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LECTURES ON MATHEMATICAL STATISTICAL MECHANICS

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Preface

In these notes we give an introduction to mathematical statistical mechanics, based on the six lectures given at the *Max Planck institute for Mathematics in the Sciences* February/March 2006. The material covers more than what has been said in the lectures, in particular examples and some proofs are worked out as well the Curie-Weiss model is discussed in section 9.3. The course partially grew out of lectures given for final year students at the University College Dublin in spring 2004. Parts of the notes are inspired from notes of Joe Pulé at University College Dublin.

The aim is to motivate the theory of Gibbs measures starting from basic principles in classical mechanics. The first part covers Sections 1 to 5 and gives a route from physics to the mathematical concepts of Gibbs ensembles and the thermodynamic limit. The Sections 6 to 8 develop a mathematical theory for Gibbs measures. In Subsection 6.4 we give a proof of the existence of phase transitions for the two-dimensional Ising model via Peierls arguments. Translation invariant Gibbs measures are characterised by a variational principle, which we outline in Section 7. Section 8 gives a quick introduction to the theory of large deviations, and Section 9 covers some models of statistical mechanics. The part about Gibbs measures is an excerpt of parts of the book by Georgii ([Geo88]). In these notes we do not discuss Boltzmann's equation, nor fluctuations theory nor quantum mechanics.

Some comments on the literature. More detailed hints are found throughout the notes. The books [Tho88] and [Tho79] are suitable for people, who want to learn more about the physics behind the theory. A standard reference in physics is still the book [Hua87]. The route from microphysics to macrophysics is well written in [Bal91] and [Bal92]. The old book [Kur60] is nice for starting with classical mechanics developing axiomatics for statistical mechanics. The following books have a higher level with special emphasis on the mathematics. The first one is [Khi49], where the setup for the microcanonical measures is given in detail (although not in used modern manner). The standard reference for mathematical statistical mechanics is the book [Rue69] by Ruelle. Further developments are in [Rue78] and [Isr79]. The book [Min00] contains notes for a lecture and presents in detail the two-dimensional Ising model and the Pirogov-Sinai theory, the latter we do not study here. A nice overview of deep questions in statistical mechanics gives [Gal99], whereas [Ell85] and [Geo79],[Geo88] have their emphasis on probability theory and large deviation theory. The book [EL02] gives a very nice introduction to the philosophical background as well as the basic skeleton of statistical mechanics.

I hope these lectures will motivate further reading and perhaps even further research in this interesting field of mathematical physics and stochastics. Many thanks to Thomas Blesgen for reading the manuscript. In particular I thank Tony Dorlas, who gave valuable comments and improvements.

Leipzig, Easter 2006 *Stefan Adams*

1 Introduction

The aim of equilibrium Statistical Mechanics is to derive all the equilibrium properties of a macroscopic system from the dynamics of its constituent particles. Thus its aim is not only to derive the general laws of thermodynamics but also the thermodynamic functions of a given system. Mathematical Statistical Mechanics has originated from the desire to obtain a mathematical understanding of a class of physical systems of the following nature:

• The system is an assembly of identical subsystems.
• The number of subsystems is large ($N \sim 10^{23}$, Avogardo's number 6.023×10^{23}, e.g. $1cm^3$ of hydrogen contains about 2.7×10^{19} molecules/atoms).
• The interactions between the subsystems are such as to produce a thermodynamic behaviour of the system.

Thermodynamic behaviour is phenomenological and refers to a macroscopic description of the system. Now "macroscopic description" is operationally defined in the way that subsystems are considered as small and not individually observed.

Thermodynamic behaviour:

(1) Equilibrium states are defined operationally. A state of an isolated system tends to an equilibrium state as time tends to $+\infty$ (*approach to equilibrium*).
(2) An equilibrium state of a system consists of one or more macroscopically homogeneous regions called *phases*.
(3) Equilibrium states can be parametrised by a finite number of thermodynamic parameters (e.g. temperature, volume, density, etc) which determine the thermodynamic functions (e.g. free energy, pressure, entropy, magnetisation, etc).

It is believed that the thermodynamic functions depend piecewise analytical (or smoothly) on the parameters and that singularities correspond to changes in the phase structure of the system (*phase transitions*). Classical thermodynamics consists of laws governing the dependence of the thermodynamic functions on the experimental accessible parameters. These laws are derived from experiments with macroscopic systems and thus are not derived from a microscopic description. Basic principles are the zeroth, first and second law as well as the equation of state for the ideal gas.

