\Lambda^*\setminus\{0\}} \frac{1}{\mathcal{E}(p)}\right] . \tag{8.19}$$

For large L the weighted sum in the bracketed can be recognized as a Riemann sum approximation of the integral defining C_d, in (8.14), which suggests that

$$\lim_{L\to\infty}\frac{1}{|\Lambda|}\sum_{p\in\Lambda^*\setminus\{0\}}\frac{1}{\mathcal{E}(p)} = C_d . \tag{8.20}$$

Proving that requires some care since $\mathcal{E}(p)^{-1}$ is not uniformly continuous over the Brillouin zone $[-\pi,\pi]^d$. The argument can be made by splitting the sum into two parts. The sum over $\|p\| \geq \epsilon$ converges by the standard theorem. By elementary estimates, which we omit here, the contribution from $\|p\| < \epsilon$ is bounded by Const $\epsilon^{(\mathrm{d}-2)}$, which vanishes in the limit $\epsilon \to 0$. The combination of these two observations allows to deduce (8.20).

The above completes the proof of (1). The second assertion follows from (1) through the application of the Lemma which is stated below.

Claim (3) follows from (2) as a generally valid implication of the non-differentiability of the pressure (which was discussed in Section 10. More explicitly: the average magnetization of Gibbs states is related to the pressure's derivative w.r.t. the magnetic field

$$\langle \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \underline{\sigma}_x \rangle = \frac{1}{\beta} \underline{\nabla}_h \Psi . \tag{8.21}$$

When the latter has different directional derivatives at $\underline{h} = \underline{0}$, to each direction corresponds at least one translation invariant Gibbs state for which the bulk-averaged magnetization is almost -surely given by the corresponding derivative. Each of these states exhibits symmetry breaking. □

In the above proof, the implication (1) $\Longrightarrow$ (2) was based on the following general statement.

Lemma 8.2. *Assume that a system of bounded spins on $\mathbb{Z}^d$, which at $h = (0, ..., 0)$ has the spin rotational symmetry, for all L large enough:*

$$\left\langle \left| \frac{1}{|\Lambda_L|} \sum_{\Lambda_L} \sigma_x^{(1)} \right|^2 \right\rangle^{(b.c.)}_{\Lambda_L, \beta, h=0} \geq B^2 \tag{8.22}$$

for some $B > 0$ and an arbitrary choice of boundary conditions. Then at the given β the system's pressure has a conical singularity in h, satisfying

$$\Psi(\beta, \underline{h}) - \Psi(\beta, \underline{0}) \;\geq\; B\beta \, \|h\| . \tag{8.23}$$

Proof By the system's rotational symmetry it suffices to consider $\underline{h} = (1, 0, ..0$. The system's finite volume pressure function satisfies

$$e^{\left\{[\Psi(\beta,\underline{h}) - \Psi(\beta,\underline{0})]\,\|\Lambda_L\|\right\}} = \left\langle \exp\{\beta\, \underline{h} \cdot \sum_{\Lambda_L} \underline{\sigma}_x\} \right\rangle \geq e^{\left\{\beta\, \underline{h}\, B \|\Lambda\|(1-\varepsilon)\right\}}\, P_L(\varepsilon) \tag{8.24}$$

with $P_L(\varepsilon)$ the probability

$$P_L(\varepsilon) := \left\langle \mathbb{1}\Big[\sum_{\Lambda_L} \sigma_x^{(1)} \geq B - \varepsilon \Big] \right\rangle . \tag{8.25}$$

An L-independent positive low bound on $P_L(\varepsilon)$ readily follows from the assumption (8.22) through the implied Chebyshev type estimate

$$B^2 \;\leq\; \left\langle \left| \frac{1}{|\Lambda_L|} \sum_{\Lambda_L} \sigma_x^{(1)} \right|^2 \right\rangle^{(b.c.)}_{\Lambda_L, \beta, 0} \;\leq\; (B - \varepsilon)^2 + B^2 P_L(\varepsilon) \tag{8.26}$$

Taking the logarithm of (8.24), dividing by the volume, and using the known convergence of $\Psi_L(\beta, \underline{h})$ to the (boundary independent) pressure function yields the claim (8.23) □

8.3 Reflection positivity - definition and examples

The criterion provided by Proposition (8.1) for symmetry breaking (SB) is based on somewhat sophisticated but still rather elementary considerations. However, verifying the assumption (8.13) is quite a challenge. At present, this has been accomplished only for systems endowed with **reflection positivity**. Our goal in this section is to introduce the concept and derive the chessboard inequality which it enables.

The concept of reflection symmetry is applicable to systems formulated over either $\mathbb{R}^d$ or a graph which is symmetric with respect to a reflection about a hyperplane, or a family of hyperplanes. Examples include the infinite graph $\mathbb{Z}^d$, and the finite graphs $\Lambda = [-L/2, L/2] \cap \mathbb{Z}^d$ taken with periodic boundary conditions. The reflection symmetry may be discussed with respect to reflections dissecting the graph through mid-points of edges, or through vertices.

The symmetry plane divides Λ, minus the plane itself, into two parts which we label as $\Lambda_\pm$. It will be convenient to include in each also the vertices which lie on the symmetry plane itself, in case there are such.

Let $\mathcal{R} : \Lambda \to \Lambda$ be the reflection with respect to such a plane. Quite naturally, any such mapping is an involution ($\mathcal{R}^2 = \mathbb{1}$) and it lifts to a mapping on observables $F : \Omega \to \mathbb{C}$ via

$$(\mathcal{R}F)(\sigma) := F(\mathcal{R}\sigma).$$

where $(\mathcal{R}\sigma)_x = \sigma_{\mathcal{R}(x)}$.

Definition 8.3. A state $\langle\cdot\rangle$ is said to be **reflection positive** (RP) about a reflection $\mathcal{R}$ iff for any pair of observables $F, G : \Omega \to \mathbb{C}$,

$$\langle \bar{F}\mathcal{R}F\rangle \geq 0\,; \qquad \langle \bar{F}\mathcal{R}G\rangle = \langle G\mathcal{R}\bar{F}\rangle\,. \tag{8.27}$$

An example of immediate relevance for our discussion is the $O(N)$ model with the nearest neighbor interactions. In Λ_L with the periodic boundary conditions the model is reflection positive with respect to reflection about any of the graph's symmetry hyperplanes, i.e. symmetry planes cutting through either sites and edges. This can be deduced from the following RP criterion of [2].

Proposition 8.4. *A sufficient condition for the Gibbs states of a spin model in Λ_L to be reflection positive with respect to a symmetry reflection $\mathcal{R}$ is that its Hamiltonian can be written as*

$$-H = A + \mathcal{R}A + \sum_{j=1}^{k} B_j \mathcal{R}B_j \tag{8.28}$$

with A and $\left\{ B_j \right\}_j$ depend only on spins in Λ_+.

Proof To start one may note that by the independence of the spins with respect to the a-priori measure, for any $\left\{ A_j \right\}_{j=1}^{m}$ which depend only on spins in Λ_+

$$\Big\langle \prod_{j=1}^{m} A_j \mathcal{R}A_j \Big\rangle_0 \geq 0 \tag{8.29}$$

where $\langle - \rangle_0$ is the $\beta = 0$ Gibbs state, or equivalently the a-priori average.

Next, under the assumption (8.28) the model's Gibbs factor is of the form

$$\exp(-\beta H) = \exp(\beta A)\,(\mathcal{R}\exp(\beta A)) \prod_{j=1}^{k} \exp(\beta B_j \mathcal{R}B_j)\,. \tag{8.30}$$

Expanding the exponentials we obtain

$$\exp\left(\beta B_j \mathcal{R} B_j\right) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \left(B_j \mathcal{R} B_j\right)^n . \tag{8.31}$$

This allows to readily verify the conditions (8.27) by which reflection positivity is defined. □

Other criteria for reflection positivity and examples of long range reflection positive interactions are presented in [2, 12]. For dimensions $1 \leq d \leq 4$ this class includes two body spin-spin interactions with power law decay, among with

$$J_{x,y} = 1/\|x-y\|^{\tau} \tag{8.32}$$

(for $x \neq y$) at $\tau \geq |d-2|_+$.

8.4 The chessboard inequality

Reflection positivity leads to inequalities. The first of these is the **Cauhcy-Schwarz inequality**.

Denoting by $\mathcal{B}$ the linear space of observables $F : \Omega \to \mathbb{C}$, the map

$$\mathcal{B}^2 \ni (F, G) \mapsto \langle \overline{F} \mathcal{R} G \rangle =: [F, G] \in \mathbb{C} \tag{8.33}$$

furnishes it with a (non-negative) inner-product $[\cdot, \cdot]$. The Cauchy-Schwarz inequality states that under such conditions, for all square integrable $F, G \in \mathcal{B}$, $|\,[F, G]\,|^2 \leq [F, F]\,[G, G]$. In the present context that translates to

$$|\langle \overline{F} G \rangle|^2 \leq \langle \overline{F} \mathcal{R} F \rangle \langle \overline{G} \mathcal{R} G \rangle . \tag{8.34}$$

As a step towards a picturesque extension of this inequality, let us first restrict it to a statement about the expectation value of a product of functions which depend on the restrictions of the spin configuration into different components of Λ. More explicitly, for a given reflection $\mathcal{R}$, Λ can be presented as the union (not necessarily disjoint) $\Lambda = \Lambda_+ \cup \Lambda_-$. Let $\mathcal{B}_\alpha$, for $\alpha \in \{-, +\}$ be the collection of functions which depends only on spins in Λ_α (i.e. functions measurable w.r.t. to the sigma-algebra generated by the spins in that set, in the terminology of Chapter 10.) In this notation, (8.34) implies that for any pair of square integrable functions $F_\alpha \in \mathcal{B}_\alpha$:

$$|\langle F_+ F_- \rangle|^2 \leq \langle \overline{F_+} \mathcal{R} F_+ \rangle \, \langle \overline{F_-} \mathcal{R} F_- \rangle \tag{8.35}$$

In words, using suggestive notation, the expectation value of a product of the form $F_+(\sigma_+)F_-(\sigma_-)$ is bounded by the geometric mean of expectations of functions obtained by extending through reflections one of the two functions $F_\pm$ throughout both domains, and complex conjugating upon each reflection. In this notation, a somewhat more explicit version of (8.35) is:

$$\Big| \int F_+(\sigma_+)\, F_-(\sigma_-)\, \rho(d\sigma) \Big|^2 \leq \int \overline{F}_+(\sigma_+)\, F_+(\sigma_-)\, \rho(d\sigma) \int \overline{F}_-(\sigma_+)\, F_-(\sigma_-)\, \rho(d\sigma) . \tag{8.36}$$

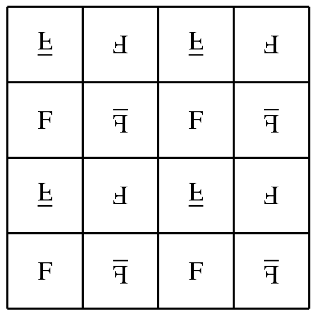
Next, let us consider a spin system in Λ_L whose state is invariant under periodic shifts, and is reflection positive with respect to a family of reflections with respect to hyper-planes, each perpendicular to a principal direction. The planes decompose Λ into the union of $K \in \mathbb{N}$ boxes, $\Lambda =$

$\bigcup_{\alpha=1}^{K} \Lambda_\alpha$ (allowing overlaps along the boundaries), to which we shall refer in a natural extension of the above notation.

Theorem 8.5 (The chessboard inequality [2])**.** *In the setup described above, assume that the system's state $\langle\cdot\rangle$ is reflection positive with respect to each of the above family of reflections. Then for any collection of functions $\{ F_\alpha \}_\alpha \subseteq \mathcal{B}$ of which each F_α is measurable with respect to $\mathcal{B}_\alpha$*

$$\boxed{\left|\langle \prod_\alpha F_\alpha(\sigma_\alpha\rangle\right| \leq \prod_\alpha \left(\langle \prod_\gamma F^\sharp_\alpha(\sigma_\gamma)\rangle\right)^{1/K}} \tag{8.37}$$

where K is the number of boxes, and $\sharp$ indicates that the reflection and complex conjugation are to be applied by repeating the period 2 pattern in each direction, as depicted in the accompanying figure.



Proof Since (8.36) is homogenous of degree 1 in each F_α, it suffices to consider the case that all these functions are normalized by the condition

$$\langle \prod_\gamma F^\sharp_\alpha(\sigma_\gamma\rangle = 1\,. \tag{8.38}$$

This reduces the task to proving the following statement:
Let $\mathcal{S} = \{F_j\}_{j=1,...,K} \subset \mathcal{B}_{\alpha_0}$ be a collection of functions measurable in a common box Λ_0, each normalized by (8.38), and let $\kappa : \{1, ..., K\} \to \{1, ..., K\}$ represent assignments of functions from $\mathcal{S}$ to the cells. Then the following maximum

$$\max_{\kappa:\{1,...,K\}\to\{1,...,K\}} \left|\langle \prod_\alpha F^\sharp_{\kappa(\alpha)}(\sigma_\alpha))\rangle\right| \tag{8.39}$$

(which need not be unique) is attained by a configuration for which $\kappa(\alpha)$ is constant.

By the Cauchy-Schwarz inequality if κ is maximizer then so is each of the two configurations which are obtained by symmetrizing κ with respect to an arbitrarily chosen reflection plane. Such reflections can be used to decrease the amount of disagreement in the nearest neighbor assignments while staying within the collection of optimizing assignments. The only maximizing configurations whose nearest neighbor disagreement cannot be further reduced corresponds to κ such that $\kappa(\alpha) = \kappa(\alpha')$ for each pair of neighboring boxes. This condition implies that among the maximizer there is one for which $\kappa(\alpha)$ takes a common value for all α, and the claim follows. (Ipso facto this also implies that under the chosen normalization, each constant κ is an optimizer.) □

8.5 The Gaussian domination bound

Armed with the chessboard inequality of [**?**], we proceed toward the proof of the Gaussian domination bound (8.13) of [1]. To refresh the memory, we consider here the $O(N)$ spin model with the interaction (8.7) and proceed under the assumption that the corresponding Gibbs state is reflection positive (which is the case for the nearest neighbor model presented in Sec. 8.2. A key step is to consider the shifted partition function, defined for $\eta : \Lambda \to \mathbb{R}^N$ as:

$$Z(\eta) := \int \exp\Big\{ -\frac{1}{2}\beta \sum_{\mathrm{x,y}} \mathrm{J_{x,y}} \, \|(\sigma_{\mathrm{x}} + \eta_{\mathrm{x}}) - (\sigma_{\mathrm{y}} + \eta_{\mathrm{y}})\|^2 \Big\} \prod_{\mathrm{u}\in\Lambda} \rho_0(\mathrm{d}\sigma_{\mathrm{u}}) \tag{8.40}$$

where $\rho_0(d\sigma)$ is the a-priori measure, which for the $O(N)$ models is the Haar measures on the $N-1$ sphere.

Lemma 8.6. *If at the given β the Gibbs state under the Hamiltonian* (8.7) *is reflection positive, then for all $\eta : \Lambda \to \mathbb{R}^N$:*

$$\boxed{Z(\eta) \leq Z(0)} \,. \tag{8.41}$$

Proof For the argument which follows it is convenient to present the a-priori measure $\rho_0(d\sigma)$ (which is supported on just the N-sphere , as the weak limit of probability measures whose support is all of $\mathbb{R}^N$,

$$\rho_0(d\sigma) \stackrel{w}{=} \lim_{\delta \searrow 0} \rho_\delta(d\sigma) \tag{8.42}$$

with $\rho_\delta(d\sigma)$ probability measures of full support over R^N, of strictly positive and bounded density $g_\delta(\sigma)$ (for an explicit example one may take $g_\delta(\sigma) = C_\delta e^{-(\|\sigma\|^2-1)/\delta^2}$ with C_δ a normalizing constant.) By continuity, it suffices to prove that for any delta the correspondingly modified partition functions satisfy

$$Z_\delta(\eta) \leq Z_\delta(0) \,. \tag{8.43}$$

For $\delta > 0$ the shift $\sigma_x \mapsto \sigma_x + \eta_x$ can be transformed into a change in the variable of integration, and the shifted partition function presented as

$$Z_\delta(h) = \int_\sigma \exp(-H(\sigma)) \prod_x \Big[T_{\eta_x}(\sigma_x) \rho_\delta(d\sigma_x) \Big] = Z_\delta(0) \, \Big\langle \prod_x T_{\eta_x}(\sigma_x) \Big\rangle \,. \tag{8.44}$$

with $T_{\eta_x}(\sigma_x) = g_\delta(\sigma_x - \eta_x)/g_\delta(\sigma_x)$.

From the expression (8.40) it should be clear that shifts by an x-independent constant have no effect on $Z_\delta(0)$, i.e. for any $y \in \Lambda$: $\Big\langle \prod_x T_{\eta_y}(\sigma_x) \Big\rangle = 1$ The chessboard inequality (8.37) (applied with the decomposition $\Lambda = \bigcup_{x\in\Lambda} \{ \, x \, \}$) allows to conclude from that for general shifts (8.43) holds. □

We are now ready for the punchline.

Theorem 8.7. *In any dimension the* $O(N)$ *spin models over* $\mathbb{Z}^d$*, with interactions of the form* (8.7) *which are reflection positive satisfy the corresponding* **gaussian domination bound** (8.13).

Proof From Lemma 8.6 (and the second form of the interaction in (8.7)) we learn that for any $\eta : \Lambda \to \mathbb{R}^N$ and any $\varepsilon > 0$

$$1 \geq \frac{Z(\varepsilon\eta)}{Z(0)} = \left\langle \exp\left(\varepsilon\beta \sum_{\mathrm{x,y}} \sigma_{\mathrm{x}} \mathrm{J}_{\mathrm{x,y}} \eta_{\mathrm{y}}\right)\right\rangle \exp\left(\varepsilon^2 \frac{1}{2}\beta \sum_{\mathrm{x,y}} \eta_{\mathrm{x}} \mathrm{J}_{\mathrm{x,y}} \eta_{\mathrm{y}}\right) \tag{8.45}$$

that is:

$$\left\langle \exp\left(\varepsilon\beta \sum_{\mathrm{x,y}} \sigma_{\mathrm{x}} \mathrm{J}_{\mathrm{x,y}} \eta_{\mathrm{y}}\right)\right\rangle \leq \exp\left(\varepsilon^2 \frac{1}{2}\beta \sum_{\mathrm{x,y}} \eta_{\mathrm{x}} \mathrm{J}_{\mathrm{x,y}} \eta_{\mathrm{y}}\right) \tag{8.46}$$

Expanding in ε the first two terms on both sides are $1 + 0\,\varepsilon$. Comparing the terms of order ε^2 one learns that for any real valued function η

$$\beta^2 \left\langle \left| \sum_{x,y} \sigma_x J_{x,y} \eta_y \right|^2 \right\rangle \leq \frac{\beta}{2} \left(\sum_{x,y} \eta_x J_{x,y} \eta_y \right). \tag{8.47}$$

Expanding in the basis of the p-waves

$$\sum_{x,y} \sigma_x J_{x,y} \eta_y = \sum_{p \in \Lambda^*} \overline{\widehat{\sigma}_p}\, \mathcal{E}(p)\, \widehat{\eta}_p \tag{8.48}$$

In evaluation this sum's second moment note that by the state's translation invariance

$$\langle \overline{\widehat{\sigma}_{p_1}} \widehat{\sigma}_{p_2} \rangle = \delta_{p_1,p_2} \widehat{S}^{(L)}_{\rho,\beta}(p)\,. \tag{8.49}$$

Thus one gets:

$$\sum_{p \in \Lambda_L^*} \mathcal{E}(p)^2 \; S^{(L)}_{\rho,\beta}(p)\; |\widehat{\eta}_p|^2 \leq \frac{1}{2\beta} \sum_{p \in \Lambda_L^*} \mathcal{E}(p)\, |\widehat{\eta}_p|^2 \tag{8.50}$$

Since this holds for any η, it readily follows that

$$\boxed{S^{(L)}_{\rho,\beta}(p) \;\leq\; \frac{1}{2\beta\, \mathcal{E}(p)}}$$

as claimed in (8.13). □

The implications of the above bound were presented in Proposition 8.1.

Notes (extensions, and other implications)

The methods and results presented in this Chapter have had quite a number of extension and applications in rigorous studies of critical phenomena. Pointers to some of those:

• *Quantum spin systems:* While the correspondence is not perfect, and new challenges appear there, many of the ideas presented above apply also to related quantum spin models. Fundamental results in this direction were presented in [2, 3].

• *Other applications of the chessboard inequality:* This inequality also provides a tool for bounding probabilities of local events, e.g. probability of observing Peierls type contours, in terms of thermodynamic quantities. It was applied in this manner in [4] for the proof of symmetry breaking **at the critical point** of Q state Potts models, at large enough Q. An interesting twist there is that the relevant contour estimates are based not on energy but on entropy bounds.

• *Reflection positivity for infinite systems:* Reflection positivity as a tool for rigorous studies goes back to studies of statistical field theory over the Euclidean space $\mathbb{R}^d$ [5]. Among its application is the spectral representation of the two point function, in which the rate of exponential decay is identified as a spectral gap [6]. (This relation which will be presented in one of the next chapters.)

• *Messager-Miracle Sole monotonicity [7]:* Reflection positive also leads to the point-wise monotonicity in x_j (in the expected direction) of the n.n. model's two point function $\langle \sigma_0 \sigma_x \rangle$.