The art of the mathematical physicist consists in finding a mathematical justification for the statements (1)-(3) from a microscopic description. A microscopic complete information is not accessible and is not of interest. Hence, despite the determinism of the dynamical laws for the subsystems, random-

ness comes into play due to lack of knowledge (*macroscopic description*). The large number of subsystems is replaced in a mathematical idealisation by infinitely many subsystems such that the extensive quantities are scaled to stay finite in that limit. Stochastic limit procedures as the law of large numbers, central limit theorems and large deviations principles will provide appropriate tools. In these notes we will give a glimpse of the basic concepts. In the second chapter we are concerned mainly with the Mechanics in the name Statistical Mechanics. Here we motivate the basic concepts of ensembles via Hamilton equations of motions as done by Boltzmann and Gibbs.

2 Ergodic theory

2.1 Microscopic dynamics and time averages

We consider in the following N identical classical particles moving in $\mathbb{R}^d, d \geq 1$, or in a finite box $\Lambda \subset \mathbb{R}^d$. We idealise these particles as point masses having the mass m. All spatial positions and momenta of the single particles are elements in the *phase space*

$$\Gamma = \big(\mathbb{R}^d \times \mathbb{R}^d\big)^{2N} \quad \text{or} \quad \Gamma_\Lambda = \big(\Lambda \times \mathbb{R}^d\big)^{2N}. \tag{2.1}$$

Specify, at a given instant of time, the values of positions and momenta of the N particles. Hence, one has to specify $2dN$ coordinate values that determine a single point in the phase space Γ respectively Γ_Λ. Each single point in the phase space corresponds to a *microscopic state* of the given system of N particles. Now the question arises whether the $2dN-$ dimensional continuum of microscopic states is reasonable. Going back to Boltzmann [Bol84] it seems that at that time the $2dN-$ dimensional continuum was not really deeply accepted ([Bol74], p. 169):

> *Therefore if we wish to get a picture of the continuum in words, we first have to imagine a large, but finite number of particles with certain properties and investigate the behaviour of the ensembles of such particles. Certain properties of the ensemble may approach a definite limit as we allow the number of particles ever more to increase and their size ever more to decrease. Of these properties one can then assert that they apply to a continuum, and in my opinion this is the only non-contradictory definition of a continuum with certain properties...*

and likewise the phase space itself is really thought of as divided into a finite number of very small *cells* of essentially equal dimensions, each of which

determines the position and momentum of each particle with a maximum precision. Here the maximum precision that the most perfect measurement apparatus can possibly provide is meant. Thus, for any position and momentum coordinates

$$\delta p_i^{(j)} \delta q_i^{(j)} \geq h, \qquad \text{for } i = 1, \ldots, N, j = 1, \ldots, d,$$

with $h = 6,62 \times 10^{-34}$ Js being Planck's constant. Microscopic states of the system of N particles should thus be represented by phase space cells consisting of points in $\mathbb{R}^{2dN}$ (positions and momenta together) with given centres and cell volumes h^{dN}. In principle all what follows should be formulated within this cell picture, in particular when one is interested in an approach to the quantum case. However, in this lectures we will stick to the mathematical idealisation of the $2dN$ continuum of the microscopic states, because all important properties remain nearly unchanged upon going over to the phase cell picture.

Let two functions $W\colon \mathbb{R}^d \to \mathbb{R}$ and $V\colon \mathbb{R}_+ \to \mathbb{R}$ be given. The energy of the system of N particles is a function of the positions and momenta of the single particles, and it is called **Hamiltonian** or **Hamilton function**. It is of the form

$$H(q,p) = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + W(q_i) \right) + \sum_{1 \leq i < j \leq N} V(|q_i - q_j|), \tag{2.2}$$

where $q = (q_1, \ldots, q_N), p = (p_1, \ldots, p_N)$. Here, the function W is called the **external-potential** at the spatial positions due to external forces (walls, pressure,...) or external fields (gravitation, magnetic field,...), and the function V is called the **pair potential**, depending only on the spatial distances of each pair of particles. Also more general many-particle interaction potentials can be considered (see [Rue69] for details). In the following we assume that the Hamiltonian $H\colon \Gamma \to \mathbb{R}$ is twice continuously differentiable and we abbreviate $n = dN$. The phase space dynamics is governed by **Hamilton's equations of motion**