• *Quadratic form versus pointwise bounds:* For the ferromagnetic n.n. interaction (8.10) the Gaussian domination inequality provides the quadratic form bound:

$$\left\langle \Big| \sum_{x \in \Lambda} g(x) \sigma_x \Big|^2 \right\rangle \leq \frac{1}{2\beta} \sum_{x,y \in \Lambda} \overline{g}(x)(-\Delta)^{-1}(x,y) g(y) \tag{8.51}$$

In dimensions $d > 2$, this can be extended, through the MMS monotonicity, into a pointwise bound in terms of the inverse Laplacian's kernel (aka the Green function) [8]

$$\left\langle \sigma_x, \sigma_y \right\rangle_{\beta_c} \leq \widetilde{C}_d \, (-\Delta)^{-1}(x,y) \approx \frac{\widetilde{C}_d}{\|x-y\|^{d-2}} \, . \tag{8.52}$$

• *The existence of an upper critical dimension:* Through correlation inequalities and other methods [8, 6, 9] it was shown that in any dimension in which the Ising model's correlation function is square summable at T_c the following critical exponents assume values which coincide with those of the model's (solvable) mean field version:

$$\boxed{\alpha = 0, \quad \widehat{\beta} = 1/2, \quad \gamma = 1, \quad \delta = 3} \, . \tag{8.53}$$

The Gaussian domination bound, extended to the model's critical point, yields

$$B := \sum_{x \in \mathbb{Z}^d} |\langle \sigma_0 ; \sigma_x \rangle|^2 \leq \frac{1}{2\beta} \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathcal{E}(p)^2 dp \tag{8.54}$$

and thus implies that the above condition ($B < \infty$) is met in dimensions $d > 4$. The values (8.53) extend also to the marginal dimension $d = 4$; in that case the sum in (8.54) may diverge, but still only at a logarithmic rate.

In the above statements the critical exponents are taken to be defined through the limits of the log ratios, as in:

$$\beta = \lim_{T \nearrow T_c} \frac{\log M(T,0)}{\log(T_c - T)}\,, \quad \gamma = \lim_{h \nearrow 0} \frac{\log M(T_c,h)}{\log(T_c - T)} \tag{8.55}$$

$M(T,h)$ being the model's mean magnetization (induced in case $h > 0$, or spontaneous at $h = 0$).

• *Long range interactions:* Among the reflection positive spin-spin coupling are also interactions with the power law decay ($J_x \approx 1/\|x\|^r$). Fisher-Ma-Nickel [11] pointed out that, in the renormalization group analysis, under sufficiently slow decay the model's effective dimension rises, and in particular the mean-field type behavior can be realized in lower dimensions. Rigorous proofs of related phenomena were presented in [2, 12].

Exercises

8.1 Explain how the chessboard inequality can be used to derive a Peierls-like bound similar to (7.12) on the probability that a given simple loop is realized as a contour in the Gibbs equilibrium state of the two dimensional Ising model with periodic boundary conditions.

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9

The Transfer Matrix method

The task of calculating the free energy of any one dimensional system with finite range interactions, of range R, can be reduced to that of finding the largest eigenvalue of an $(R+1) \times (R+1)$ matrix – the model's "transfer matrix" T. As is the case with many other techniques, this method can be simply demonstrated on the corresponding Ising model.

This technique goes back to Ernst Ising's early study of the model which was presented to him by his thesis advisor Wilhelm Lenz. The principal question was whether the one dimensional string of binary variables with short range coupling may offer a mathematical example of a system undergoing a phase transition. His solution of the $1D$ case (of 1925) yields:

- "Good news": the model is **solvable**, in the sense that its pressure in the infinite volume limit, and other properties, can be obtained in closed form.
- "Disappointment": the resulting pressure is analytic in β and h and hence the one dimensional system does not exhibit phase transitions at positive temperatures (and by related analysis neither does any other one dimensional model with finite range interactions).

The interest in what is now known as the Ising model was restored by Sir Rudolf Peierls (in 1935) who showed that in higher dimensions it actually does exhibit a phase transition. While Peierls' argument (cf. Chapter 7) makes no use of this methods, the transfer matrix formulation resurfaces in the Schultz-Mattis-Lieb (1964) presentation of Onsager's (1944) exact solution of the model's two dimensional version (with the nearest neighbor interaction). Success, as far as exactly calculable results go, seems to stop in $2D$. However, the transfer matrix approach continues to play a role also in higher dimension, as will be seen in the chapter which follows this one.

9.1 Solution of the $1D$ Ising model

The key observation from which this approach has started, is that the partition function of the $1D$ Ising model, with the nearest neighbor interaction

$$H(\sigma) = -J \sum_n \sigma_n \sigma_{n+1} - h \sum_n \sigma_n \,, \quad \sigma_n \in \{\pm 1\} \,, \tag{9.1}$$

and the periodic boundary conditions, $\sigma_0 \equiv \sigma_L$ in $[0, L]$, can be presented as the trace of a 2×2 matrix $T = \begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix}$:

$$
\begin{aligned}
Z^{\text{per}}_{[0,L]}(\beta, h) &= \sum_{\sigma_1,\ldots\sigma_L=\pm} \exp\left(\beta \sum_{n=1}^{L} \left[J\sigma_n\sigma_{n+1} + h\frac{\sigma_n + \sigma_{n+1}}{2} \right]\right) \\
&= \sum_{\sigma_1,\ldots\sigma_L=\pm} T_{\sigma_1,\sigma_2}\, T_{\sigma_2,\sigma_3} \cdots T_{\sigma_{L-1},\sigma_L}\, T_{\sigma_L,\sigma_1} \\
&= \sum_{\sigma_1=\pm} T^L_{\sigma_1,\sigma_1} \equiv \operatorname{tr}(T^L)
\end{aligned}
\tag{9.2}
$$

with

$$
\begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix} = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix} . \tag{9.3}
$$

A was made here self adjoint by splitting each site's external field term equally between the two edges which reach that site. This feature is is not essential for the computation of the free energy, but it simplifies the subsequent discussion of the correlation functions. Upon diagonalization, the self adjoint matrix can be presented as

$$
T \;=\; U^{-1} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U \tag{9.4}
$$

with U a unitary matrix, and $\{\lambda_1, \lambda_2\}$ the eigenvalues of T, ordered so that $|\lambda_1| \geq |\lambda_2|$.

In these terms,

$$
Z^{\text{per}}_{[0,L]}(\beta, h) = \operatorname{tr}(T^L) \;=\; \lambda_1^L + \lambda_2^L \;=\; \lambda_1^L \left[1 + \left(\frac{|\lambda_2|}{|\lambda_1|} \right)^L \right] , \tag{9.5}
$$

from which it readily follows that

$$
\psi(\beta, h) \;=\; \lim_{L\to\infty} \frac{1}{L} \ln Z^{\text{per}}_{[0,L]}(\beta, h) \;=\; \boxed{\ln \lambda_1(\beta, h)} . \tag{9.6}
$$

Being the roots of the characteristic polynomial, the eigenvalues satisfy

$$
0 = \det(T - \lambda \mathbb{1}) \;=\; \lambda^2 - 2\,\lambda\, e^{\beta J} \cosh(\beta h) + (e^{2\beta J} - e^{-2\beta J}) . \tag{9.7}
$$

The two solutions of this quadratic equation are

$$
\lambda_{1,2} = e^{\beta J} \cosh(\beta h) \pm e^{\beta J} \sqrt{\sinh^2(\beta h) + e^{-4\beta J}} . \tag{9.8}
$$

From which one gets the exact value of the model's pressure

$$
\boxed{\psi(\beta, h) = \beta J + \ln\left[\cosh(\beta h) + (\sinh^2(\beta h) + e^{-4\beta J})^{\frac{1}{2}}\right]} . \tag{9.9}
$$

A significant implication of this explicit solution is:

Theorem 9.1. *The infinite-volume pressure of the one-dimensional Ising model is real analytics in (β, h), at all finite (β, h) with no discontinuity in the magnetization*

$$m(\beta, h) = \frac{1}{\beta}\frac{\partial\psi}{\partial h}(\beta, h) = \frac{\sinh\beta h}{[\sinh^2(\beta h) + e^{-4\beta J}]^{\frac{1}{2}}} \tag{9.10}$$

The above calculation can be extended to any finite range interaction. In case of binary spin systems with interactions of range R the dimension of the space on which the transfer matrix acts will change to 2^R. The matrix may not be self adjoint, but the pressure will still be expressible in terms of just the highest eigenvalue, as in (9.6).

9.2 Spectral gap and the decay of correlations

The transfer matrix allows also to compute the corresponding equilibrium expectation values of local quantities. Of particular interest is fact that in one dimension at any $\beta < \infty$ the spins decorrelate exponentially, in the distance between the sites. As we shall see the rate of this decay is given by the "spectral gap"

$$\alpha = \ln|\lambda_1| - \ln|\lambda_2| = \ln|\lambda_1/\lambda_2| \; > \; 0\,. \tag{9.11}$$

The strict positivity can be read off the exact solution (9.8), or more generally explained by the Perron–Frobenius theorem which is presented below.

For an exact expression for the spin-spin correlation let us S denote the spin operator

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{9.12}$$

In terms of the spectral representation of T (which in this case is self adjoint):

$$T^n = \lambda_1^n \; |\Phi_1\rangle\langle\Phi_1| \; + \; \lambda_2^n \; |\Phi_2\rangle\langle\Phi_2| \tag{9.13}$$

where where $|\Phi_j\rangle\langle\Phi_j|$ (in Dirac's notation) is the projection on T's corresponding eigenspace, and the two eigenvalues of T are $\lambda_1 > 0$ and $\lambda_2 = \lambda_1 e^{-\alpha}$ at $\alpha > 0$.

Applying the cyclicity of the trace, and noting that $\langle\Phi_n| S \,|\Phi_m\rangle\langle\Phi_m| S \,|\Phi_n\rangle = |\langle\Phi_n| S \,|\Phi_m\rangle|^2$, we get

Previous typos fixed

$$\langle\,\sigma_x\rangle_{[0,L]}^{(per)} = \frac{\operatorname{tr} T^x\, S\; T^{L-x}}{\operatorname{tr} T^L} = \frac{\operatorname{tr} S\; T^L}{\operatorname{tr} T^L} = \langle\Phi_1| S\,|\Phi_1\rangle + \langle\Phi_2| S\,|\Phi_2\rangle\, e^{-\alpha L} \tag{9.14}$$

$$\langle\,\sigma_0\,\sigma_x\rangle_{[0,L]}^{(per)} = \frac{\operatorname{tr} S\, T^x\, S\; T^{L-x}}{\operatorname{tr} T^L} = \tag{9.15}$$

$$= \frac{1}{(1 + e^{-\alpha L})}\left\{|\langle\Phi_1| S\,|\Phi_1\rangle|^2 + |\langle\Phi_1| S\,|\Phi_2\rangle|^2 \cdot \left[e^{-\alpha|x|} + e^{-\alpha(L-|x|)}\right] + |\langle\Phi_2| S\,|\Phi_2\rangle|^2\, e^{-\alpha L}\right\}.$$

For the truncated correlation function in the infinite volume limit ($L \to \infty$) this reduces to:

$$\langle \sigma_{x_1}; \sigma_{x_2} \rangle_\beta := \langle \sigma_{x_1} \sigma_{x_2} \rangle_\beta - \langle \sigma_{x_1} \rangle_\beta \langle \sigma_{x_1} \rangle_\beta = |\langle \Phi_1 | S \, |\Phi_2 \rangle|^2 \, e^{-\alpha(\beta)|x|} \tag{9.16}$$

Here both the spectral gap α and the eigenvectors $|\Phi_j\rangle$ depend on β, but $\alpha(\beta) > 0$ for all $0 \leq \beta < \infty$.

9.3 The Perron–Frobenius theorem

As the above discussion shows, it is useful to know that the leading eigenvalue of the transfer matrix T is non-degenerate. A sufficient condition for that is provided by the following general result.

Theorem 9.2 (Perron-Frobenius). *Let $T = (T_{ij})$ be a $W \times w$ matrix with non-negative entries, for which at some $k \geq 0$: $(T^k)_{ij} > 0$ for all i, j . Then:*

1. *The matrix T has a positive eigenvalue $r > 0$ (the Perron-Frobenius eigenvalue) which dominates the rest of the spectrum in the sense that all other eigenvalues of T are of magnitude dominated by $r\, e^{-\alpha}$ for some $\alpha > 0$.*
2. *The maximal eigenvalue is simple, and the corresponding eigenvector is strictly positive.*
3. *Under iterations:*
$$\lim_{L \to \infty} \frac{1}{r^L} T^L = |v\rangle\langle w| \tag{9.17}$$
with $|v\rangle$, and $\langle w|$, the right and left eigenvectors of T, correspondingly, at the eigenvalue r.[1]

We omit here the proof, which can be found in text on probability and/or linear algebra. However let us expand a bit on the implication of this general statement.

• *Exponential decay:*

The Perron–Frobenius theorem has an exception clause: it does not apply to models for which $\mathbb{Z}$ can be spilt into subgraphs with the interactions not crossing that division. An example of that would be systems whose interactions are limited to sites of the same parity. However, on a second thought, even for such situations the Perron–Frobenius theorem, applied within the corresponding sub-lattices, allows to conclude exponential decay of correlations for any finite range model with translation invariant interactions.

• *Analyticity of the pressure:*

For finite range systems the matrix elements of T are manifestly analytic in β, and in the other parameters of the Hamiltonian I am Can one conclude that also the leading eigenvalue of the transfer matrix, which yields the pressure function, is analytic in the model's parameters?

By general theory, which we shall skip here, the answer is yes - as long as the spectral gap stays positive. In other words, only a level crossing could yield non-analyticity of the pressure. The possibility of that at some real β is precluded by the Perron-Frobenius theorem. Hence, Ising's observation that the one dimensional n.n. Ising model has no phase transition at $T > 0$ extends to

[1] The right and left eigenvectors satisfy: $T|v\rangle = r|v\rangle$, $\langle w|T = r\langle w|$. In case T is Hermitian $\langle w| = |v\rangle^\dagger$.

more general analyticity statement of one dimensional systems of finite range interactions. (This however does not preclude singularities of the pressure at complex β, which may for instance occur at a zero of the partition functions.)

9.4 Other boundary conditions

For computing the system's pressure it suffices to calculate it for the periodic boundary conditions, which as we saw are rather convenient for this task. However one wants to understand also the structure of the partition function under other boundary conditions, for instance at specified values of σ_0 and σ_L. The corresponding transfer matrix expression is:

$$Z_L^{\sigma_0,\sigma_L} \;=\; \sum_{\sigma_1,\ldots,\sigma_{L-1}=\pm} T_{\sigma_0\sigma_1} T_{\sigma_1\sigma_2} \cdots T_{\sigma_{L-1}\sigma_L} = (T^L)_{\sigma_0\sigma_L} \;=\; \langle\sigma_0|\, T^L \,|\sigma_L\rangle \tag{9.18}$$

where $|\sigma\rangle$ is the vector given by

$$|+\rangle \;=\; \begin{pmatrix}1\\0\end{pmatrix}, \quad \text{and} \quad |-\rangle \;=\; \begin{pmatrix}0\\1\end{pmatrix}, \tag{9.19}$$

and $\langle\sigma|$ is the corresponding transpose, or dual, vector (in Dirac's notation).

Writing the self adjoint matrix T in terms of its spectral representation, that is expanding in terms of the projections onto the eign-space of T:

$$P_j = |\Phi_j\rangle\langle\Phi_j| \tag{9.20}$$

with $|\phi_j\rangle$ the corresponding eigenvector, one has

$$T \;=\; \lambda_1 P_1 + \lambda_2 P_2 \quad \text{and} \qquad T^L \;=\;=\; \lambda_1^L P_1 + \lambda_2^L P_2\,. \tag{9.21}$$

Substituting that in (9.18) one gets

$$Z_L^{\sigma_0,\sigma_L} \;=\; \lambda_1^L \left(\langle\sigma_0|\, P_1 \,|\sigma_L\rangle \;+\; e^{-\alpha L} \langle\sigma_0|\, P_2 \,|\sigma_L\rangle \right) \tag{9.22}$$

Consistently with the Perron-Froebenius theorem, the leading eigenvector $|\Phi_j\rangle$ can be adjusted to be strictly positive in the basis of the two vectors $|\pm\rangle$ in which T was defined. Denoting

$$\kappa(+) := \langle + |\Phi_1\rangle\,,\;\; \kappa(-) := \langle - |\Phi_1\rangle > \;0 \tag{9.23}$$

one learns that

$$Z^{\sigma_0,\sigma_L} = \kappa(\sigma_0)\kappa(\sigma_L)\lambda_1^L \left[1 + O(e^{-\alpha L})\right], \tag{9.24}$$

Thus the boundary conditions produce a local multiplicative effect on the free energy, with correlations between the two ends decaying exponentially fast in the system's size.

Notes

To summarize, let us note three main observations based on the above considerations.

i) One dimensional systems of compact spins with finite range translation invariant and bounded interactions do not exhibit phase transition. The pressure function of any such systems is real-analytic in temperature and coupling constants.
ii) The computation of the pressure of such one dimensional system requires just the transfer matrice's highest eigenvalue.
iii) The correlations, expressed in the covariance of local functions, decay at an exponential rate, given by a "spectral gap". So do the effects of the boundary conditions.

Valuable applications of the transfer matrix perspective beyond $1D$ would be presented in Chapters which follow.

The transfer matrix' appearance hints on links between classical statistical mechanics and quantum structures. And more is true. As we shall see (time permitting) the transfer matrix of the two dimensional n.n. Ising spin model can be cast as the Hamiltonian of a systems of free fermions (!). Its integrability is related to the solvability of planar Ising models.

The application to transfer matrices does not exhaust the relevance of the Perron-Frobenius theorem for physics. Other examples will be listed on these pages later.

Exercises

9.1 i. For the Ising model with the nearest neighbor interactions and periodic boundary conditions on $[0, L]$ express in terms of the transfer matrix the finite volume expectation value of a product of n spins at specified sites,

$$\langle \prod_{j=1}^{n} \sigma_{x_j} \rangle_{[0,L]}^{(per)} = ...$$

ii. Write down the corresponding expression for the + boundary conditions.

9.2 Using what is known about the spectrum of the one dimensional transfer matrix T prove that in the one dimensional Ising model the spin-spin correlations decay exponentially in the distance, that is satisfy

$$\left| \langle \sigma_x \sigma_y \rangle_{[0,L]}^{(per)} - \langle \sigma_x \rangle_{[0,L]}^{(per)} \langle \sigma_y \rangle_{[0,L]}^{(per)} \right| \leq \mathrm{C}\ \mathrm{e}^{-\alpha\, \mathrm{dist_L}\{\mathrm{x,y}\}} \left[1 + \mathrm{O}(\mathrm{e}^{-\alpha \mathrm{L}}) \right] \tag{9.25}$$

equation modified a bit

at some $\alpha > 0$, with the distance at periodic boundary conditions

$$\mathrm{dist_L}\{\mathrm{x, y}\} = \min\{|\mathrm{x} - \mathrm{y}|, \mathrm{L} - |\mathrm{x} - \mathrm{y}|\}\,.$$

Identity α in terms of the spectrum of T.

9.3 Consider a one dimensional system of Ising spins with nearest and next-nearest neighbor interaction, of the form

$$H(\sigma) = -\sum_{\{x,y\}} J_{x-y}\sigma_x\sigma_y - h\sum_x \sigma_x\,, \tag{9.26}$$

with $J_u \neq 0$ only for $|u| \leq 2$.

Hint modified

i. Express the system's pressure in terms of a finite dimensional transfer matrix.

   Hint: you may find it useful to present the system in terms of two component variables, e.g. writing $\tau_x = (\sigma_x, \sigma_{x+1})$. In this case the variables τ take 4 values, and correspondingly the transfer matrix can be formulated as a 4×4 matrix advancing from τ_n to τ_{n+1}, or alternatively directly to τ_{n+2}.

ii. Prove, possibly relying on the above quoted Perron-Froebenius theorem, that also in this system the truncated spin - spin correlations decay exponentially fast.

10

Gibbs States in the Infinite Volume Limit

The infinite volume limit provides a natural framework for the description of of phase transitions in statistical mechanics. After all, the finite-volume pressure functions and Gibbs measures are analytic in the control parameters such as $\{\beta, J, h\}$. It is in the infinite volume limit that discontinuities, and other forms of non-analyticity, show up.

To be clear: singularities can also be detected in finite systems, but their manifestation requires a fine tuned discussion of the rates of change, and effects of boundary conditions. The infinite volume limit captures the asymptotic behavior deep within the system, keeping track of the residual effects of the boundary conditions but omitting the boundary itself. Thus, somewhat paradoxically, the infinite volume description is a simplification which captures less than in the fully comprehensive analysis of finite system. It is an example of the generally valid observation that limits involve selection and loss of information.

10.1 Configuration spaces in the infinite volume limit

Following is an informal introduction of the notation which will be employed in describing a systems of local variables, often denoted σ_x and called "spins", indexed by the vertex set of a lattice, or more generally a transitive graph $\mathbb{G}$.

We denote by S the local variable's configuration space. By default it will be assumed that it is a compact metric space. Basics examples include:

i) $S = \{+1, -1\}$ – for Ising spin models

ii) $S = \{1, \ldots, Q\} \subset \mathbb{N}$ – for Q-state Potts spin models

iii) $S = \{\sigma \in \mathbb{R}^n : |\sigma| = 1\}$ – for n-components spins (for which one may study the conditions for symmetry breaking of the continuous $O(n)$ symmetry).

iv) $S = \cup_n (0, 1]^n$ – for a gas of particles (though this case will not be much discussed here).

For the systems of such variables associated with the vertices of a graph $\mathbb{G}$ we denote:

- $\Omega = S^{\mathbb{G}}$ – the configuration space of the system of variables $\{\sigma_x\}_{x\in\mathbb{G}}$:
  The points of this space, often denoted $\sigma \in \Omega$ (or, on other occasions $\omega \in \Omega$) are functions $\sigma : \mathbb{G} \to S$.
- (Ω, Σ) – the measurable space built on Ω. The collection of the corresponding measurable functions is denoted by $\mathcal{B}$. We shall expand on this below.

- $\rho(d\sigma)$ – a "natural" a-priori measure on (Ω, Σ). When normalized, it presents what may be regarded as the fully chaotic state. Typically it will be a product measure

$$\rho(d\sigma) \;=\; \otimes_{x\in\mathbb{G}}\rho_0(d\sigma_x)\,. \tag{10.1}$$

  E.g., for the Q state Potts models, ρ_0 is the point measure assigning equal weights to the Q possible values of σ_x, and for the $O(n)$ models this would be the Haar measure on S.

The proper introduction of the above terms will be incomplete without a description of the relevant topology on Ω and the Σ-algebra of measurable sets, on which the probability is defined.

For a simple example which may illuminate the formal definition, let us recall that the unit interval $[0, 1]$ may be viewed as the configuration space of an infinite system of binary variables n_j with values in $S = \{0, 1\}$ in terms of which

$$x = \sum_{n=1}^{\infty} \frac{1}{2^n}\,\sigma_n\,, \tag{10.2}$$

Thus (except for the ambiguity which occurs at the countable collection of points of finite binary expansions) points $x \in [0, 1]$ may be represented as infinite spin configurations:

$$x \longleftrightarrow \{\sigma_j\}_{j=1}^{\infty}\,. \tag{10.3}$$

Similarly, doubly-infinite sequences of binary variables correspond to points in the unit square $[0, 1]^2$. Under this correspondence, the Lebesgue measure, dx_1dx_2 on $[0, 1]^2$, corresponds to the product measure on $S^{\mathbb{Z}}$ with respect to which σ_n form an iid sequence of binary variables with probabilities $(1/2, 1/2)$.

A point worth noting is that from the above perspective, the Lebesgue measure is just one from the family of measures μ_p on $\{0, 1\}^{\mathbb{Z}}$, for which σ_n are iid Bernoulli $0, 1$ valued random variables of mean p. Furthermore, for different values of p these measures are mutually singular – i.e. of disjoint supports (cf. (10.10)).

A natural choice for $\Omega = S^{\mathbb{G}}$ is the product topology, which is the minimal topology with respect to which all functions of the form $F(\sigma) = F_\Lambda(\sigma_\Lambda)$, with Λ ranging over finite subsets or $\mathbb{G}$, are continuous. A key result for such a construction is:

Theorem 10.1 (Tychonoff)**.** *The product of any collection of compact topological spaces is compact with respect to the product topology.*

For countable products, as in the case of main interest here, the product structure is especially simple: i) the topology can be based on the notion of sequential convergence (i.e., one does not need invoke "nets"), and ii) a countable product of a metric space is also metrizable. Among the possible metrics is:

$$d(\sigma, \sigma') = \sum_x \alpha_x \frac{d(\sigma_x, \sigma'_x)}{1 + d(\sigma_x, \sigma'_x)}. \tag{10.4}$$

with $\sum_x \alpha_x < \infty$.

Convergence in $\Omega = S^{\mathbb{G}}$ is equivalent to the statement that the finite volume restrictions of the configuration converge, i.e.

$$\omega_n \to \omega \quad\Longleftrightarrow\quad \omega_n|_\Lambda \to \omega_n|_\Lambda \quad \text{for all finite } \Lambda \subset \mathbb{G}\,. \tag{10.5}$$

The product topology provides also a convenient starting point for the construction of the corresponding Borel Σ algebra of measurable sets, with which the product space $\Omega = S^{\mathbb{G}}$ becomes a measurable space.

10.2 Some relevant Σ-algebras

To build the intuition let us introduce some relevant sets of functions and the corresponding Σ-algebras of measurable sets.

Definition 10.2. For each finite Λ, a function $f : \Omega \to \mathbb{C}$ is **measurable in** Λ if $f(\sigma)$ is measurable and depends on just the restriction of σ to Λ, i.e. on σ_Λ.

We denote by $\mathcal{B}_\Lambda$ the linear space of such functions, and by Σ_Λ the σ-algebras of correspondingly measurable sets (i.e. sets $A \subset \Omega$ whose indicator functions $\mathbb{1}_A$ are in $\mathcal{B}_\Lambda$).

The collection of **local functions** is, naturally,

$$\mathcal{B}_0 \;=\; \bigcup_{\Lambda \subset \mathbb{G}, |\Lambda| < \infty} \mathcal{B}_\Lambda \tag{10.6}$$

Building on that, and in line with the general method of measure theory, the **sigma algebra** of sets measurable in an infinite region $\widetilde{\Lambda} \subset \mathbb{G}$ is constructed in two steps: first taking the union of sets measurable in finite subsets of $\widetilde{\Lambda}$, and then extending it into the minimal collection of sets which is closed under the taking of complements and countable unions and intersections:

$$\Sigma_{\widetilde{\Lambda}} = \overline{\bigcup_{\Lambda \subset \widetilde{\Lambda}, |\Lambda| < \infty} \Sigma_\Lambda} \,. \tag{10.7}$$

The corresponding collection of measurable functions, which is related to it through the natural analog of (**??**), is denoted $\mathcal{B}_{\widetilde{\Lambda}}$.

The above notions allow one to formulate also what may at first sight appear somewhat surprising: the collection of functions which are **measurable at** ∞, defined as

$$\boxed{\mathcal{B}_\infty = \bigcap_{|\Lambda| < \infty} \mathcal{B}_{\mathbb{G} \setminus \Lambda} \,.} \tag{10.8}$$

In essence, elements of $\mathcal{B}_\infty$ are measurable functions whose values are not affected by an arbitrary flips of the configuration in any finite volume. At first encounter with the concept one may wander whether this does not require the function to be constant. After all, any pair of configurations can be "morphed" into each other through a countable collection of local changes, none of which affects the value of $f(\sigma)$. The question is answered by the following example.

Example 10.3. For sequences $\{\sigma_j\}_{j=1}^{\infty} \in [0,1]^{\mathbb{Z}}$, the function

$$\overline{M}(\sigma) \;:=\; \overline{\lim_{L \to \infty}} \, \frac{1}{L} \sum_{n=1}^{L} \sigma_n \tag{10.9}$$

is insensitive to any finite collection of terms in the sequence. Since it is also measurable (cf. exercise Ex. 10.1) $\overline{M}(\sigma)$ is measurable at ∞.

As an application of this concept, the above function permits to easily show that the Bernoulli measures μ_p under which σ_j form iid variables of mean p are mutually singular. Denoting

$$\Omega_p \ = \ \{\sigma \in \Omega \ : \ \overline{M}(\sigma) = p\} \tag{10.10}$$

the law of large numbers implies that for each $p \in [0, 1]$ the measure μ_p is fully supported in Ω_p. For different values of p these are clearly disjoint sets.

In statistical mechanics functions in $\mathcal{B}_\infty$ play a similar role in classifying the extremal Gibbs states of infinite systems. To introduce this notion properly let us briefly recapitulate the probabilistic notion of conditional expectation.

10.3 Conditional expectations - general terminology

The most basic conditional probability is that of an event A conditioned on event B, in which case it is

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)} \,. \tag{10.11}$$

The next step is to consider a finite partition of the probability space into disjoint union $\Omega = \sqcup_\alpha B_\alpha$ of sets of positive probability. Denoting by Σ_0 the σ-algebra of functions whose value depends only on which of basic elements of this partition does the point (or, in our case, configuration) belong, one has:

- the conditional probability of an event A, conditioned on Σ is the function

$$\mathbb{P}(A \,|\, \Sigma_0)(\sigma) := \mathbb{P}(A|B_\alpha) \quad \text{where } B_\alpha \text{ is the set containing } \sigma \,. \tag{10.12}$$

- $\mathbb{E}(f \,|\, \Sigma_0)(\sigma) \ = \$ the mean value of f averaged on the cell B_α to which σ belongs is .

The notions of conditional probability and of conditional expectation can be extended to the case where the partition corresponds to a (measurable) fibration into sets of zero measure, even though in that case the above definition breaks down, at least if taken in the literary sense. Their standard extension is based on the following basic result of probability theory.

Proposition 10.4 (Regular conditional expectation)**.** *Let (Ω, Σ, μ) be a probability space and $\Sigma_0 \subseteq \Sigma$ a sub σ-algebra. Then there is a unique linear map associating to each bounded Σ-measurable function $f \in L^\infty(\Omega, \Sigma)$ the function $\mathbb{E}(f \,|\, \Sigma_0)(\sigma)$ such that*

i. $\mathbb{E}(f \,|\, \Sigma_0)(\sigma)$ *is measurable with respect to* Σ_0.

ii. for all pairs of bounded measurable functions $f, g \in L^\infty(\Omega, \Sigma)$: if g measurable with respect to Σ_0 then

$$\boxed{\mathbb{E}(f\, g \,|\, \Sigma_0)(\sigma) = g(\sigma) \cdot \mathbb{E}(f \,|\, \Sigma_0)(\sigma)} \tag{10.13}$$

iii. for all $f \in L^\infty(\Omega, \Sigma)$

$$\boxed{\int f(\sigma)\, \mu(d\sigma) \ = \ \int \mathbb{E}(f \,|\, \Sigma_0)(\sigma)\, \mu(d\sigma)} \,. \tag{10.14}$$

To broaden the perspective, it may be added that the conditional expectation mapping

$$P_{\Sigma_0} \ : \ f \mapsto \mathbb{E}(f \,|\, \Sigma_0) \tag{10.15}$$

extends in $L^2(d\mu)$ into an orthogonal projection, onto the subspace

$$\mathrm{Range}\, \mathrm{P}_{\Sigma_0} \ = \ \{\mathrm{f} \in \mathrm{L}^2(\mathrm{d}\mu) \ : \ f \text{ is } \Sigma_0 \text{ measurable}\}\,. \tag{10.16}$$

For any monotone decreasing sequence of Σ-algebras $\Sigma_1 \supset \Sigma_2 ... \supset \Sigma_n ...$ the corresponding projections commute and have the **towering** property:

$$\boxed{P_{\Sigma_n} P_{\Sigma_k} \ = \ P_{\Sigma_n} \quad \text{for all } n \geq k}\,. \tag{10.17}$$

A noteworthy implication is that for any bounded (or just square integrable) function f the sequence $P_{\Sigma_n} f$ converges in the $L^2(d\mu)$ sense.

In probabilistic terms, the towering property means that for bounded functions f the sequence $P_{\Sigma_n} f$ forms a martingale. The *martingale convergence theorem* [5], allows to extend the above to the statement that for any such sequence the pointwise limit

$$\lim_{n\to\infty} P_{\Sigma_n} f(\sigma) \tag{10.18}$$

exists for μ-almost every σ, and yields the function $P_{\Sigma_\infty} f$ for $\Sigma_\infty = \cap_n \Sigma_n$.

10.4 States and observables

In a convention which seems to serve well quantum, classical, and statistical mechanical systems, the term **state** indicates an expectation value functional on the corresponding sets of observables.

In classical statistical mechanics **observables** correspond to continuous functions $f : \Omega \to \mathbb{C}$, whose collection forms the space $C(\Omega, \mathbb{C})$. An **expectation value functional** is a *linear mapping* $\rho : C(\Omega) \to \mathbb{C}$ such that

i) $\rho(f) \ > \ 0$, for all positive functions f
ii) $\rho(1) = 1$.

(from which it follows that: $|\rho(f)| \leq \|f\|_\infty$).

While the principle is common, the more constructive characterization of the states varies between classical and quantum systems. For classical systems one has the "Riesz representation" theorem.

Theorem 10.5 (Riesz-Markov-Kakutani)**.** *Let Ω be a compact metric space, and $\rho : C(\Omega) \to \mathbb{C}$ a linear functional satisfying the above three conditions. Then there exists a Borel probability measure μ on (Ω, Σ) such that*

$$\rho(f) = \int_\Omega f(\omega)\, d\mu(\omega)\,. \tag{10.19}$$

Thus, a **state** of an infinite classical system, of the type introduced above, is a Borel probability measure on its configuration space Ω. (States of quantum systems are discussed in [1, 6, 3].)

A natural notion of convergence of states is given by the convergence of expectation values of local observables.

Definition 10.6. Let $\Lambda_n \nearrow \mathbb{G}$ (e.g. $\mathbb{G} = \mathbb{Z}^d$) and μ_{Λ_n} be a sequence of finite volume states. We say $\lim_{n\to\infty} \mu_{\Lambda_n} = \mu$ if

$$\lim_{n\to\infty} \int f(\sigma)\, d\mu_n(d\sigma) \tag{10.20}$$

exists for all local continuous functions ($f \in \mathcal{B}_0$ in the terminology introduced below), and equals $\int f(\sigma)\, \mu(d\sigma)$.

10.5 The Dobrushin-Lanford-Ruelle condition

We now turn to systems of spin variables associated with the sites of a graph whose vertices are all of finite degree, with a Hamiltonian of the form

$$H = \sum_{A \subset \mathbb{G}} J_A\, \phi_A(\sigma_A) \tag{10.21}$$

with $\sup_\sigma |\Phi_A(\sigma_A)| = 1$. The interactions need not be translation invariant, but unless stated otherwise we limit to the case

$$\sup_{x\in\mathbb{G}} \sum_{A\subset\mathbb{G}: A\ni x} |J_A| \; < \; \infty \tag{10.22}$$

which implies that the energy change due to any single spin flip is finite.

For infinite systems the Gibbs prescription for the equilibrium states

$$\rho_\beta(d\sigma) = \frac{e^{-\beta H^{(\mathrm{b.c.})}(\sigma)} \rho_0(d\sigma)}{Z^{(\mathrm{b.c.})}}. \tag{10.23}$$

may at first glance not make much sense, since the Gibbs's factor is exponential in the system's size and thus typically either 0 or ∞. However this formula carries a local implication which continues to make sense even in the infinite volume limit.

We refer here to the observation that among the configurations with prescribed values in the complement of a finite set Λ the relative weights of the different configurations within Λ are governed by the finite volume Gibbs measure with σ_{Λ^c} serving as the boundary conditions.

More explicitly: for any finite subdomain Λ of an arbitrarily large finite systems the local conditional expectations $\mathbb{E}_\rho(f \,|\, \Sigma_\Lambda)(\sigma)$ are given by:

$$\boxed{\mathbb{E}_\rho(f \,|\, \Sigma_\Lambda)(\sigma) = \int f(\eta_\Lambda, \sigma_{\Lambda^c}) \frac{e^{-\beta H_\Lambda(\eta_\Lambda|\sigma_{\Lambda^c})}}{Z_\Lambda^{(\sigma_{\Lambda^c})}} \rho_0(d\eta_\Lambda) \overset{def}{=} \nu_{\Lambda,\beta}(f \,|\, \sigma)} \tag{10.24}$$

with $H_\Lambda(\eta_\Lambda|\sigma_{\Lambda^c})$ the collection of only those energy terms which involve η_Λ:

$$H_\Lambda(\eta_\Lambda|\sigma_{\Lambda^c}) = \sum_{\substack{A\subset\mathbb{G} \\ A\cap\Lambda\neq\emptyset}} J_A \phi_A((\eta_\Lambda, \sigma_{\Lambda^c}))\,. \tag{10.25}$$

It should be emphasized here that the function $\nu_\Lambda(f\,|\sigma)$ depends on σ only through σ_{Λ^c}, i.e. the configuration's restriction to the complement of Λ.

In physical terms the condition (10.24) states that the configuration within Λ is in thermal equilibrium with the rest of the system (the latter serving as a heat bath).

In mathematical terms this allows to extract from the Gibbs formula a relation which contin- ues to make perfect sense even in the infinite volume limit.

As suggested by R. Dobrushin and, independently, by O. Lanford and D. Ruelle this condi- tion can be taken as the defining characteristics of Gibbs states, which retains its validity even in the infinite volume limit. This motivates the following definition.

Definition 10.7. (The DLR condition) A probability measure μ on $(\Omega_{\mathbb{G}}, \Sigma)$ is a **Gibbs state** for the Hamiltonian H iff its conditional expectation $\mathbb{E}_\mu(f \,|\, \Sigma_0)(\sigma)$ for any finite region is given by $\nu_{\Lambda,\beta}(f \,|\, \sigma)$ of (10.24).

Before moving on let us comment that the DLR condition plays a role also in the Metropolis-Hastings algorithm (or Glauber dynamics), which has been used for numerical computations of equilibrium expectation values. There, in order to sample the configuration at close to its equilib- rium distribution, sites (or blocks) are repeatedly picked at random and have their spins redrawn with the DLR conditional probability distribution. Gibbs measures are clearly stationary under such dynamics. In finite volumes, under such evolution the probability distribution converges at an exponential rate to its unique equilibrium state. As the system grows in size the rate of convergence may degrade, and in infinite volume limit the uniqueness of the stationary measure may be lost.

10.6 The question of Gibbs state's uniqueness

Within the context of compact spin space and finite range bounded interactions the **existence** of infinity volume Gibbs states is a simple consequence of compactness. In particular, Prokhorov's theorem [5], which asserts that the collection of probability measures on a compact separable metric space is sequentially compact, allows to deduce the existence of converging sequences for any sequence of finite volume Gibbs equilibrium measures with arbitrary boundary conditions. To this one may add:

Theorem 10.8 (Stability under limits)**.** *Any probability measure μ which can be presented as the (weak) limit $\lim_{n\to\infty} \mu_{\Lambda_n}$ of a sequence of finite volume equilibrium states, of a common Hamilto- nian of finite range and $\beta < \infty$ is a Gibbs state.*

The proof, which we omit here, can be based on the continuity of the integral version of the DLR condition expressed in (**??**). The statement and its proof have a rather direct extension to long range interactions for which

$$\boxed{\sup_{x\in\mathbb{G}} \sum_{A\ni x} |J_A| < \infty\,.} \tag{10.26}$$

One may note that this condition is somewhat more restrictive than (5.8) which was required for the convergence of the pressure function.

The corresponding question of Gibbs state's **uniqueness** has a less uniform answer. It is of interest since non-uniqueness of the Gibbs state is the hallmark of **first order phase transitions**.

First order phase transitions, in Ehrenfest's classification, correspond to the discontinuity in the density of an extensive quantity, such as the energy or the magnetization. In thermodynamic terms this corresponds to non-differentiabilty, in the form of a kink-singularity, of the pressure as a function of the conjugate intensive parameter (such as the temperature, or the external field). The statistical mechanical manifestation of the phenomenon is the co-existence of two distinct Gibbs state, which represent distinct limits of the Gibbs states for which the relevant parameter is approaching its value from above, in one case, and below in the other.

For couplings at which there is more than one Gibbs state the different states may be reached in a number of ways:

i) taking infinite volume limits which different boundary conditions
ii) manipulation of infinite Gibbs states through control parameters, e.g. external magnetic filed $\underline{h}$ being taken to $\underline{0}$ while its orientation is fixed
iii) an ergodic decomposition of a state which spontaneously emerges in a mixed state (e.g. Ising model with free boundary conditions, at low temperatures).

10.7 Extremal state decomposition

For the case the Gibbs state is not unique the following observation provide some useful notions, and a relevant criterion.

The defining condition (10.24) implies that the collection of Gibbs states at specified H and β is closed under convex combinations. I.e. any measure of the form

$$\mu(\cdot) \; = \; \int_{\mathcal{I}} \mu_\alpha(\cdot)\, \kappa(d\alpha) \tag{10.27}$$

with μ_α a family of Gibbs states indexed (measurably) by $\alpha \in \mathcal{I}$ and κ a probability measure on $\mathcal{I}$, is also a Gibbs state on (Ω, Σ). The proof is left as an exercise (Ex. 10.3).

Definition 10.9. A Gibbs state is said to be an **extremal** (or **pure**) Gibbs measure, if it does not admit a decomposition into a convex combination of distinct Gibbs states.

Theorem 10.10. *Any Gibbs state has a unique representation as a linear combination of extremal Gibbs states. A Gibbs state μ is extremal if and only if any function measurable at infinity (i.e. $g \in \mathcal{B}_\infty$) is μ-almost surely constant.*

Let us note that the first statement may be rephrased as saying that with respect to the convex decomposition of states, the collection of Gibbs states at specified H and β forms a **simplex**.

Proof Taking a sequence of finite volumes with $\Lambda_n \nearrow \mathbb{G}$ one may conclude from (**??**) that for any Gibbs state μ (at a specified Hamiltonian and β) and bounded function $f \in \mathcal{B}$:

$$\mu(f) \; = \; \int_\Omega \mathbb{E}_\mu(f \,|\, \mathcal{B}_\infty)(\sigma)\, \mu(d\sigma) \tag{10.28}$$

with
$$\mathbb{E}_\mu(f\,|\,\mathcal{B}_\infty)(\sigma) \;=\; \lim_{n\to\infty} \mathbb{E}_\mu(f\,|\,\mathcal{B}_{\Lambda_n^c})(\sigma) \;=\; \lim_{n\to\infty} \nu_{\Lambda,\beta}(f)(\sigma) \tag{10.29}$$

The limit on the left exists by the Martingale Convergence Theorem [5], which guarantees almost sure convergence of the conditional expectations conditioned on a monotone family of Σ-algebras. Its expression on the right, in terms of a function which does not depend on μ, is by the Gibbs state's defining DLR property.

Applying standard separability arguments, μ is supported on the subset $\Omega_0 \subset \Omega$ of configurations for which the above limit exists for all continuous functions $f \in C(\Omega)$.

It follows that Gibbs measures are fully characterized by their restriction to functions measurable with respect to Σ_∞.

In addition, from the tower property of nested expectations it follows that for every $\sigma \in \Omega_0$ the linear functional: $f \mapsto \mathbb{E}(f\,|\,\mathcal{B}_\infty)(\sigma)$ is itself a Gibbs measure. And for each function g which is the pointwise limit of functions in $B_0 \cap B_{\Lambda_n^c}$, with $\Lambda_n \nearrow \mathbb{G}$, this conditional measure is supported on the collection of configurations σ' with $g(\sigma') = g(\sigma)$.

This allows to conclude that these Gibbs states are not further decomposable, and are pairwise either equal or mutually singular. □

It is hard to resist here a comment on the beauty of the probabilistic concepts involved in the above discussion. Whereas finite systems' equilibrium states are explicitly affected by the boundary conditions, in the infinite limit the boundary seems to disappear out of sight. The σ algebra Σ_∞ of sets measurable at infinity provides a handle for referring to the boundary conditions after the boundary itself was erased from the picture. A similar device can be seen in the Martin boundary in the theory of random walks on graphs.

10.8 A uniqueness criterion

The above considerations yield the following criterion for the uniqueness of the infinite system's Gibbs state (at a specified β).

Theorem 10.11. *A sufficient condition for H to have a unique Gibbs state at given β is that for any pair of Gibbs states there exists $C < \infty$ such that*

$$\boxed{\mu_1(f) \;\le\; C\,\mu_2(f)} \tag{10.30}$$

for all positive bounded local functions $f \in \mathcal{C}_0$.

Proof Since any Gibbs state is decomposable into convex combinations of extremal Gibbs states, if there is more than one then there have to exist at least two distinct extremal Gibbs states μ_1 and μ_2. By virtue of their extremity, these Gibbs states are mutually singular, i.e. there is a set $A \in \Omega$ (which would be measurable at infinity) for which

$$\mu_1(A) \;=\; 1\,, \quad \text{and} \quad \mu_2(A) \;=\; 0\,. \tag{10.31}$$

Condition (10.30) rules such a possibility out since any measurable set can be approximated in probability arbitrarily well by locally measurable sets, and for such sets $(\widetilde{A})$ (10.30) implies that $\mu_1(\widetilde{A}) \le C\mu_2(\widetilde{A})$. □

10.9 Implications for first order phase transition

Corollary 11.2 allows to set a fairly good criterion for delineating this possibility for a broad class of one dimensional systems with long range interactions.

Theorem 10.12. *For a one-dimensional system with a Hamiltonian of the form*

$$H(\sigma) = -\sum_{A\subset\mathbb{Z}} J_A \Phi_A(\sigma_A)\,, \tag{10.32}$$

if the following condition holds, at some finite U, for a collection of sites $x \in \mathbb{Z}$ which includes a sequence $x_n^+ \to \infty$ and a sequence $x_n^- \to -\infty$

$$\boxed{\sum_{\substack{A\cap[x_n,\infty)\neq\emptyset \\ A\cap((-\infty,x_n]\neq\emptyset}} |A|\,|J_A| \le U\,,} \tag{10.33}$$

then at every positive temperature the system has only one Gibbs state.

Proof Given a positive local function $f \in \mathcal{B}_0$, let Λ be the smallest interval $[x_n^{(-)}, x_n^{(+)}]$ such that $f \in \mathcal{B}_\Lambda$ is measurable within Λ. Then, by the DLR equation, for any Gibbs state $\mu(f) = \int \mathbb{E}_{\Lambda^c}(f|\sigma)\,\mu(d\sigma)$ with

$$\mathbb{E}(f\,|\,\mathcal{B}_{\Lambda^c})(\sigma) = \int f(\eta_\Lambda)\frac{e^{-\beta H_\Lambda(\eta_\Lambda|\sigma_{\Lambda^c})}}{Z_\Lambda^{(\sigma_{\Lambda^c})}}\rho_0(d\eta_A). \tag{10.34}$$

Included in $e^{-\beta H_\Lambda(\eta_\Lambda|\sigma_{\Lambda^c})}$ are only the interaction terms which involve η_Λ. Of these, let $H_\Lambda^\circ(\eta_\Lambda)$ be the collection of terms which do not involve any of the spins outside Λ. The assumed condition, provides the following estimate on the omitted terms:

$$|H_\Lambda^{\text{b.c.}}(\eta_\Lambda, \sigma_{\Lambda^c}) - H_\Lambda^\circ(\eta_\Lambda)| \le 2U. \tag{10.35}$$

The claimed bound then follows using the simple bound stated next. This implies that any pair of Gibbs states satisfy (10.31) (at $D = e^{2\cdot 4U}$) and hence, by Corollary 11.2, the system has a unique Gibbs state. □

Lemma 10.13. *Let $\mu_j(d\sigma)$ at $j = 1, 2$ be a pair of probability measures on a common space Ω, related by:*

$$\mu_2(d\sigma) = \frac{e^{\mathcal{A}(\sigma)}\mu_0(d\sigma)}{\int e^{\mathcal{A}(\tilde\sigma)}\mu_1(d\tilde\sigma)}\,. \tag{10.36}$$

Then for any positive measurable function f

$$\boxed{\int f(\sigma)\,\mu_2(d\sigma) \le e^{2\,\|\mathcal{A}\|_\infty}\int f(\sigma)\,\mu_1(d\sigma)} \tag{10.37}$$

where $\|\mathcal{A}\|_\infty := \sup_{\sigma\in\Omega}|\mathcal{A}(\sigma)|$.

This criterion provided by Theorem 10.12 allows to rule out first order phase transitions for one dimensional models with finite range interactions.

The above argument also yields a relevant criterion for one-dimensional systems with long range interactions, e.g. the $1D$ Ising model with

$$\boxed{J_{x,y} = \frac{1}{|x-y|^r}\,.} \tag{10.38}$$

For this case it implies that there is no first order phase transition if $r > 2$.

As it turns out $r = 2$ is the actual borderline, since at that value the model does exhibit a phase transition (and one of rather interesting characteristics [7, 8, 9, 10]). For long range interactions of random sign the threshold is pushed further [11].

Another application of the theory of extremal states will be presented below in the discussion of continuous symmetry breaking.

Exercises

10.1 (Measurability of percolation) For the Ising model on $\mathbb{Z}^2$ we say that a configuration $\sigma \in \Omega \equiv \{-1,+1\}^{\mathbb{Z}^2}$ exhibits +percolation if there exists an infinite path in $\mathbb{Z}^2$ along which $\sigma_x = +1$. Denoting the collection of such configurations by $K^+(\subset \Omega)$ explain why is this set measurable, i.e., $K^+ \in \Sigma$. *Hint: look at* (7.18) *and consider its implications.*

10.2 (Extremal state decomposition) For the 2D Ising model with the nearest neighbor interaction the *wired* boundary conditions correspond to the restriction that the boundary spins take a common value, and consequently:

$$\mu^{(w)}_{\beta,h} \;=\; \lim_{L\to\infty} \frac{1}{2}\left[\mu^{(+)}_{\Lambda_L;\beta,h} \;+\; \mu^{(-)}_{\Lambda_L;\beta}\right] \tag{10.39}$$

where $\Lambda_L = [-L, L]^2$. (The limit is known to exists through a monotonicity argument which at this point may be omitted).

i. Show that at $h = 0$ and temperatures low enough so that

$$3e^{-2\beta} < 1 \tag{10.40}$$

these states satisfy:

$$a)\quad \mu^{(w)}_{\beta,0}(K^+ \cap K^-) \;=\; 0, \qquad b)\quad \mu^{(w)}_{\beta,0}(K^+ \cup K^-) \;=\; 1 \tag{10.41}$$

Remark If you answered Question 7.1 fell free to just quote the relevant estimates which you may have used there.

ii. Show that under the above conditions the sigma algebra of functions measurable at infinity Σ_∞ is not trivial with respect to μ. Then show how can this information be used to decompose the measure $\mu^{(w)}$ into a sum of two mutually singular Gibbs states.

iii. Optional: Explain how the FKG inequality allows to conclude that under the above condition (10.40) symmetry breaking is detectable also in the mean magnetization

$$\mu^{(+)}_{\beta,0}[\sigma_0] = \int \sigma_0 \mu^{(+)}_{\beta,0}(d\sigma)$$

. That is, show that (10.40) implies:

$$\mu^{(+)}_{\beta,0}[\sigma_0] \neq 0 . \tag{10.42}$$

(Note: this yields an improved bound on the critical temperature, still based on just the Peierls contours analysis.)

Remark: the FKG inequality and the related coupling principle allow to deduce :
i) the finite volume Gibbs equilibrium states with the +, and correspondingly −, boundary conditions have translation invariant limits
ii) the limiting measures admit monotone coupling in which one of configurations pointwise dominates the other.
In your answer you may take these statements for granted, but do explain their meaning.

10.3 Prove that any linear combination of Gibbs states, as in (10.27) is also a Gibbs state.

Notes

The infinite system formalism is discussed in greater detail in [1, 2, 3]. Deeper discussion of the relevant probability theory can be found in [5, 4], the latter presenting a generalization of the DLR condition to singular conditional distributions.

One dimensional system with the borderline long range interaction (10.38) at $r = 2$ are discussed in [7, 8, 9, 10]). Among its notable features is the unusual behavior of the spontaneous magnetization as function of the temperature. In particular, in this case $\mu^{(+)}_{\beta_c,0}(\sigma_0) \neq 0$. The phenomenon was initially predicted in [7] (in hindsight the argument was insufficient, since the necessity for that was presented as an alternative to another unusual behavior, which as it turns out also occurs [10]. The topic was revisited in another remarkable work [8] where one finds an early formulation and application of (non-rigorous) renormalization group flow. The discontinuity of the spontaneous magnetization in 1D models of discrete spins with the $1/r^2$ interaction was established rigorously through an altogether different analysis in [9].

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11

Symmetry breaking, and conditions under which it does not occur

11.1 Spontaneous symmetry breaking: the concept

A **symmetry** of a statistical mechanical systems is an invertible measurable mapping $R : \Omega \to \Omega$ which preserves both ρ_0 and H, in the sense that:

i. the a-priori measure is R-invariant: $\rho_0(R^{-1}A) = \rho_0(A)$ for all $A \in \Sigma$.
ii. and so are the energy terms $\phi_\Lambda(R\sigma) = \phi_\Lambda(\sigma)$.

With each such transformation on Ω there is an induced mapping on functions and on measures, which for economy of notation will be denoted by the same symbol. These are naturally defined so that for each measurable function $f \in \mathcal{B}$, measure μ on (Ω, Σ) and measurable set $A \subset \Omega$

$$Rf(\sigma) = f(R\sigma)\,, \qquad R\mu(\{A\}) \;=\; \mu(R^{-1}\{A\})\,. \tag{11.1}$$

By implication the expectation-value functionals $\mu[f] \equiv \int f(\sigma)\mu(d\sigma)$, satisfy [1]

$$R\mu[f] := \int f(\sigma)\, R\mu(d\sigma) = \int f(\sigma)\, \mu(R^{-1}(d\sigma)) = \int f(R\sigma)\, \mu(d\sigma) =: \mu[Rf] \tag{11.2}$$

Examples include:

i. (Discrete symmetry) The global spin flip $(R\sigma)_x = -\sigma_x, \forall x \in \mathbb{G}$ defined within the Ising model at $h = 0$.
ii. (Continuous rotational symmetry) The $O(N)$ rotations acting on the N-component spins $\sigma \in \mathcal{S}^{N-1}$, in the model with
$$H = -\sum_{x,y} J_{x,y}\, \underline{\sigma}_x \cdot \underline{\sigma}_y\,. \tag{11.3}$$
iii. (A non-compact symmetry group) The shifts $(R_\delta\phi)_x = \phi_x + \delta$ acting within the lattice Gaussian free field, with $\phi : \mathbb{Z}^d \to \mathbb{R}$ and
$$H = -\sum_{x,y} J_{x-y} |\phi_x - \phi_y|^2\,. \tag{11.4}$$

In this case the finite volume equilibrium states may be stabilized by fixing the spins in the complement of $[-L, L]^d$ say at $\phi = 0$. In the limit $L \to \infty$ the corresponding probability

[1] The definitions of the induced actions listed in (11.1) apply also in case the measurable mapping R is not **one to one**. However, the mappings of main interest here are invertible, with R^{-1} acting similarly to R.

distribution of ϕ may converge to a limit as is the case for $D > 2$, or fluctuate away (in the sense that $|\phi_x| \stackrel{\mathcal{D}}{\to} \infty \ \forall x$) as is the case for $D = 2$.

When a Gibbs state is acted upon, i.e. transformed, by the system's symmetry the resulting measure will continue to satisfy the DLR condition. Thus, if μ is a Gibbs state then so is $R\mu$, and if μ is an extremal Gibbs state then so is $R\mu$.

Definition 11.1. A (statistic mechanical) *system* exhibits **symmetry breaking** if, at the specified temperature, it admits a Gibbs state which is not invariant under one of the system's symmetries (mappings preserving both the a-priori measure ρ_0 and the Hamiltonian H).

It may be added that for systems of spins with values in a compact space, with interaction satisfying the finite energy condition (10.26), at any β for each symmetry R there is at least one R-invariant Gibbs state. That need not be the case in the non-compact situation. E.g. this fails to be the case in the last of the above three examples (the Gaussian free field) in two dimensions.

An example of symmetry breaking is found in the $2D$ Ising model at low enough temperatures, for which its existence was established by Peierls. (An improvement of his upper bound on β_c is presented in Exercise 10.2, based on symmetry considerations and an application of the FKG inequality.)

In the Ising model, states of broken symmetry emerge naturally as limits of finite volume Gibbs equilibrium states with $+$, or correspondingly $-$ boundary conditions.

Symmetry breaking can also find its expression in the fact that infinite volume states which do have the symmetry (e.g. limits of free of periodic boundary condition states) are not extremal, and instead decompose into linear combinations of non-symmetric Gibbs measures. In this case the combined state would also fail to be ergodic under translations. This manifestation of the phenomenon is conveyed by the term **spontaneous** symmetry breaking.

11.2 Criterion for the absence of symmetry breaking

By the observation made above, symmetry breaking may take place only if the system has more than one Gibbs state. Thus a direct consequence of Theorem 10.11 is:

Corollary 11.2. *Let (H, ρ_o) be a statistic mechanical system with symmetry R. If for some β there exists $D < \infty$ such that for all Gibbs states at the given temperature and all positive bounded local functions $f \in \mathcal{B}_0$:*

$$\boxed{\mu(Rf) \ \le \ D\,\mu(f)} \tag{11.5}$$

then at the specified temperature the symmetry R is not broken.

11.3 The $1/|x-y|^2$ threshold for discrete symmetry breaking in $1D$

As was first pointed out by Ising, in one dimension the nearest neighbor Ising model does not exhibit symmetry breaking. His analysis (which in essence was based on the finite dimensional transfer matrix) can be extended to translation invariant interactions of finite range in one dimension.

A more general sufficient condition for the absence of symmetry breaking in one dimensional Ising models is provided by Theorem 10.12. In particular it implies that for Ising spin systems with interactions of the form

$$H(\sigma) \ = \ -\sum_{x,y\in Z} J_{x,y}\sigma_x\sigma_y\,. \tag{11.6}$$

there is no symmetry breaking if

$$J_{x,y} \le \frac{C}{|x-y|^r}\,, \qquad r > 2\,. \tag{11.7}$$

This is a relevant criterion, since symmetry breaking does occur for $J_{x,y} = 1/|x-y|^2$. (For coupling of random sign the borderline is pushed further; cf. previous section's references [8, 9, 11].)

11.4 The Mermin Wagner theorem

While discrete symmetries can be broken already in two dimensions, under the natural assumptions the continuous spin rotational symmetries can be broken only in dimensions $d > 2$. This is the content of the following celebrated result. As in the discrete case, this rule does not cover interactions which decay by only a sufficiently slow power law, in which case symmetry breaking can occur also in lower dimensions.

Theorem 11.3. *(Mermin-Wagner [1]) For two dimensional systems of spin variables with a rotational symmetry, of finite range bounded interactions*

$$H(\sigma) \ = \ \sum_{A\subset\mathbb{G}} J_A\Phi_A(\underline{\sigma}_A) \tag{11.8}$$

whose interaction terms
i) vary smoothly under site-dependent rotations, i.e. mappings $\sigma \mapsto \widehat{R}\sigma$ with

$$[\widehat{R}\sigma]_x = R_{\theta_x}\sigma_x\,, \tag{11.9}$$

ii) are invariant under uniform rotations ($R_\alpha := \widehat{R}_\theta$ at constant $\theta_x = \alpha$), i.e. satisfy

$$\Phi_A(R_\alpha\sigma) = \Phi_A(\sigma)\,, \tag{11.10}$$

any infinite volume Gibbs state is invariant under uniform spin rotations.

In other words: continuous rotational symmetries, under the natural assumptions are not broken in dimensions $D \le 2$.

Let us note that since general rotations of N component spins can be presented as products of rotations mixing just two of the spin's components, it suffices to focus on that case.

For a proof, we may employ Corollary 11.2. By this criterion, the Mermin-Wagner theorem can be deduced from the following estimate.

Lemma 11.4. *For a system with an $O(2)$ symmetry (as defined above) with interactions of finite range, satisfying*

$$\left|\frac{\partial^2}{\partial\theta(x)\,\partial\theta(y)}\;\Phi_A(\widehat{R}_\theta\sigma)\right| \ \le\ B\ <\infty\,, \tag{11.11}$$

Let $\mu^{\#}_{\Lambda}(d\sigma_\Lambda)$ be a finite volume Gibbs equilibrium state in $\Lambda = [-(L+K), L+K]$ with the boundary conditions, indicated here by #, provided by an arbitrarily fixed spin configuration in Λ^c. Then for all **positive** *local functions $f \in \mathcal{B}_{[-K,K]^d}$, at $K \leq L/2$ and uniform rotations R_α,*

$$\boxed{\mu^{\#}(R_\alpha f) \;\geq\; e^{-\beta C\, L^{D-2}}\; \mu^{\#}(f)} \tag{11.12}$$

with $C < \infty$ which depends only on B and the interaction's range.

Proof of Lemma 11.4 For any function f measurable in $\widetilde{\Lambda} = \Lambda(K)$ the action of uniform rotation by angle α can also be accomplished through an x-dependent rotation which acts uniformly within $[-K,K]^2$ and then gradually tapers off to the identity at distance R (the interaction range) to the boundary.

To ease the reference to such tapered rotations let us denote:

$$\tau(x) \;=\; \begin{cases} 1 & \|x\|_\infty \leq K \\ \frac{L-\|x\|_\infty}{L-K} & K \leq \|x\|_\infty \leq L \\ 0 & \|x\|_\infty \geq L\,, \end{cases} \tag{11.13}$$

and for the given α let $\widehat{R}_{\alpha\tau}$ be the non-uniform rotation in which σ_x is rotated by

$$\theta(x) \;=\; \alpha\,\tau(x)\,. \tag{11.14}$$

Since $f \in \mathcal{B}_{\Lambda(K)}$ depends only on the spins over which $\theta(x)$ takes the constant value α we have the equality

$$\boxed{\mu^{\#}(R_\alpha f) \;=\; \mu^{\#}(f(\widehat{R}_{\alpha\tau}\sigma))\,.} \tag{11.15}$$

Next, using a simple change of the variable of integration, into $\sigma' = \widehat{R}_{\alpha\tau}\sigma$, the term on the right may be re-expressed as

$$\begin{aligned} \mu^{\#}(f(\widehat{R}_\alpha\sigma)) &= \int_{\Omega_\Lambda} f(\widehat{R}_{\alpha\tau}\sigma_\Lambda)\frac{e^{-\beta H^{\#}_\Lambda(\sigma_\Lambda)}}{Z^{\#}_\Lambda}\rho(d\sigma_\Lambda) \\ &= \int_{\Omega_\Lambda} f(\sigma'_\Lambda)\frac{e^{-\beta H^{\#}_\Lambda(\widehat{R}^{-1}_{\alpha\tau}\sigma'_\Lambda)}}{Z^{\#}_\Lambda}\rho(d\sigma'_\Lambda) \\ &= \int_{\Omega_\Lambda} f(\sigma'_\Lambda)e^{-\beta[R^{-1}_{\alpha\tau}H-H](\sigma')}\frac{e^{-\beta H(\sigma')}}{Z^{\#}_\Lambda}\rho(d\sigma'_\Lambda) \end{aligned} \tag{11.16}$$

which may be summarized by:

$$\boxed{\mu(R_\alpha f) \;=\; \mu(f e^{-\beta[H(\widehat{R}^{-1}_\alpha)-H]})\,.} \tag{11.17}$$

The next goal is to show that for positive f the effect of this "tilt" of the expectation value functional is uniformly bounded.

For simplicity of presentation let us carry the analysis first for the simplest example, of the $O(2)$ spin models with $H = -\sum_{|x-y|=1} \underline{\sigma}_x \cdot \underline{\sigma}_y$ (often referred to as the XY model). In that case, using the symmetry:

$$H(\widehat{R}^{-1}_{\alpha\tau}\sigma) - H(\sigma) = \sum_{|x-y|=1} \left[\underline{\sigma}_x \cdot \underline{\sigma}_y - (R^{-1}_{\alpha\tau(x)}\underline{\sigma}_x)\cdot(R^{-1}_{\alpha\tau(y)}\underline{\sigma}_y)\right]$$
$$= \sum_{|x-y|=1} [\underline{\sigma}_x \cdot \underline{\sigma}_y - \underline{\sigma}_x \cdot R_{\alpha[\tau(x)-\tau(y)]}\underline{\sigma}_y] \tag{11.18}$$

The rotation can be written as $R_t = e^{t\mathcal{L}}$ with $t = \alpha[\tau(x) - \tau(y)]$ and $\mathcal{L}$ the corresponding generator, which in the natural representation of the two components spin space is $\mathcal{L} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. The rotation of relevance is at small angles, $t = O(\frac{\alpha}{L})$. Expanding R_t to the first order one gets

$$e^{t\mathcal{L}} = \mathbb{1} + t\mathcal{L} + T_2(t) \tag{11.19}$$

with $T_2(t)$ a 2×2 matrix of norm $\|T_2(t)\| \le |t|^2$. Hence

$$H(\widehat{R}^{-1}_{\alpha\tau}\sigma) - H(\sigma) = \frac{\alpha}{2}\sum_{|x-y|=1}[\tau(y)-\tau(x)]\,(\underline{\sigma}_x, \mathcal{L}\,\underline{\sigma}_y) + \frac{1}{2}\sum_{|x-y|=1}\Big(\underline{\sigma}_x, T_2(\alpha[\tau(y)-\tau(x)])\,\underline{\sigma}_y\Big)$$
$$= \alpha\,\delta_1(H) + \delta_2(H)\,, \tag{11.20}$$

with $\alpha J\delta_1(H)$ the sum of the1st order terms and $\delta_2(H)$ the remnant. Substituting (**??**) in (11.17) one gets

$$\mu(R_\alpha f) \;=\; \mu(f e^{\alpha J\delta_1(H) + J\delta_2(H)})\,. \tag{11.21}$$

Following the natural bounds one gets the following estimates for the two terms

$$\begin{aligned} |\delta_1(H)| \;&\le C\sum|\tau(x)-\tau(y)| \;\le\; 4J\,L^{D-1} \\ |\delta_2(H)| \;&\le C\sum|\tau(x)-\tau(y)|^2 \;\le\; CJ\,L^{D-2}\,. \end{aligned} \tag{11.22}$$

which if the dimension is $D \le 2$ is bounded uniformly in L_0.

For $D \le 2$ the second order term is bounded! Hence its contribution to (11.21) is within our tolerance level. However the first order term appears problematic.

As an aside, let us note that at the ground state configuration, with all spins parallel the first order term vanishes due to the anti-symmetry of the rotation's generator $\mathcal{L}$. This observation may have played a role in the original brilliant insight that it may be correct to ignore here $\delta_1(H)$. However, as is this argument cannot be sustained at positive temperatures.

The difficulty can be bypassed by taking advantage of the fact that the desired rotation can also be produced by rotating in the opposite direction, by the angle $2\pi - \alpha$, i.e.

$$R_\alpha = R_{-(2\pi-\alpha)} \tag{11.23}$$

This yields an alternative version of equation (11.21):

$$\mu(R_\alpha f) \;=\; \mu(f e^{-(2\pi-\alpha)\delta_1(H) + \widetilde{\delta}_2(H)}) \tag{11.24}$$

with $\delta_1(H)$ the same function as in (11.21), and $\widetilde{\delta}_2(H)$ while different from the corresponding term there still satisfies the second order bound (11.22).

The fact that the basic equality holds regardless of the sign in front of $\delta_1(H)$ suggests that this term may not be so relevant after all. To translate this into a proof, let us consider the interpolation of the two expressions, defined as:

$$Q(t) = \mu(f e^{(1-t)[\alpha\delta_1(H)+\delta_2(H)]} e^{t[-(2\pi-\alpha)\delta_1(H)+\widetilde{\delta}_2(H)]}). \tag{11.25}$$

The function $t \mapsto \ln Q(t)$ is convex in t (in other words $Q(t)$ is log-convex) with

$$Q(0) \;=\; Q(1) \;=\; \mu(R_\alpha f)\,. \tag{11.26}$$

Applying the Jensen inequality(a) to $\ln Q(t)$ we learn that for all $0 \le t \le 1$

$$Q(t) \;\le\; Q(0)^{1-t} Q(1)^t \;=\; \mu(R_\alpha f)\,. \tag{11.27}$$

For $t = t_\alpha$ selected by the condition

$$(1-t)\alpha - t(2\pi - \alpha) \;=\; 0 \tag{11.28}$$

the linear term in $Q(t)$ vanishes, and we get from (11.27)

$$\mu(R_\alpha f) \;\ge\; Q(t_\alpha) = \mu(f) e^{(1-t_\alpha)\delta_2 + t_\alpha \widetilde{\delta}_2} \;\ge\; e^{-\beta C L^{D-2}} \mu(f)\,. \tag{11.29}$$

Thus $\mu(R_\alpha f) \ge e^{-\beta C L^{D-2}} \mu(f)$ as claimed.

While the above estimates focused on the Heisenberg interaction $(\underline{\sigma}_x \cdot \underline{\sigma}_y)$, it is easy to see that the argument extends also to the more general class of Hamiltonians described in Lemma 11.2. □

[a] The bound (11.27) could alternatively be arrived at through the Hölder's inequality applied to the expectation value integral in (11.25).

Notes

• The Mermin-Wagner theorem is, in essence, driven by the observation that in $d = 2$ dimensions a function $\theta : \mathbb{R}^2 \to R$ which for $\|x\| \ge L$ is pinned at $\theta = 0$ can be raised up to $\theta = 1$ for $\|x\| = R$ at an elastic-energy cost which for each $0 < R$ vanishes in the limit $L \to \infty$[2]. In contrast, in dimensions $d > 2$ this quantity is bounded below by $c_d R^{d-2}$, uniformly in $L \ge R$. More explicitly:

$$\min\left\{ \int_{\substack{x\in\mathbb{R}^d \\ R\le\|x\|\ge L}} \|\underline{\nabla}\theta(x)\|^2\, dx \,\middle|\, \theta \in C^1(\mathbb{R}^d)\,, \;\; \begin{array}{ll} \theta(x) = 1 & \text{for } \;\|x\| = R \\ \theta(x) = 0 & \text{for } \;\|x\| = L \end{array} \right\} = \begin{cases} \frac{\pi}{\log L/R} & d = 2 \\ C_d\, R^{d-2}/[1-(R/L)^{d-2}] & d > 2 \end{cases} \tag{11.30}$$

The minimizing function is unique by a convexity argument, and thus also rotation invariant. It is given by a harmonic function, which in $2D$ is

$$\theta(x) \;=\; \frac{\log(L/\|x\|)}{\log(L/R)} \tag{11.31}$$

[2] The tools provided by the decomposition into extremal Gibbs state, allow to employ the simpler variational bound which states that this energy is bounded by a constant.

In higher dimensions the minimizer is a multiple of $[R/\|x\|)^{d-2} - (R/L)^{d-2}]$.

• For systems endowed with rotational symmetry it is natural to consider the effects of the addition of a "symmetry breaking field" to the symmetric Hamiltonian H_0, turning the latter into

$$H_h(\sigma) = H_0(\sigma) - \sum_x \underline{h} \cdot \underline{\sigma}_x \,. \tag{11.32}$$

Clearly, if the original system is symmetric under the uniform rotations R_α, then the extended pressure function is both convex in $\underline{h}$ and symmetric under rotations, satisfying

$$\Psi(\beta, R_\alpha \underline{h}) = \Psi(\beta, \underline{h}) \tag{11.33}$$

If the function is differentiable at $\underline{h} = \underline{0}$ then by symmetry its derivative there has to vanish. The alternative is a kink discontinuity at $\underline{h} = \underline{0}$, which then corresponded to symmetry breaking. Thus, the thermodynamic manifestation of the Mermin-Wagner theorem is that for systems with the continuous rotational symmetry, in two dimension the pressure $\Psi(\beta, \underline{h})$ is differentiable in $\underline{h}$ at $\underline{h} = \underline{0}$, with zero derivative there.

• The argument presented above can be adapted also to quantum systems, cf [5].

Exercises

11.1 (Implications of symmetry on the Gibbs state decomposition)
Let (Ω, ρ_0, H) describe a statistic mechanical system symmetry R, as defined in the opening of this chapter. Prove that the system's infinit-volume Gibbs state's over $\mathbb{R}^d$ have the following properties:

i. If μ is a Gibbs state then also the rotated state $R\mu$ is a Gibbs state.

ii. If μ is an **extremal Gibbs state** then so is $R\mu$.

iii. If, at a given temperature β^{-1}, each of the system's Gibbs states is absolutely continuous with respect to its spin-rotated version, then each of the system's Gibbs states is **rotation invariant**.

References

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12

Partial order and FKG monotonicity

Monotonicity considerations are very helpful in the study of the Gibbs states of variety of models, yielding non-perturbative results which may be seen as intuitive yet hard to establish by other means. As a demonstration of such tools, in this section we shall highlight the natural **partial order** structure on the Ising model's configuration space, and present the fundamental theorem on the subject due to C.M. Fortuin, P. W. Kasteleyn and J. Ginibre.

The method is applicable to ferromagnetic Ising models on arbitrary graphs including under site dependent external magnetic field $h(x)$. It allows to prove for such systems that:

i) the infinite volume limit for the ferromagnetic Ising model's Gibbs states with the +(alternatively the −) boundary conditions exist
ii) in finite as well as infinite volumes all the system's Gibbs states are are bracketed between the states constructed with + and − boundary conditions
iii) for translation-invariant ferromagnetic Hamiltonians the +and the − limiting states are translation invarianat
iv) at (β, h) at which the pressure is differentiable in the magnetic field h the system has exactly one infinite volume Gibbs state.

In the chapter which follows the concepts presented here will be extended to a broader family of models.

12.1 Partial order and the FKG condition for Ising systems

Before turning to the Ising models, let us linger for a moment on the **monotonicity structure** of the real line, $\mathbb{R}$, which is a prime example of a totally ordered set, ordered by the relation $x \geq y$.

Monotonicity of a function $f : \mathbb{R} \mapsto \mathbb{R}$ expresses its order-preserving property[1]. Related to it one has the following general statement.

[1] Except where stated otherwise, throughout our discussion monotonicity terms are meant to be understood in their weak sense, e.g. "monotone increasing" means the same as "non-decreasing".

Theorem 12.1. *For any probability measure μ on $\mathbb{R}$, and any pair of increasing functions $f, g, : R \mapsto \mathbb{R}$*

$$\mu[fg] \geq \mu[f]\mu[g] \ . \tag{12.1}$$

where $\mu[F]$ denotes the expectation value of a function F with respect to μ.

Proof The claim is an easy consequence of the observation that

$$\int_{x,y\in\mathbb{R}} [f(x) - f(y)] \, [g(x) - g(y)] \, \mu(dx)\mu(dy) \ \geq \ 0 \tag{12.2}$$

which holds thanks to the simultaneous monotonicity of f and g. □

Unlike the real line, the space of Ising model's configurations is not totally ordered. Nevertheless, it admits the following natural **partial order**.

Definition 12.1. For any pair of spin configurations $\sigma, \tilde{\sigma} : V \to \{ \pm 1 \}$, one is said to dominate the other ($\tilde{\sigma} \geq \sigma$) if the relation hold pointwise. That is:

$$\boxed{\tilde{\sigma} \geq \sigma \Longleftrightarrow \tilde{\sigma}_x \geq \sigma_x \qquad \forall x \in V} \ . \tag{12.3}$$

The partial order on the set of configurations $\Omega = \{-1, +1\}^V$ gives rise to the following notions.

Definition 12.2. 1) A function $f : \{ \pm 1 \}^V \to \mathbb{R}$is called **increasing** iff

$$\sigma \geq \tilde{\sigma} \Longrightarrow f(\sigma) \geq f(\tilde{\sigma}) \ .$$

2) For a pair of probability measures μ, ν on Ω, μ is said to **dominate** ρ ($\mu \geq \nu$) iff for all increasing $f : \{ \pm 1 \}^V \to \mathbb{R}$:

$$\mu[f] \ \geq \ \nu[f] \ . \tag{12.4}$$

3) A probability measure μ on $\Omega_V \equiv \{ \pm 1 \}^V$is said to have the **positive association property** iff for any pair of increasing functions $f, g : \ \Omega \to \mathbb{R}$

$$\boxed{\mu[fg] \ \geq \ \mu[f] \, \mu[g]} \tag{12.5}$$

$$\tag{12.6}$$

One may note that an equivalent formulation of the last property is that for any positive and monotone increasing function f,

$$\boxed{\mu_f \geq \mu} \, . \tag{12.7}$$

where μ_f is the f**-tilted** measure that is defined by

$$\mu_f[g] \ = \ \frac{\mu[f g]}{\mu[f]} \, . \tag{12.8}$$

By the seminal result of Fortuin, Kasteleyn and Ginibre [3], a sufficient condition for the positive association property is provided by the following condition on the measure ρ.

Definition 12.3. A probability measure on $\Omega_V = \{\pm 1\}^V$ with density $\rho(\sigma)$ with respect to the independent product measure is said to satisfy the **FKG lattice condition** iff

$$\boxed{\rho(\sigma \wedge \widetilde{\sigma})\ \rho(\sigma \vee \widetilde{\sigma})\ \geq\ \rho(\sigma)\ \rho(\widetilde{\sigma})} \tag{12.9}$$

where the configurations on the left are defined by

$$(\sigma \wedge \widetilde{\sigma})_x := \min(\{\sigma_x, \widetilde{\sigma}_x\}) \qquad (x \in V) \tag{12.10}$$

$$(\sigma \vee \widetilde{\sigma})_x := \max(\{\sigma_x, \widetilde{\sigma}_x\}) \qquad (x \in V)\ . \tag{12.11}$$

It may be of help to note a number of points concerning the above notion.

- The notation in (12.10) is motivated by the observation that the partial order on Ising configurations corresponds to the inclusion order on the corresponding sets of sites at which $\sigma_x = +1$. From this perspective $\wedge$ and $\vee$ are naturally associated with the union and the intersection of the corresponding sets.

- The validity of the FKG condition (12.9) is unaffected by changes of ρ through the multiplication by arbitrary single site factors, e.g. under the addition to $H(\sigma)$ of a term of the form $U(\sigma) = \sum_{x\in V} h_x \sigma_x$ (i.e. the addition of an arbitrary magnetic field, or the imposition of an arbitrarily selected, but then held fixed, boundary configuration).

- The term **lattice** is invoked in Definition 12.3 in reference not to the graph but to configuration space's partial order structure.

For completeness we shall spell the more general setting which is invoked by the lattice notion. First however let us sketch the proof that the key condition is satisfied by Ising spin systems with only ferromagnetic pair interaction.

Lemma 12.4. *The ferromagnetic Ising model's Gibbs measures with the free, periodic, or arbitrarily fixed boundary conditions each obey the FKG lattice condition* (12.9).

Proof Stripping the weight $\rho(\sigma)$ of the single spin factors which, as noted above, do not affect the validity of the condition (12.9) one is left with a product of only the two-body terms, which contribute to $\rho(\sigma)$ in proportion to the amount of agreement among interacting spins. The switch from the pair $(\sigma, \widetilde{\sigma})$ to $(\sigma \wedge \widetilde{\sigma}, \sigma \vee \widetilde{\sigma})$ corresponds to the migration of + spins to the first factor, and − spins to the second. Such a switch only enhances the total amount of agreement among interacting pairs. □

12.2 A more generally stated FKG lattice condition

Now that we have a sense of where this discussion is headed, let us fill some gaps in the above presentation of the terminology.

Definition 12.5 (Partial order)**.** A partial order on an set Ω is a binary relation $\preceq$ which is:

i) reflexive: $\omega \leq \omega$, $\forall \omega \in \Omega$,

ii) antisymmetric: $\omega \leq \widetilde{\omega}$ and $\widetilde{\omega} \leq \omega$ implies $\omega = \widetilde{\omega}$.

iii) transitive: $\omega \leq \widetilde{\omega}$ and $\omega \leq z$ implies $\omega \leq z$.

When that applies, we refer to $\omega \leq \widetilde{\omega}$ as "$\widetilde{\omega}$ dominates ω" and may write it interchangeably as $\widetilde{\omega} \geq \omega$.

Definition 12.6 (Lattice)**.** A partially ordered set $(\Omega, \leq)$ is called a **lattice** if for any pair $\omega, \widetilde{\omega} \in \Omega$ there exist:

i) a unique minimal upper bound, denoted $\omega \vee \widetilde{\omega}$
(i.e. a unique element which is dominated by all elements that dominate both ω and $\widetilde{\omega}$)

ii) a unique maximal lower bound, denoted $\omega \wedge \widetilde{\omega}$
(i.e. a unique element which dominates all elements that are dominated by both ω and $\widetilde{\omega}$).

Furthermore, a lattice is called **distributive** iff

$$\omega \wedge (\omega' \vee \omega``) = (\omega \wedge \omega`) \vee (\omega \wedge \omega``) \qquad (\omega, \omega`, \omega`` \in X)\ . \tag{12.12}$$

Examples: The above structure can be noted in the **inclusion** relation among the collection of subsets of a set S. That is, letting $\Omega = \{A : A \subset X\}$ (the "power set" of X), with

$$A \leq B \Longleftrightarrow A \subseteq B\,. \tag{12.13}$$

We already encountered such a lattice in the discussion of the Ising model, whose configuration $\sigma : V \to \{-1, +1\}$ can be alternatively represented by the set $\{x \in V\ :\ \sigma_x = +1\}$. **The symbols** $\vee$ **and** $\wedge$ **which appeared in** (12.10) **are motivated by this representation.**

Other examples include one component spin models of spins taking values over a compact set $S \subset \mathbb{R}$, and coupled through ferromagnetic Ising-like interaction terms $J_{x,y}\sigma_x\sigma_y$.

In the above terminology the more generally stated FKG inequality is:

Theorem 12.2 (The FKG inequality [3])**.** *For a probability measure on a distributive lattice Ω_V, of density ρ with respect to a product measure, a sufficient condition for the positive association property* (12.5) *is that corresponding version of the lattice condition* (12.9) *is satisfied for any pair $\sigma, \widetilde{\sigma} \in \Omega_V$ i.e.*

$$\boxed{\rho\,(\sigma \wedge \widetilde{\sigma})\ \rho\,(\sigma \vee \widetilde{\sigma})\ \geq\ \rho\,(\sigma)\ \rho\,(\widetilde{\sigma})}\,. \tag{12.14}$$

with $\sigma \wedge \widetilde{\sigma}$ and $\sigma \vee \widetilde{\sigma}$ defined as above, in terms of the specified order.

Proof of the statement, which we shall omit here, may be found in the original article [3], in numerous works which followed, e.g. [4], and in the textbook on the subject [3].

12.3 Implications for the ferromagnetic Ising spin model

To demonstrate the uses of the above theory, let us return to the Ising model on a locally finite graph $\mathbb{G} = (\mathcal{V}, \mathcal{E})$ (e.g. the d-dimensional $\mathbb{Z}^d$) with a ferromagnetic Hamiltonian of the form

$$H(\sigma) = -\sum_{(x,y)\in\mathcal{E}} J_{x,y}\sigma_x\,\sigma_y - \sum_x (h + \eta_x)\sigma_x \tag{12.15}$$

with $J_{x,y} = J_{y,x} \geq 0$, satisfying $\sum_{y\in\mathcal{V}} |J_{x,y} < \infty$ for each x, and the parameter h is a uniform addition to the possibly site dependent external magnetic field η_x.

As noted in Lemma 12.4, the Gibbs measures of such models, in finite volume $\Lambda \subset \mathcal{V}$ with boundary condition given by specified exterior configurations σ_{Λ^c} satisfy the **FKG lattice condition** (12.14). Hence these measures have the positive association property (12.5).

Among the implications, one has the following.

Lemma 12.7 (Monotonicity in the dependence on the boundary conditions)**.** *For Ising spin systems as specified above, for any fixed Λ the finite volume Gibbs measures conditioned on different exterior spin configurations are monotone in the boundary spins, in the sense discussed above. More explicitly (in the notation of* (10.24)*) for any pairs of exterior configurations the conditional distributions satisfy:*

$$\sigma^1 \leq \sigma^2 \;\Rightarrow\; \nu^{\sigma^1}_{\Lambda,\beta} \;\leq\; \nu^{\sigma^2}_{\Lambda,\beta}\,. \tag{12.16}$$

In particular, each such finite volume Gibbs distribution is bracketed between the corresponding + and − finite volume states

$$\nu^{-}_{\Lambda,\beta} \;\leq\; \nu^{\widetilde{\sigma}}_{\Lambda,\beta} \leq\; \nu^{+}_{\Lambda,\beta}\,. \tag{12.17}$$

where ± indicates the corresponding boundary conditions.

To recall: (12.17) means that for any monotone increasing spin function f, and any choices of the boundary conditions

$$\nu^{-}_{\Lambda,\beta}(f) \;\leq\; \nu^{\widetilde{\sigma}}_{\Lambda,\beta}(f) \;\leq\; \nu^{+}_{\Lambda,\beta}(f)\,. \tag{12.18}$$

The proof of Lemma 12.7 is left here is as an exercise to the reader (Ex. 12.1). But let us list here a **series of consequences**.

1) **Monotonicity in L**
For any monotone increasing sequence of finite subsets $\Lambda_L \subset \mathcal{V}$ with $\cup\Lambda_L = \mathcal{V}$ the sequence of Gibbs states constrained to take a constant value in the complements of Λ_L is monotone in L, when viewed as a sequence of states of the system defined over all of $\mathcal{V}$:
    the + constrained states **decrease** as $L \nearrow$
    the − constrained states **increase** as $L \nearrow$.
(In each case, the relevant condition is in effect relaxed as $L \nearrow$).

2) **Construction of the infinite volume ± states**
The limits define the infinite volume + and − states, with

$$\nu^{+}_{\mathcal{V},\beta}(f) := \lim_{L\to\infty} \nu^{+}_{\Lambda_L,\beta}(f), \quad \nu^{-}_{\mathcal{V},\beta}(f) := \lim_{L\to\infty} \nu^{-}_{\Lambda_L,\beta}(f) \tag{12.19}$$

for any local function $f \in \mathcal{B}_0$.
(Note: the convergence is initially deduced for monotone functions, but these include all finite products of the form $f(\sigma) = \prod_J [(\sigma_{x_j} + 1)]$. By implication the convergence extends to all polynomials in the spin variables. But any local function can be written in that form. $\square$)

3) **The ± bracketing relation**
Any infinite volume Gibbs measure $\nu_{\mathcal{V},\beta}($ is bracketed between the + and − states, in the sense that for any monotone local function

$$\nu^{-}_{\mathcal{V},\beta}(f) \;\le\; \nu_{\mathcal{V},\beta}(f) \;\le\; \nu^{-}_{\mathcal{V},\beta}(f)\,. \tag{12.20}$$

(The condition is proven by combining (12.18) with the DLR expression for the expectation values as an average over finite volume conditional expectation, conditioned on σ_{Λ^c}.)

4) **Translation invariance**
For the models on $\mathcal{V} = \mathbb{Z}^d$ (and more generally transitive locally finite graphs) with translation invariant Hamiltonian the + and − Gibbs states are translation invariant.
(Proof idea: by monotonicity, any two sequences of increasing finite volumes which are nested in the sense that one asymptotically covers the other, yield the same state.)

5) **Condition for uniqueness of the Gibbs state**
On any infinite graph, at any given (β, h) the systems admits exactly one infinite volume Gibbs state if and only if

$$\forall x \in \mathcal{V}: \qquad \nu^{+}_{\mathcal{V},\beta}(\sigma_x) \;=\; \nu^{-}_{\mathcal{V},\beta}(\sigma_x) \tag{12.21}$$

The last implication rests on the following very useful **monotone coupling** criterion.

Theorem 12.8 (Holley [4])**.** *On any distributive lattice, a probability measures μ dominates ν, i.e.*

$$\mu \ge \nu \tag{12.22}$$

if and only if the two admit a monotone coupling, in the sense that there exists a probability measure $\kappa(d\sigma^{(1)}\, d\sigma^{(2)})$ on the product space $\Omega \times \Omega$ such that

i) *$\kappa(d\sigma^{(1)}\, d\sigma^{(2)})$ is supported the collection of pairs $(\sigma^{(1)}, \sigma^{(2)})$ for which*

$$\sigma^{(1)} \ge \sigma^{(2)} \tag{12.23}$$

ii) *the marginal distribution of κ on the first component is given by μ and on the second component by ν, in the sense that for any (measurable) function $f : \Omega \to \mathbb{R}$:*

$$\begin{aligned} \int_{\Omega\times\Omega} f(\sigma^{(1)})\; \kappa(d\sigma^{(1)}\, d\sigma^{(2)}) &= \int_\Omega f(\sigma)\, \mu(d\sigma) \\ \int_{\Omega\times\Omega} f(\sigma^{(2)})\; \kappa(d\sigma^{(1)}\, d\sigma^{(2)}) &= \int_\Omega f(\sigma)\, \nu(d\sigma)\,, \end{aligned} \tag{12.24}$$

One many note that in one direction this statement is trivial, since if such a coupling exists then for any monotone increasing funcition $f : \Omega \mapsto \mathbb{R}$

$$\mu(f) - \nu(f) \;=\; \int_{\Omega\times\Omega} \Big[f(\sigma^{(1)}) - f(\sigma^{(2)})\Big]\kappa(\sigma^{(1)}\, d\sigma^{(2)}) \;\ge\; 0 \tag{12.25}$$

where the inequality holds since by (12.23) the integrand is non-negative almost surely in κ. The point of Holley's theorem is that the converse relation is also true.

Notes

An alternative tool for the proof of some of the results, including the convergence of selected states to the infinite volume limit, is provided by Griffiths' spin correlation inequalities [4]. These, and other related inequalities will be presented in a separate chapter.

While the above discussion is focused on the structure of Gibbs equilibrium states, monotonicity considerations and the coupling of measures prove also very useful tools for the study of stochastic time evolutions. Fruitful links between the two perspectives, of equilibrium and dynamics, can be found in Holley's derivation of Theorem 12.8, and other subsequent results.

The criterion (12.21) for the uniqueness of Gibbs state was found useful in the proof by Aizenman and Wehr [6] of a strong version of the Imry-Ma phenomenon [5], which is that in the two dimensional Random Field Ising model, under arbitrarily weak random field, at any (β, h) the system has only one infinite volume Gibbs state. The main part of the analysis is to prove the quenched free energy's differentiability in h. The above criterion allows then to boost the result to a Gibbs uniqueness statement. We are not aware of other tools enabling that globally, i.e. beyond perturbative regimes.

In the next chapters we shall encounter applications of the FKG inequality in other contexts. One of these is the family of Fortuin-Kastelyn random cluster models. Other applications will show up in the study of thermal and ground states of certain quantum spin chains.

Exercises

12.1 Prove Lemma 12.7.
(Hint: Given an ordered pair of boundary conditions, $\sigma_{\Lambda^c} \leq \widetilde{\sigma}_{\Lambda^c}$, write explicitly the factor by which should the Gibbbs measure conditioned on σ_{Λ^c} be "tilted" in order to produce the one conditioned on $\widetilde{\sigma}_{\Lambda^c}$. Consider this factor's monotonicity properties, and their implications.)

12.2 Spell the proofs of translation invariance of the + and − Gibbs states of the Ising model with translation invariant interactions (in the sense explained in item (4) in the above list).

12.3 Derive the criterion (12.21) for the uniqueness of the model's infinite volume Gibbs state.
(Hint: under monotone couplings, equality in the mean magnetization implies coalescence.)

References

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(Additional references on related topics are mentioned in the next section, and are listed there.)

13

Fortuin-Kasteleyn random cluster models

The Fortuin-Kasteleyn random cluster model provides a stochastic geometric perspective on the correlation and phase transitions in discrete spin models. It leads to new insights, and links a range of classical and even quantum spin system. It would be natural to present the model starting with a brief presentation of R.B. Potts' extension of the Ising model [1].

13.1 The Q-state Potts model

In the Q-state Potts model the spin variables assume not just 2 but Q distinct values, weighted equally in the model's a-priori measure. The corresponding configuration space for such a system on a graph of vertex set $\mathcal{V}$ is

$$\Omega_Q := \{ \sigma : \mathcal{V} \to \{ 1, \ldots, Q \} \} . \tag{13.1}$$

In an extension of the ferromagnetic Ising interaction, the Potts Hamiltonian rewards agreement among interacting pairs:

$$\boxed{H(\sigma) = \sum_{\{ x,y \} \subset \mathcal{V}} J_{xy} \left(1 - \delta_{\sigma_x, \sigma_y} \right) - \sum_{x \in \mathcal{V}} \delta_{\sigma_x, 1}} \tag{13.2}$$

with h a magnetic-field like parameter which allows to tune up a symmetry breaking term (which for $h > 0$ gives preference to $\sigma_x = 1$ over the other $(Q-1)$ values.

At $h = 0$ the model has an obvious symmetry, of global permutation of the spin values. like the Ising model, in dimensions $d > 1$ the Potts model (over $\mathbb{Z}^d$, with non-degenerate interactions) undergoes a phase transition, and exhibits symmetry breaking at low temperatures. The corresponding order parameter is

$$M(\beta) \; := \; \lim_{h \searrow 0} \left[\langle \delta_{\sigma_x, 1} \rangle_{\beta, \rho} - \frac{1}{Q} \right] \cdot \frac{Q}{Q-1} \tag{13.3}$$

where $\langle -- \rangle_{\beta,\rho}$ is the expectation in the corresponding infinite volume Gibbs state, normalized to range between $M = 0$ (indicating no bias) to $M = 1$ (probability one for $\sigma_x = 1$).

Existence and translation invariance of the infinite volume state will be derived in this section by arguments which are reminiscent of those presented in the preceding section.

Among the model's notable features:

i) At $Q = 2$ the Potts models coincides with the Ising model (except for a factor of 2 in the definition of the coupling). However at other values of Q it **does not** share the Ising model's $h \mapsto -h$ symmetry.

ii) For the nearest neighbor interaction over $\mathbb{Z}^2$, unlike in the Ising model, at $Q > 4$ the Potts model's order parameter is **discontinuous** at the phase transition, at which it jumps from $M(\beta_c - 0) = 0$ to a strictly positive value $M(\beta_c + 0) > 0$ [**?**, **?**, 1].

iii) Also notable is the fact that the above behavior is **not "universal"** in the sense that it is not stable under the extension to broader finite range interactions. (Under sufficient broad couplings the discontinuity occurs already at $Q = 3$).

iv) On planar graphs, at $h = 0$ the model is in a **duality relation** with a similar model of the same value of Q, formulated on the dual graph, at a dual temperature. In the case of $Q = 2$ this relation coincides with the Ising model's Kramers-Wannier duality.

v) The model's critical temperature on the self dual planar graph $\mathbb{Z}^2$ is calculable as the **self dual** value of β. (The alternative would have been the existence of two critical points, and an intermediate phase. This option is ruled out for a range of models, including Potts models at all values of $Q \in \mathbb{N}$.)

(Reference will be provided in the discussion of the yet broader family of random cluster models to which we turn next.)

13.2 Extension into a system of spin & bond-percolation variables

A convenient starting point for the transition to a random cluster model is the observation that for two ferromagneticaly linked spins the Gibbs factor can be presented as:

$$\boxed{e^{\beta J_{xy}\left(\delta_{\sigma_x,\sigma_y}-1\right)} \;=\; \lambda_{xy}\delta_{\sigma_x,\sigma_y} + \left(1-\lambda_{xy}\right)} \quad \text{at } \lambda_{xy} := 1 - e^{-\beta J_{xy}}. \tag{13.4}$$

This elementary rewriting of the bi-valued function of σ can be read as a decomposition of a ferromagnetic measure into a convex combination of two drastically different measures. The one weighted by λ_{xy} is a joint distribution in which the two spins are locked together, assuming always the same value though that value may vary. In the other, of weight $\left(1-\lambda_{xy}\right)$, the spins fluctuate independently.

Inserting this decomposition into the model's Gibbs factor, and then distributing the resulting product, one obtains the following presentation of the model's partition function

$$
\begin{aligned}
Z^{\text{Potts}}_{\beta,Q} &= \sum_{\sigma\in\Omega} \exp\left(\beta \sum_{\{x,y\}\in\mathcal{E}} J_{xy}\left(\delta_{\sigma_x,\sigma_y} - 1\right)\right) \\
&= \sum_{\sigma\in\Omega} \prod_{\{x,y\}\in\mathcal{E}} \left[\left(1-\lambda_{xy}\right) + \lambda_{xy}\delta_{\sigma_x,\sigma_y}\right] = \sum_{\sigma\in\Omega} \sum_{n:\mathcal{E}\to\{0,1\}} \prod_{b\in\mathcal{E}} \lambda_b^{n_b}\,(1-\lambda_b)^{1-n_b}\,\delta^{n_b}_{\sigma_{b_x},\sigma_{b_y}} \\
&= \boxed{\sum_{n:\mathcal{E}\to\{0,1\}} Q^{C(n)} \prod_{b\in\mathcal{E}} \lambda_b^{n_b}\,(1-\lambda_b)^{1-n_b} \;=: Z^{\text{FK}}_{\beta,Q}}
\end{aligned}
\tag{13.5}
$$

where we use $n : \mathcal{E} \to \{0,1\}$ for keeping track of which of the two factors of (13.4) appears in a given product, and use the abbreviating symbol b for edges $\{b_{x},_y\, by\}$.

The transition to the third line is based on the observation that for a given edge configuration (n) the spins are constrained to be **constant over each of the n- connected clusters**, in a decomposition for which an edge $b \in \mathcal{E}$ is regarding as connecting iff $n_b = 1$. $C(n)$ denotes here the number of clusters in the corresponding decomposition.

This representation of the partition function allows to change our perspective and consider the systems as having two sets of degrees of freedom (σ, n). One of these is the Potts system of spins assigned to the graph's sites $\sigma : \mathcal{V} \to \{1, ..., Q\}$ and the other, described by the edge configuration $n : \mathcal{E} \to \{0, 1\}$, is a bond-percolation system, whose configurations' probability depends on both the number of occupied edges and the resulting number of connected clusters.

In this picture, the joint probability of (σ, n) is

$$
\mu(\sigma, n) = \frac{1}{Z} \prod_{b\in\mathcal{E}} \lambda_b^{n_b}\,(1-\lambda_b)^{1-n_b}\,\delta^{n_b}_{\sigma_{b_x},\sigma_{b_y}} \tag{13.6}
$$

The marginal distribution of σ, obtained by summing over n, is the Potts model we started with. The marginal distribution of the edges is given by the weights of with which each configuration n contributes to the last sum in (13.5), times $1/Z^{\text{FK}}_{\beta,Q}$.

A notable feature of this system is the simplicity of the conditional distribution of each of its two components conditioned on the other:

$\eta \Rightarrow \sigma$: Conditioned on the configuration of $\{n_b\}$ the spins are constant within each of the connected clusters, and for the different clusters form independent random variables, of uniform distribution over $\{1, ..., Q\}$.

$\sigma \Rightarrow \eta$: Conditioned on the spin configuration $\{\sigma_x\}$, the edge variable assume values 0 or 1 independently of each other, with the conditional probability for $n = 1$ given by:

$$
\Pr(n_{x,y} = 1 \,|\, \sigma) \;=\; \begin{cases} \lambda_{x,y} & \text{if } \sigma_x = \sigma_y \\ 0 & \text{if } \sigma_x \neq \sigma_y \end{cases} \tag{13.7}
$$

Under this representation the covariance between two spins can be traced to the probability of their sites being n-connected. An explicit relation in this vein is

$$\tau(x,y) := \frac{Q}{Q-1}\, \mathbb{E}^{\rm Potts}_{Q}\left[\left(\delta_{\sigma_x,\sigma_y} - \frac{1}{Q}\right)\right] = \Pr\left(x \overset{n}{\leftrightarrow} y\right) . \tag{13.8}$$

Under this relation, the model's potential **long range order** (in the infinite volume limit), which is characterized by the spin-spin covariance satisfying

$$\lim_{|y|\to\infty} \tau(o,y) \neq 0\,, \tag{13.9}$$

coincides with **percolation**, i.e. the emergence of an infinite n-connected cluster in the system of randomly occupied edges described by the $\{\, n_b \,\}$ variables.

Such stochastic geometric representations of covariance provide a useful handle on the spread of correlations, and tools for the study of their critical behavior.

A creative use of the $\sigma \longleftrightarrow n$ relation was made by R.H. Swendsen and J-S Wang [5] who used these rules for the construction of a non-local or cluster algorithm for Monte Carlo simulation for large systems near criticality. The algorithm is based on successive alternating refreshments of η and σ. Typically, as T approaches T_c the convergence rate of Monte Carlo simulations slows down, as the spins develop longer correlations. However, in their algorithm that is partially offset by the emergence of large size flips in the dynamical process which drives the system towards its Gibbs equilibrium state.

13.3 The Fortuin-Kasteleyn random cluster model

The Fortuin-Kasteleyn random cluster model, on a pre-specified graph $\mathbb{G} = (\mathcal{V}, \mathcal{E})$, has as its configurations random sets of edges, which are naturally described by the edge function $n : \mathcal{E} \to \{\, 0, 1 \,\}$. Its probability distribution has the form which we encountered in (13.5), except that Q is no longer restricted to be an integer.

More explicitly, in the FK state's on a finite graph the probability of an edge configuration is given by

$$\rho^{FK}_{\beta,Q}(\{\, n \,\}) \;=\; \frac{1}{Z^{\rm FK}_{\beta,Q}}\, Q^{C(n)} \prod_{b\in\mathcal{E}} \lambda_b^{n_b}\, (1-\lambda_b)^{1-n_b} \tag{13.10}$$

where λ_b are the model's basic parameters, and the weights are normalized to yield a probability measure by the factor $Z^{\rm FK}_{\beta,Q}$ (c.f. (13.5)) which also forms the model's partition function.

For the simplicity of presentation it is sometimes more convenient to focus on the case of constant couplings, in which these would be presented as

$$\lambda_b = 1 - e^{-\beta} \tag{13.11}$$

with a common parameter $\beta \in [0, \infty)$.

At $Q = 1$ the FK-random cluster model reduces to an independent bond percolation model.

At varying Q the FK random cluster model interpolates between percolation and the Ising and Potts models (linked to them through the relation (13.5)) and allows to even extrapolate beyond those (cf. Notes), though as we shall see some of its behavior is modified for $Q < 1$.

As a percolation model, the basic derived quantities concern the structure of the model's connected clusters. Of particular interest is the model's percolation transition, and more detailed questions related to: `To be filled in!`

13.4 Boundary conditions

Having encountered already the effects of boundary conditions, one may ask what choice would be of particular relevance for the FK random cluster measures. The question shows up in discussions of such measures on finite subgraphs corresponding to the restriction to a finite subsets of vertices $\lambda \subset \mathcal{V}$ of the vertex set of a potentially infinite graph $\mathbb{G} = (\mathcal{V}, \mathcal{E})$. The following types of boundary conditions would enter our discussion.

- **Free:** the edges over which n is defined consist of only those whose both endpoints are in Λ. Equivalently, one may consider n as defined over all the edges of $\mathcal{E}$ but interpret the free boundary conditions as stating that $n_{x,y} = 0$ for all edges which are not contained in Λ.
- **Wired:** the inner boundary of λ, that is the set of sites $u \in \lambda$ which share an edge with a site in Λ^c, is regarded as all interconnected. Equivalently, n is regarded as having the value $n_{u,v} = 0$ over all all edges which have at least one site outside of λ.
- **Mixed:** the inner boundary of Λ is partitioned into sets which are declared by fiat as connected clusters. Given such a partition, sites of Λ which are connected internally to boundary sites in the same cluster are regarded as connected.
- **Periodic:** these are applicable in case the graph is disjointly covered by graph isomorphic copies of Λ. For each such tiling corresponds a natural enhancement of the edges of Λ which may be regarded as the periodic extension of its edge set.

The choice of the boundary conditions affects the count of the number of connected clusters $C(n)$, and through it the probability of the configuration n, as well as the partition function (except if $Q = 1$).

The periodic boundary conditions provide a convenient choice for producing translation invariance in finite volume setup. However the proof of the finite volume states' convergence in the infinite volume limit is not the easiest with this choice. In fact, we are not aware of a simple general argument which is directly applicable to this case.

In contrast, for the 'wired' and the 'free' b.c. convergence of the finite volume states of any monotone sequence of restrictions of the graph to finite volumes Λ_L would be an easy conclusion of the monotonicity arguments to which we turn next.

The limiting 'wired' and 'free' states need not be equal, but when they coincide then convergence is implied for any sequence of mixed and, when applicable, periodic boundary conditions.

13.5 Monotonicity

The FKG monotonicity theory that was presented in the preceding section in the context of the Ising model, is applicable also in the context of the FK random cluster models.

A natural partial order on the set of the model's configurations is $n : \mathcal{E} \to \{0, 1\}$ is

$$\tilde{n} \geq n \Longleftrightarrow \tilde{n}_b \geq n_b \qquad \forall b \in \mathcal{E} . \tag{13.12}$$

Describing the configurations $n \in \{0, 1\}^{\mathcal{E}}$ in terms of the corresponding subsets of occupied edges, $\{ b \in \mathcal{E} \,|\, n_b = 1 \}$, the configuration space is immediately recognizable as forming a distributive lattice under this order, in the sense explained in Section 12.2. What is also true, though a bit less immediate, is that the lattice FKG condition (12.14) is valid also in this context.

Theorem 13.1. *For $Q \geq 1$, in any finite volume the FK random cluster probabilities $\mathbb{P}^{FK}_{\beta,Q}$ defined by* (13.10) *satisfy the FKG lattice condition*

$$\rho\,(\sigma \wedge \widetilde{\sigma})\;\; \rho\,(\sigma \vee \widetilde{\sigma}) \;\geq\; \rho\,(\sigma)\;\; \rho\,(\widetilde{\sigma}) \;.$$

Proof The two side in the desired relation are affected equally by the single edge factors in the measure's density, $\prod_{b\in\mathcal{E}} \lambda_b^{n_b}\,(1-\lambda_b)^{1-n_b}$. Hence what needs to be proved (for the specified range of $Q \geq 1$) is that the number of connected clusters satisfies

$$C\,(n \wedge n') + C\,(n \vee n') \;\geq\; C\,(n) + C\,(n') \;. \tag{13.13}$$

for all pairs (n, n').

Equivalently stated, the condition is $C\,(n \vee n') - C\,(n) \;\geq\; C\,(n') - C\,(n \wedge n')$. Expressing it in terms of the intersection $k = n \wedge n'$, we see that what needs to be show is:

$$C\,(n' \vee n) - C\,(n) \;\geq\; C\,(n' \vee k) - C\,(k) \tag{13.14}$$

for all n' and $k \preceq n$. In other words: what needs to be shown is that for each n' the **difference** which its "addition to n" makes on the number of clusters, i.e. $C\,(n' \vee n) - C\,(n)$, is a monotone **increasing** function of n.

In case n' has a single bond b with $n'_b = 1$ this condition is satisfied since

$$C\,(n \vee \mathbb{1}_b) - C\,(m) = \begin{cases} 0 & \text{the endpoints of } b \text{ are already connected through } n \\ -1 & \text{otherwise} \end{cases}$$

which is a monotone increasing function of n (being the negative of an obviously decreasing function).

The general statement follows by a telescopic decomposition of the relevant condition, for which the addition of n' is presented as the concatenation of a series of single edge additions, the effect of each of which is monotone by the above argument. □

Before turning to the tangible implication of the FKG monotonicity of the random cluster model, let us note that in the case of Ising model we now have two notions of monotonicity: one is based on the partial order of the spin configurations (discussed in section 12), and the other based on the partial order of the edge configurations, that are associated with the model's presentation as a $Q = 2$ Potts model. The two notions do not overlap, but rather supplement each other.

13.6 Implications for the random cluster measures

The above proven FKG condition for the FK random cluster measures has implications which may ring similar to what we already encountered in the discussion of the Ising model. In addition, we shall see relations which allow comparisons between FK models at different values of Q - **which throughout this section we discuss only for $Q \geq 1$.**

Theorem 13.2. *At $Q \geq 1$ for each finite graph, the random cluster measure*

$$\rho^{FK}_{\beta,Q}(\{ n \}) \; = \; \frac{1}{Z^{FK}_{\beta,Q}} \, Q^{C(n)} \prod_{b \in \mathcal{E}} \lambda_b^{n_b} \, (1-\lambda_b)^{1-n_b} \tag{13.15}$$

has the following monotonicity properties:

i) it is **increasing** *in the parameters $\lambda = \{ \lambda_b \}_{b \in \mathcal{E}}$*

ii) it **decreasing** *in Q*

iii) for Q and $\{ \lambda_b \}$ evolving under a parameter t at rates satisfying

$$\forall b \in \mathcal{E} : \quad \frac{d}{dt} \ln \frac{\lambda_b}{1-\lambda_b} \; \geq \; \frac{d}{dt} \ln Q \; \geq \; 0 \tag{13.16}$$

the measures are monotone **increasing** *in t.*

The last case is listed to show how the decrease of the measure as $Q \nearrow$ can be more than compensated by a suitable increase of β, in the sense of (13.4).

Sketch of the proof Combining Theorems 12.2 and 13.1 one learns that for $Q \geq 1$ the random cluster measures have the positive association property. One of its implicaitons is that tilting the measure by a factor of the form $e^{f(n)}$ with a function $f(n)$ that is monotone increasing, or monotone decreasing, in n changes the measure accordingly.

The three monotonicity statements follow through simple considerations of the effect of increase in the corresponding parameters on

$$\log \left[Q^{C(n)} \prod_{b \in \mathcal{E}} \lambda_b^{n_b} \, (1-\lambda_b)^{1-n_b} \right] . \tag{13.17}$$

The pertinent for the first statement is then that in the sense of the partial order considered here:

i) each n_b is a monotone increasing function of n

ii) $C(n)$ is a monotone decreasing function of n (adding an edge either decreases the number of connected clusters by 1, or leave that number invariant)

iii) the sum $C(n) + \sum_b n_b$ is monotone increasing in n.

□

The arguments which were presented in Section 12.3 in the context of the Ising model though its σ-based partial order lead in the present case to the following conclusions. (Note: the partial order discussed here is different, and the implications do not overlap, but the logic is similar.)

1) **Bracketing relations**
In any finite volume, the random cluster probability measure corresponding to the wired boundary conditions dominates that with the free boundary conditions, and any state of mixed boundary conditions in bracketed between the two:

$$\rho^{FK,\,\mathrm{Free}}_{\beta,Q,\Lambda} \ \le\ \rho^{FK,\,\mathrm{Mixed}}_{\beta,Q,\Lambda} \ \le\ \rho^{FK,\,\mathrm{Wired}}_{\beta,\Lambda} \tag{13.18}$$

2) **Monotonicity in Λ**
For any monotone increasing sequence of finite subsets $\Lambda_L \subset \mathcal{V}$ the random cluster measures in Λ_L with the **free** and **wired** boundary conditions are monotone in the following sense

$$\rho^{FK,\,\mathrm{Free}}_{\beta,Q,\Lambda} \ \nearrow \qquad \text{and} \qquad \rho^{FK,\,\mathrm{Free}}_{\beta,Q,\Lambda} \ \searrow \qquad (\text{as } \Lambda \ \nearrow) \tag{13.19}$$

3) **Infinite volume limits of the "wired" and "free" states**
For any sequence of finite subdomains Λ_L with $\cup\Lambda_L = \mathcal{V}$ the the corresponding wired and free measures converge (as probability measures on the common space $\{0,1\}^{\mathcal{V}}$). Their limits form an ordered pair of random cluster measures

$$\rho^{FK,\,\mathrm{Free}}_{\beta,Q,\mathcal{V}} \ \le\ \rho^{FK,\,\mathrm{Wired}}_{\beta,Q,\mathcal{V}} \tag{13.20}$$

4) **Semicontinuity in β**
for each $\beta \ge 0$ and $Q \ge 1$

$$\lim_{\widetilde{\beta}\nearrow\beta} \rho^{FK,\,\mathrm{F/W}}_{\widetilde{\beta},Q,\mathbb{Z}^d} \ =\ \rho^{FK,\,\mathrm{Free}}_{\beta,Q,\mathbb{Z}^d} \le \rho^{FK,\,\mathrm{Wired}}_{\beta,Q,\mathbb{Z}^d} = \lim_{\widetilde{\beta}\searrow\beta} \rho^{FK,\,\mathrm{F/W}}_{\widetilde{\beta},Q,\mathbb{Z}^d} \tag{13.21}$$

where W/F indicates that the limits can be taken with either of the boundary conditions.

5) **Translation invariance**
For the models on $\mathcal{V} = \mathbb{Z}^d$ (and more generally transitive locally finite graphs) with translation invariant edge parameters the limiting wired and free random cluster measures are translation invariant.

We omit here the discussion of more general definition of the infinite volume version of random cluster measures, which can be formulated in terms of a suitable DLR-type condition (or **specification** in the terminology of [9]).

However, it may be of interest to state here a"thermodynamic" criterion for the coincidence of the infinite graph's wired and free boundary measures on $\mathbb{Z}^d$.

Definition 13.1. For the random cluster model on $\mathbb{Z}^D$, with translation invariant edge density parameters $\lambda_{x,y} = 1 - e^{-\beta J_{x-y}}$ with positive and summable J_u, the following function is referred to as the model's thermodynamic pressure

$$\varphi(\beta, Q) := \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \log Z^{FK}_{\beta,Q} \tag{13.22}$$

The following result holds true in greater generality, but for simplicity of presentation it is stated here for the nearest neighbor case.

Theorem 13.2. *For the translation invariant random cluster measures on $\mathbb{Z}^d$ the with nearest neighbor connections at $\lambda = 1 - e^{-\beta}$, and $Q \geq 1$, the infinite volume wired and free states at given (β, Q) coincide if and only if at that point $\varphi(\beta, Q)$ is differentiable in β, or equivalently*

$$\frac{\partial}{\partial\beta - 0}\varphi(\beta, Q) = \frac{\partial}{\partial\beta + 0}\varphi(\beta, Q)\,. \tag{13.23}$$

The proof of this statement is a recommended exercise. It is reachable through the combination of thermodynamic convexity considerations, FKG monotonicity, and Holey's Theorem. The Ising version of such a statement was first presented by J.L. Lebowitz [11] using thermodynamic convexity combined with correlation inequalities, some of which were developed by him for this purpose.

13.7 The percolation phase transition in random cluster models

`Basic notions and results to be filled in. Among those:`

• The bound

$$\beta_c(Q') \geq \beta_c(Q) \geq \frac{Q}{Q'}\beta_c(Q') \qquad (Q' \geq Q \geq 1)\,. \tag{13.24}$$

which follows from Theorem 13.2

• The almost sure **uniqueness of the infinite cluster** [**?**, **?**], and its implications [**?**].

• The notion and proofs of sharpness of the phase transition. [**?**, **?**, **?**, **?**]

• Critical exponent bounds [**?**]

• Highights of the 2D results [**?**]

13.8 Duality relations in $2D$

• Geometric duality of planar models.

• The self duality of the planar FK random cluster measures

• The explicit relations, in which $A(n) \approx B(n)$ means equality up to an additive graph-dependent constant:

$$n_b + n^*_{b^*} = 1 \tag{13.25}$$

$$C(n^*) - C(n) \approx \|n\| \tag{13.26}$$

$$Q^{C(n)} \approx \sqrt{Q}^{\,C(n)+C^*(n^*)} \sqrt{Q}^{\,\|n\|} \tag{13.27}$$

where $\|n\| := \sum_{b \in \mathcal{E}} n_b$.

• The more symmetric reformulation of the model in terms of separating loops, each bounding either a connected cluster or a dual connected clusters.

• The self dual model, and the fractal structure of its typical configurations.

Notes

References

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PART III. Quantum statistical mechanics

14

Quantum Statistical Mechanics

14.1 A brief summary of QM principles

Text to be filled in.

15

Quantum spin arrays

15.1 Pauli matrices

Pauli-sigma matrices:

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 := \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Together with $\sigma_0 := \mathbb{1}_{2\times 2}$ they span the $\mathbb{R}$ vector space of 2×2 Hermitian matrices.

Basics properties: for all $i, j = 1, 2, 3$ (with summation convention over repeating indices)

$$\sigma_i^2 = \mathbb{1}_{2\times 2}\,, \quad \mathrm{tr}\,(\sigma_i) = 0\,, \quad \det(\sigma_i) = -1 \tag{15.1}$$

$$\text{(commutation relations)} \qquad \left[\sigma_i, \sigma_j\right] \equiv \sigma_i\sigma_j - \sigma_j\sigma_i = 2\mathrm{i}\varepsilon_{ijk}\sigma_k \tag{15.2}$$

$$\text{(anit-commutation relations)} \qquad \left\{\sigma_i, \sigma_j\right\} \equiv \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}\mathbb{1}_{2\times 2} \tag{15.3}$$

where ε_{ijk} is the antisymmetric Levi-Civita symbol, and i the imaginary unit in $\mathbb{C}$.

15.2 Quantum spin operators

A triplet (vector) of operators $\underline{S} = (S_1, S_2, S_3]$ which satisfy the angular-momentum commutation relations

$$\left[S_i, S_j\right] = \mathrm{i}\varepsilon_{ijk}S_k \tag{15.4}$$

Except for the degenerate case of the one-dimensional $\mathcal{H}_0$ (in which case each of the three operators act as multiplication by 0) the operators S_j do not commute.

The first non-trivial case is that of a q-bit whose state space is the two dimensional Hilbert space $\mathbb{C}^2$, spanned by a pair of orthogonal vectors $|+\rangle\,, |-\rangle$. The spin commutation relations are realized there by the triplet of operators which in the preselected basis act as

$$S_j = \frac{1}{2}\sigma_j^{(\mathrm{Pauli})} . \tag{15.5}$$

Building on that, it is found that in every finite dimensional Hilbert space these commutation relations can be realized in a triple of self adjoint operators which act irreducibly on $\mathcal{H}$.

It is convenient to write the dimension as $\boxed{\dim \mathcal{H} = 2S + 1}$, with $S \in \frac{1}{2}\mathbb{Z}_+$, and denote the corresponding space as $\boxed{\mathcal{H}_S}$ (e.g. the above q-bit space is $\mathcal{H}_{1/2}$). The following properties then follow from the commutation relations combined with irreducibility.

i) The collection of linear combination of the form

$$\underline{v} \cdot \underline{S} := \sum_{J=1}^{3} v_j S_j \tag{15.6}$$

with $\underline{v}$ a classical vector in $\mathbb{R}^3$ is closed under addition and commutation. Upon exponentiation (into $U_{\underline{\theta}} = e^{i\underline{\theta}\cdot\underline{S}}$) it generates the group of unitary transformations of $\mathcal{H}_S$. Its induced action on the linear space of operators of the form $\underline{v} \cdot \underline{S}$ is isomorphic to rotations in $\mathbb{R}^3$.
(The corresponding action of $U_{\underline{\theta}}$ on the Hilbert space $\mathcal{H}_S$ deserves a comment, but that will be made elsewhere.)

ii) For each unit vector ($\|v\| = 1$) the spectrum of $\underline{v} \cdot \underline{S}$ over $\mathcal{H}_S$ is non-degenerate, and given by

$$\mathrm{spec}(\underline{\mathrm{v}} \cdot \underline{\mathrm{S}}) \; = \; \{ -\mathrm{S}, -\mathrm{S}+1, ..., \mathrm{S} \} \tag{15.7}$$

The eigenvectors of S_3 in $\mathcal{H}_S$ are by customarily denoted $|m, S\rangle$, so that

$$S_3 \, |m, S\rangle \; = \; m \, |m, S\rangle \; . \tag{15.8}$$

iii) Within $\mathcal{H}_S$ the operator $\underline{S} \cdot \underline{S}$ acts as a constant. More explicitly:

$$\underline{S} \cdot \underline{S} \; = \; S(S+1) \; \mathbb{1}_S \; . \tag{15.9}$$

iv) For $S > 0$ the spin flip $\underline{S} \mapsto -\underline{S}$ is not realizable through a unitary transformation (since this is not a symmetry of the commutation relations), but $(S_1, S_2, S_3) \mapsto (S_3, S_1, S_2)$ is realizable in that manner.

A semiclassical analogy can be drawn between the quantum spin operators acting in $\mathcal{H}_S$, and the classical 3-component angular momentum. The classical phase space of the latter is the sphere $\{\underline{v} \in \mathbb{R}^3 \,|\, \|\underline{v}\| = S\}$, equipped with its natural symplectic structure (i.e. that Poisson bracket on the sphere, whose algebraic structure echoes the quantum spin's commutation relation).

While not perfect, the analogy does shed light on a number of features of quantum system. For example, the spin quantization rule over $\mathcal{H}_S$ can be taken as a quantum analog of the law which Archimedes discovered about 225 BCE, on the remarkable constancy of the areas of the slices of a sphere, cut by equidistant planes[1]

[1] In simple terms: passing an orange through a bread slicing machine will get one peals of equal area.

15.3 Composite systems

The natural description of the Hilbert space for multi-component system, whose individual states spaces are $\mathcal{H}^{(n)}$ is the corresponding tensor product space,

$$\otimes_j \mathcal{H}^{(j)} \equiv \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes ...$$

For any choice of orthonormal bases B_j for the separate component, a basis for $\otimes_j \mathcal{H}^{(j)}$ can be selected as the collection of product vectors

$$|m_1\rangle_1 \otimes |m_2\rangle_2 \otimes ... \equiv |m_1, m_2, ...\rangle_{1,2,...} , \tag{15.10}$$

with $|m_j\rangle_j$ ranging over the elements of B_j. A general vector in the product space is a linear combination of such.

A general operator in $\otimes_j \mathcal{H}^{(j)}$ is a linear combination of products of operators each of which acts on a specific component.

In particular, one-particle operators are operators which act on only one of the components at a time. These take the form of linear combinations of

$$\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes A_u \otimes \mathbb{1} ... \otimes \mathbb{1} \equiv A_u \tag{15.11}$$

the abbreviated notation being used when its deemed that its action is clear within the context.

Likewise we shall denote by $A_u B_v$ the two-body operator which acts with A_u on the u-component and with B_v on the v-component. If the two components are distinct and disjoint the corresponding sets of operators commute, in their action in the tensor product Hilbert space.

15.4 Spin addition and irreducible decompositions of product spaces

`To be filled in`

The vector sum of a pair of spin vectors associated with different components, produces another triplet of operators

$$\underline{S}^{(u,v)} := \underline{S}^{u} + \underline{S}^{u} \tag{15.12}$$

With $\underline{S}^{u}$ and $\underline{S}^{u}$ commute with each other, the sum's three components $S_j^{(u,v)}$ inherit the angular momentum commutation relations

$$\left[S_i^{(u,v)}, S_j^{(u,v)}\right] = \mathrm{i}\varepsilon_{ijk} S_k^{(u,v)} , \tag{15.13}$$

and thus $\underline{S}^{(u,v)}$ also forms a spin triplet.

However, $\underline{S}^{(u,v)}$ does not act irreducibly on the $\mathcal{H}^{(u)} \otimes \mathcal{H}^{(u)}$. Stated equivalently, the group of unitary operators of the form $e^{i\underline{\theta}\cdot\underline{S}^{(u,v)}}$ does not act transitively on the product space.

Instead, the tensor product decomposes into a direct sum of subspaces in each of which the $\underline{S}^{(u,v)}$ is irreducible. Sorting the details of this decomposition is the first step towards **group representation theory**. Among its basic results is the statement that for any pair of spin values S_1 and S_2

$$\mathcal{H}_{S_1} \bigotimes \mathcal{H}_{S_1} = \bigoplus_{S=|S_1-S_2|}^{|S_1+S_2|} \mathcal{H}_S \,. \tag{15.14}$$

That is, the tensor product space decomposes into the direct sum of spin spaces at spin values ranging from $|S_1 - S_2|$ to $S_1 + S_2$, with in unit increments.

Once again, the analogy with classical vectors gives this rule in a rather intuitive interpretation, as the length of the sum of two vectors in $\mathbb{R}^3$ does have such a range. Looking at it more quantitatively, one may want to check that the dimensions of the corresponding spaces add up (as they do). In case $S_1 = S_2 = 1/2$ this translates to $2 \cdot 2 = 1 + 3$, and for more general values of $S_1, S_2 \in \frac{1}{2}\mathbb{Z}_+$:

$$(2S_1 + 1) \cdot (S_2 + 1) = \sum_{S=|S_1-S_2|}^{S_1+S_2} [2S + 1] \,. \tag{15.15}$$

In view of (15.14), for each S_1, S_2 one has two distinct bases for the resulting Hilbert space. The natural basis for the product space $\mathcal{H}_{S_1} \otimes \mathcal{H}_{S_1}$ consists of the vectors

$$\boxed{\{\, |m_1, m_2\rangle_{S_1,S_2} \,\}} \qquad \text{with } \; m_j \in \{-S_j, -S_j + 1, ..., S_j\} \text{ for } j = 1, 2 \;. \tag{15.16}$$

Another base for this Hilbert space, this time viewed a direct sum of spaces indexed by $S \equiv S^{1,2}$, consists of the vectors

$$\boxed{\{\, |m, S\,\rangle \,\}} \qquad \text{with } S \in \{\; |\, S_1 - S_2|, |S_1 - S_2| + 1, ..., |S_1 + S_2\,\} \text{ and } \; m \in \{-S, -S + 1, ...S\,\} \tag{15.17}$$

The transformation between the two bases is described by the Clebsch-Gordan coefficients, or alternatively the Wigner $3 - j$ symbols and/or the Racah W-coefficients. We shall not present their full theory here. However, the following example will play a role in our discussion.

Among the states of a pair of equal spins, with $S_1 = S_2 = S$ there is a unique state at which the total spin is $S^{1,2} = 0$. Its classical analog is the configuration in which the two spins are exactly anti-aligned. In contrast to the classical picture of such a state, for quantum spins this situation is realizable in a unique state.

For two q-bits, i.e. $S_1 = S_2 = 1/2$, this state is

$$|m = 0, S^{1,2} = 0\rangle \;=\; \frac{1}{\sqrt{2}} \Big[\, |+,-\rangle_{1/2,1/2} - |-,+\rangle_{1/2,1/2} \,\Big] \,. \tag{15.18}$$

It provides a prime example of an entangled state.

For general values of $S_1 = S_2 = S$ the **singlet** state (so called because it spans the 1 dimensional subspace in the decomposition of the spin sum space) is

$$|m = 0, S^{1,2} = 0\rangle \;=\; \frac{1}{\sqrt{2S + 1}} \sum_{m=S}^{S} (-1)^m \, |m, -m\rangle_{S,S} \tag{15.19}$$

The rank one orthogonal projection on the dimensional space spanned by this vector is

$$P^{(0)}_{1,2} = \frac{1}{2S+1} \sum_{m,m'=-S}^{S} (-1)^{m'-m} \, |m', -m'\rangle \, \langle m, -m| \tag{15.20}$$

(in Dirac's notation). The oscillatory factor $(-1)^{m'-m} = (-1)^{m'+m}$ can be removed through a unitary transformation $U_{1,2} = U_1 \otimes U_2$ which acts on each component as $U_j \, |m\rangle_j = (-1)^m \, |m\rangle_j$.

15.5 The quantum Heisenberg spin model, and its flattened extension

A demonstration of the quantum models which have been built on the above structure, can be found in the Heisenberg spin chain. It is among the earliest quantum spin arrays for which non-trivial results were obtained (if not the first). Yet it continues to attract interest due to both new results, and perspectives, and to mathematical challenges which still remain open.

On general graphs the Hilbert space associated with the states of an array of quantum spins, of magnitude S, associated with a vertex set $\mathcal{V}$ is the tensor product space

$$\mathcal{H} = \otimes_{u \in \mathcal{V}} \mathcal{H}^{(u)}_S \, .$$

In the Heisenberg model, the Hamiltonian for such a systems is taken to be the operator

$$H := \pm \sum_{\{u,v\} \subset \mathcal{V}} \underline{S}_u \cdot \underline{S}_v = \pm \sum_{\{u,v\} \subset \mathcal{V}} \sum_{i=1}^{3} S_{i,u} \, S_{i,v} \tag{15.21}$$

with the **plus** sign corresponding to an **anti-ferromagnet** and the minus sign to a ferromagnet.

Questions of interest include the spectrum of H, and the nature of the spin spin correlations (and nowadays also quantum entanglement) in its low energy states and in its thermal equilibrium states (defined below).

The exact determination of this Hamiltonian's spectrum by H. Bethe [8], for $S = 1/2$, ushered in the Bethe-ansatz method (analyzed further in [10, 11]), which since then has found various other applications [9, 14].

For $S = 1/2$, the dot product $\underline{S}_u \cdot \underline{S}_v$ can assume only 2 values, which correspond to the two possible values of the magnitude ($S_{1,2} = 0$ or $S_{1,2} = 1$) of the sum vector $(\underline{S}_u + \underline{S}_v)$. The interaction can therefor be equivalently presented in terms of the singlet projection operator $P^{(0)}_{u,u+1}$ which was presented above. The explicit relation is

$$\mathbf{S}_u \cdot \mathbf{S}_{u+1} = \frac{1}{4} - P^{(0)}_{u,u+1} \quad \text{(in case } S_1 = S_2 = 1/2) \, . \tag{15.22}$$

(The deduction of this simple relation from (15.9) is a recommended exercise.)

The strict equivalence of the Hamiltonians based on these two interactions holds only for

$S = 1, 2$. At higher values of S the operator

$$H_{\mathrm{AF}} = -(2S+1) \sum_{u=-L+1}^{L-1} P^{(0)}_{u,u+1}\,. \tag{15.23}$$

can be viewed as a "flattened" extension of Heisenberg's anti-ferromagnetic Hamiltonian.

However, the spin chain with H_{AF} as its Hamiltonian has also been of independent interest (cf. [15, 12, 13, **?**]). In particular, it bears a surprising relation with other models, both quantum and classical (explained by the picture which will be drawn next).

15.6 Notes

`To be added`

References

Cited references are listed within the bibliography of the next section.)

16

Quantum statistical mechanics

16.1 Quantum Gibbs state

In mathematical discussions of physics the term **state** is often taken to mean an expectation value functional by which values are assigned to the systems' observables ($A \mapsto \langle A \rangle$) in a manner corresponding, in a somewhat idealized sense, to experimentally realizable protocols.

With the quantum observables being represented by self adjoint operators, the state functionals are to be: i) linear, ii) positive, and iii) normalized.

In the finite dimensional case, these conditions are met by mapping of the form

$$A \mapsto \operatorname{Tr} A\rho \tag{16.1}$$

where A ranges over self adjoint operators, Tr is the trace over the corresponding Hilbert space, and ρ (often referred to as density operator) is a positive self adjoint operator of trace 1.

The trace of an operator B can be presented in different manners, one of which is as

$$\operatorname{Tr} B = \sum_j \langle \Psi_j | \, B \, | \Psi_j \rangle \tag{16.2}$$

where $|\Psi_j\rangle$ is sampled over an arbitrary orthonormal base. It is famously independent of the choice of the basis, and has the cyclic invariance property

$$\operatorname{Tr} ABC \;=\; \operatorname{Tr} CAB \,. \tag{16.3}$$

Included in the above are **pure states**, each corresponding to a singe vector $|\Psi\rangle \in \mathcal{H}$, for which the state density operator is presentable as $\rho = |\Psi\rangle\langle\Psi|$. In such case

$$\langle A \rangle \;=\; \langle \Psi | \, B \, | \Psi \rangle \;=\; \operatorname{Tr} \left(B \, |\Psi\rangle \langle \Psi| \, \right) \tag{16.4}$$

where the equality can be viewed as an extension, enabled by Dirac's notation, of the trace cyclcity (16.3).

16.1.1 Gibbs thermal states

The Hamiltonian of a quantum system like its other observables is a self adjoint operator. Regarding its eigenvectors as microstates, a natural definition of a thermal equilibrium states is

$$\langle A \rangle_\beta := \sum_j \langle \Psi_j | A | \Psi_j \rangle \, e^{-\beta E_j} \; = \; \frac{1}{Z} \operatorname{Tr} A \, e^{-\beta H} \tag{16.5}$$

with $|\Psi_j\rangle$ the Hamiltonians eigenstates, E_j its eigenvalues, and Z the system's partition function

$$Z = \operatorname{Tr} e^{-\beta H} \, . \tag{16.6}$$

The structural analogies with classical systems are obvious. As in that case, for β very large the thermal average concentrates mainly on the low energy states, whereas for $\beta = 0$ it is given by a tracial average, which as a state is universally invariant under arbitrary unitary evolutions.

Thermodynamic functions continue to make sense, and convexity arguments which we discussed in that case continue to apply [1, 2, 3]

In particular, the the quantum pressure function for quantum extensive systems defined $\mathbb{Z}^d$, or other homogeneous graphs of finite dimension, is given by

$$\Psi(\beta, \mathcal{J}) \; := \; \lim_{L \to \infty} \frac{1}{|\Lambda(L)|} \log Z_{\Lambda(L)}(\beta, \mathcal{J}) \, , \tag{16.7}$$

for which the limit converges (cf. [1]) under conditions similar to those assumed in Theorem 5.5.

16.2 A seeding strategy for the exploration of systems' ground states

The operator $\mathrm{e}^{-\beta H}$ provides also a potentially useful tool for the analysis of the systems' ground state vectors, as those can be presented as limits of

$$|\Psi_{L,\beta}\rangle = \frac{e^{-\frac{\beta}{2} H_{AF}^{(L)}} \, |\Phi_L\rangle}{\langle \Phi_L | \, e^{-\beta H_{AF}^{(L)}} \, |\Phi_L\rangle^{1/2}} \tag{16.8}$$

starting from convenient "seed states" $|\Phi_L\rangle$.

One needs however to pay attention to the potential effects of the interchange of the two limits of interest, $\beta \to \infty$ and $L \to \infty$, and seek to identify sequences of seed states for which these commute in the weak sense. That is: seek seed states for which the following expectations values of functionals of local operators converge regardless of the order in which the limits are evaluated

$$A \mapsto \lim_{\substack{\beta \to \infty \\ L \to \infty}} \langle \Psi_{L,\beta} | \; A \; | \Psi_{L,\beta} \rangle \tag{16.9}$$

Of great help for this task is the identification of convenient bases in which the matrix elements of $e^{-\beta H_L}$ are non-negative. This is of relevance since:

i) positivity pre-empts the need to consider possible cancellations effects

ii) it allows to bring in the Perron Frobenius theorem, which we encountered already in section 9.3 (in the discussion of the transfer matrix method).

The latter, when applicable, can be used to assure that at least for each of the finite volumes the selected seed states allow to reach all the system's ground states.

16.2.1 A functional integral representation

And as in the classical case typically the Hamiltonian of an extensive quantum spin array is a sum of local operators:

$$H = -\sum_{\alpha \in \mathcal{I}} K_\alpha \,, \tag{16.10}$$

where $\mathcal{I}$ is an index set used to label the contributing local interaction terms. An example is offered by the Heisenberg model, described by (15.21).

Since typically the different terms in the Hamiltonian do not all commute with each other It is usually a non-trivial challenge to determine even just the ground state of H, and of course its thermal states. In contrast to classical systems, for quantum system the ground states are described by a function $|\Psi\rangle \in \mathcal{H}$, not just a configuration, and that raises the difficulty (even ignoring the question of degeneracy).

A tool which we shall explore here is offered by the following functional integral representation of the operator $e^{-\beta H}$

$$e^{\beta \sum_\alpha K_\alpha} \;=\; \mathbb{1} + \sum_{n=1}^{\infty} \int_{0<t_1<t_2<\ldots t_n<\beta} \sum_{\alpha_1,\ldots\alpha_n} \mathcal{T}\left(\prod_{j=1}^{n} K_{\alpha_j,t_j} \right) dt_1 \ldots dt_n \,. \tag{16.11}$$

where $\mathcal{T}$ is the time ordering operator, which arranges the collection of non-commuting terms in the order of t_j, as in:

$$\mathcal{T}\left(\prod_{j=1}^{n} K_{\alpha_j,t_j} \right) = K_{\alpha_n,t_n} \cdot \ldots \cdot K_{\alpha_2,t_2} \cdot K_{\alpha_1,t_1} \,. \tag{16.12}$$

For a proof of (16.11) one may sum up the expression on the right and note that[1]

$$\text{RHS of (16.11)} = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} (-H)^n \;=\; e^{-\beta H} \,. \tag{16.13}$$

Our next step is to give (16.11) a probabilistic flavor. Pulling our the factor of $e^{\beta|\mathcal{I}|}$, the sum & integral on the right can be presented as a probability average of the time ordered product of operators, associated with a Poisson random point process over the set $\mathcal{I} \times [0,\beta]$, whose points

[1] Alternatively, one may regard (16.11) as the Dyson expansion of the solution of the differential equation for $\beta \mapsto e^{-\beta H}$.

(α, t) are associated with the action of K_α at "time" t:

$$e^{\beta \sum_\alpha K_\alpha} = e^{\beta|\mathcal{G}|} \sum_{n=0}^{\infty} \int_{0<t_1<\cdots<t_n<\beta} \left[\sum_{\alpha\in\mathcal{G}} K_\alpha \right]^n \mathrm{d}t_1 \ldots \mathrm{d}t_n$$

$$= e^{\beta|\mathcal{G}|} \int_{\Omega_{\mathcal{G},\beta}} \mathcal{T}\left(\prod_{j=1}^{|\omega|} K_{\alpha_j,t_j} \right) \rho_{\mathcal{G},\beta}(\mathrm{d}\omega) \tag{16.14}$$

In the second line, the integral represents the expectation value with respect to a Poisson point process on $\mathcal{G} \times [0,\beta]$ whose configurations $\omega \in \Omega_{\mathcal{G},\beta}$ are presented as $\omega = \{(\alpha_j, t_j)\}_{j=1}^{|\omega|}$. The corresponding probability measure on $\Omega_{\mathcal{G},\beta}$ is written as $\rho_{\mathcal{G},\beta}(\mathrm{d}\omega)$

Under this representation the partition function $Z_{\Lambda,\beta} = \mathrm{Tr}\, e^{-\beta H}$ is given by

$$\boxed{Z_{\Lambda,\beta} = e^{\beta|\mathcal{G}|} \int_{\Omega_{\mathcal{G},\beta}} \mathrm{Tr}\left[\mathcal{T}\left(\prod_{j=1}^{|\omega|} K_{\alpha_j,t_j} \right)\right] \rho_{\mathcal{G},\beta}(\mathrm{d}\omega}\,. \tag{16.15}$$

And for any vector $|\Phi\rangle \in \mathcal{H}$

$$\boxed{\langle\Phi|\, e^{\beta H_\Lambda}\, |\Phi\rangle = e^{\beta|\mathcal{G}|} \int_{\Omega_{\mathcal{G},\beta}} \langle\Phi| \left[\mathcal{T}\left(\prod_{j=1}^{|\omega|} K_{\alpha_j,t_j} \right)\right] |\Phi\rangle\ \rho_{\mathcal{G},\beta}(\mathrm{d}\omega)\,.} \tag{16.16}$$

The above expansion into the average over configurations ω casts the ground states of d-dimensional quantum spin arrays in a form which resembles statistical mechanics in $(d + 1)$ dimensions [7, **?**]. This representations is particularly useful as a tool in case the integrand can be transformed into positive real function of ω. We shall next see some examples where that turns out to be the case.

16.3 A specific example

To get a sense of the possibilities which the above representation leads to, consider the case of a one-dimensional spin array of spins of magnitude S, attached to the sites of $\Lambda_L = \{-L, -l+1, ..., L\}$, with the Hamiltonian given by with the "flattened" anti-ferromagnetic interaction (15.23) (which explained there)

$$H_{\mathrm{AF}} = -(2S + 1) \sum_{u=-L+1}^{L-1} P^{(0)}_{u,u+1}\,. \tag{16.17}$$

Each of the individual terms in this sum affects the state vector of a neighboring pair, on which its acts as

$$(2S+1)\,P^{(0)}_{1,2} = \sum_{m,m'=-S}^{S} (-1)^{m'-m}\,|m',-m'\rangle\,\langle m,-m|$$
$$= U_L \left[\sum_{m,m'=-S}^{S} |m',-m'\rangle\,\langle m,-m| \right] U_L^* \tag{16.18}$$

where U_L is the unitary operator introduced next to (15.20) under which the oscillatory factors disappear.

The matrix elements of $\langle\Psi|\,e^{-\beta H_{AF}}\,|\Psi\rangle$ are particularly simple to trace when the this operators is applied to the following "seed vector"

$$|D_L\rangle := \bigotimes_{j=1}^{L} \Big(\sum_{m=-S}^{S} (-1)^m\,|m,-m\rangle_{-L+2j-1,-L+2j} \Big)$$
$$= U_L \bigotimes_{j=1}^{L} \Big(\sum_{m=-S}^{S} |m,-m\rangle_{-L+2j-1,-L+2j} \Big). \tag{16.19}$$

The state vector $|D_L\rangle$ describes what may be called a "dimerized state" in which the spins in $\Lambda_L = \{-L+1,\ldots,L-1,L\}$ are linked pairwise into the ground states of the projection $P^{(0)}_{u,u+1}$ corresponding to the linked pairs. The "drama" here is that there is no state in which all pairs are linked in this manner.

More explicitly: in the absence of a frustration-free state (i.e. one in which all pairs are in the ground state of their pair interaction) the state vector $|D_L\rangle$ offers a natural starting point for the seed strategy presented in (16.9). However, the local structure of the dimerized state changes between the even and odd values of L as $L \to \infty$.

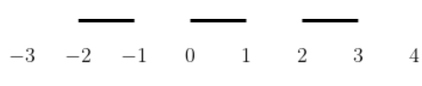

Figure 16.1 The natural pairing or $\Lambda_L = \{-L+1,\ldots,L-1,L\}$ which is used for for the odd / even seed vectors (here $L = 3,4$). Notice the difference at $u = 0$.

In this case, the interaction terms are

$$K_{u,u+1} = (2S+1)\,P^{(0)}_{u,u+1}\,, \tag{16.20}$$

The matrix elements of $\langle D_L|\prod_{j=1}^{|\omega|} K_{\alpha_j,t_j}\,|_L\rangle$ which contribute in the expansion (16.23) do not vanish if and only if at each incident at which an interaction term appears, the values of m_u, m_{u+1} before and after satisfy

$$m_u + m_{u+1} = 0 \ \text{, and (independently)} \qquad m'_u + m'_{u+1} = 0\ . \tag{16.21}$$

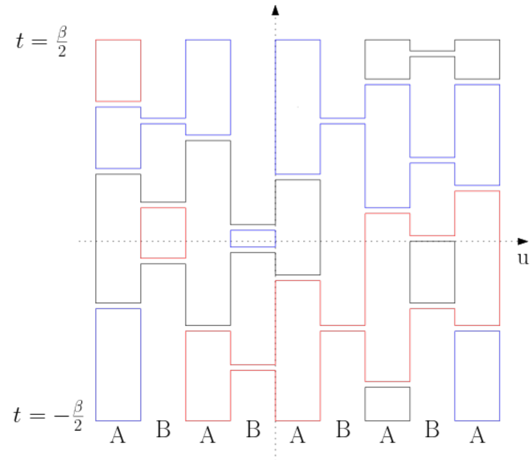

Figure 16.2 A configuration of randomly placed horizontal rungs and the resulting loops by which ithe matrix elements $\langle D_L | \prod_{j=1}^{|\omega|} K_{\alpha_j, t_j} |_L\rangle$ for the Hamiltonian H_{AF} are shown to be given by $(2S+1)^{N_\ell(\omega)}$.

and, in the natural orthonormal basis transformed by U_L, the contributing factor is 1 if the condition is met.

Counting such consistent configurations, one may note that we get a factor of $(2S+1)$ (the number of accessible values of $m \in \{-S, -S+1, ..., S\}$) per loop. From which it follows that

$$\langle D_L | \prod_{j=1}^{|\omega|} K_{\alpha_j, t_j} |D_L\rangle = (2S+1)^{N_\ell(\omega)} \tag{16.22}$$

with $N_\ell(\omega)$ the number of loops generated by ω.

Thus

$$\boxed{\langle \Phi | e^{\beta H_\Lambda} |\Phi\rangle = e^{\beta|\mathcal{G}|} \int_{\Omega_{\mathcal{G},\beta}} (2S+1)^{N_\ell(\omega)} \rho_{\mathcal{G},\beta}(d\omega)\,.} \tag{16.23}$$

One may note in the above expression an eery resemblance to the partition function of a planar Fortuin-Kasteleyn random cluster model at (!), for which the analog of the loops of ω are the loops which pass between the connected clusters of the model and those of its dual. In the present case the duality is between the A and B connected clusters, in the sense indicated in Figure 16.2. The corresponding values of the $H_A F$ and FG modele are

$$(2S+1) \Longleftrightarrow \sqrt{Q}\,. \tag{16.24}$$

Furthermore, in this stochastic-geometric representation of the present model the present case the spin-spin correlation of in the state $|\Psi_{L,\beta}\rangle$ seeded by $|D\rangle_L$, as in (16.8), reduces, up to a deterministic oscillatory factor, to the loop-weighted probability that the two sites are (at an equal time) on the same loop of ω:

$$\langle\psi_{L,\beta}|\,\underline{S}_x\cdot\underline{S}_y\,|\psi_{L,\beta}\rangle \;=\; (-1)^{x-y}\;C_S\;\frac{\int_{\Omega_{\mathcal{G},\beta}} \mathbb{1}[(x,0)\stackrel{\omega}{\longleftrightarrow}(y,0)]\;(2S+1)^{N_\ell(\omega)}\;\rho_{\mathcal{G},\beta}(\mathrm{d}\omega)}{\int_{\Omega_{\mathcal{G},\beta}}(2S+1)^{N_\ell(\omega)}\;\rho_{\mathcal{G},\beta}(\mathrm{d}\omega)}\,. \qquad (16.25)$$

with

$$C_S \;=\; 3\cdot\frac{1}{2S+1}\sum_{m\in\{-S,-S+1,\dots,S\}} m^2 \qquad (16.26)$$

where the alternating sign is due to the fact that the rules (16.21) constrain $(-1)^u S_{3,u}$ to assume only equal values between connected sites of $\Lambda\times[0,\beta]$, with no correlation in their spins if the two are not connected.

This relation between a purely stochastic geometric random system of loops and the quantum spin model, echoes the relation between the FK random cluster model, and the Q-state Potts model, at integer values of Q.

However, whereas the classical Potts spin correlations correspond to the probability that the two sites in the same connected cluster the quantum spin correlations correspond to the probability that the sites lie along the boundary of a connected cluster - of the model or its dual.

Further analysis links the interesting changes which occur in the two cases as the parameters mentioned in (16.24) cross the value 2:

i) In the quantum H_{AF} model: for $S = 1/2$ the even and odd seeded states converge, in the limit $L,\beta\to\infty$, to a common limiting ground state, in which the above long-range order is replaced by a slow decay of spin-spin correlation (which decay by only a power law, as calculated by Bethe). In contrast: for $S > 1/2$ the H_{AF}'s even and odd seeded ground states converge separately to a pair of distinct infinite volume ground states, each of exponential decay of correlations.

ii) In the classical FK random cluster model, for $Q > 4$ the system exhibits a discontinuity in its magnetization which at the model's critical point jumps from $M(\beta_c - 0) = 0$ to $M(\beta_c + 0 > 0$.

Given the similarities of the relevant loop models, one could expect a relation between these phenomena. Both occur where $(2S+1)$ and, correspondingly $\sqrt{Q}$, cross the value 2. Indeed the two phenomena are linked. And their proofs are simplified by arguments which repeatedly cross between the classical and quantum projections of their common stochastic geometric scaffolding.

Further discussion of this relation, and perspective, can be found in [17], and references therein.

Notes

`To be expanded.`

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