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad i = 1, \ldots, N, \tag{2.3}$$

where the dot denotes as usual differentiation with respect to the time variable. If J denotes the $2n \times 2n$ matrix

$$\begin{pmatrix} 0 & \mathbb{1}_n \\ -\mathbb{1}_n & 0 \end{pmatrix},$$

$\mathbb{1}_n$ the identity in $\mathbb{R}^n$, the Hamilton vector field is given as

$$v\colon \Gamma \to \Gamma,\ x \mapsto J\nabla H(x)$$

with $x = (q,p) \in \mathbb{R}^{2n}$ and

$$\nabla H(x) = \Big(\frac{\partial H}{\partial q_1}, \dots, \frac{\partial H}{\partial q_N}, \frac{\partial H}{\partial p_1} \dots, \frac{\partial H}{\partial p_N}\Big).$$

With the vector field v we associate the differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) = v(x(t)), \tag{2.4}$$

where $x(t)$ denotes a single microstate of the system for any time $t \in \mathbb{R}$. For each point $x \in \Gamma$ there is one and only one function $x\colon \mathbb{R} \to \Gamma$ such that $x(0) = x$ and $\frac{\mathrm{d}x(t)}{\mathrm{d}t} = v(x(t))$ for any $t \in \mathbb{R}$. For any $t \in \mathbb{R}$ we define a phase space map

$$\phi_t\colon \Gamma \to \Gamma,\ x \mapsto \phi_t(x) = x(t).$$

From the uniqueness property we get that $\Phi = \{\phi_t\colon t \in \mathbb{R}\}$ is a one-parameter group which is called a **Hamiltonian flow**. Hamiltonian flows have the following property.

Lemma 2.1 *Let Φ be a Hamiltonian flow with Hamiltonian H, then any function $F = f \circ H$ of H is invariant under ϕ:*

$$F \circ \phi_t = F$$

for all $t \in \mathbb{R}$.

Proof. The proof follows from the chain rule and $\langle x, Jx\rangle = 0$. Recall that if $G : \mathbb{R}^n \to \mathbb{R}^m$ then $G'(x)$ is the $m \times n$ matrix

$$\left(\frac{\partial G_i}{\partial x_j}(x)\right)_{\substack{i=1,\dots,m\\ j=1,\dots,n}} \qquad \text{for } x \in \mathbb{R}^n.$$

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} F(\phi_t(x)) &= F'(\phi_t(x)) \frac{\mathrm{d}\phi_t}{\mathrm{d}t}(x) \\
&= f'(H(\phi_t(x)))\ H'(\phi_t(x))\ \frac{\mathrm{d}\phi_t}{\mathrm{d}t}(x) \\
&= f'(H(\phi_t(x)))\ (\nabla H(\phi_t(x)))^T\ \frac{\mathrm{d}\phi_t}{\mathrm{d}t}(x) \\
&= f'(H(\phi_t(x)))\ \langle \nabla H(\phi_t(x)),\ \frac{\mathrm{d}\phi_t}{\mathrm{d}t}(x)\rangle \\
&= f'(H(\phi_t(x)))\ \langle \nabla H(\phi_t(x))\ ,\ J\ \nabla H(\phi_t(x))\rangle.
\end{aligned}$$

□

The following theorem is the well known Liouville's Theorem.

Theorem 2.2 (Liouville's Theorem) *The Jacobian* $|\det \phi_t'(x)|$ *of a Hamiltonian flow is constant and equal to* 1.

Proof. Let $M(t)$ and $A(t)$ be linear mappings such that

$$\frac{\mathrm{d}M(t)}{\mathrm{d}t} = A(t)M(t)$$

for all $t \geq 0$, then

$$\det M(t) = \det M(0) \exp\Big(\int_0^t \text{ trace } A(s)\mathrm{d}s\Big).$$

Now

$$\frac{\mathrm{d}\phi_t(x)}{\mathrm{d}t} = (v \circ \phi_t)(x).$$

Thus

$$\frac{\mathrm{d}\phi_t'(x)}{\mathrm{d}t} = v'(\phi_t(x))\phi_t'(x)$$

so that $\det \phi_t'(x) = \exp \int_0^t \text{trace } v'(\phi_s(x))\mathrm{d}s$ because $\phi_0'(x)$ is the identity map on Γ. Now

$$v(x) = J\ \nabla H(x) \text{ and } v'(x) = JH''(x),$$

where $H''(x) = \left(\frac{\partial^2 H}{\partial x_i \partial x_j}\right)$ is the *Hessian* of H at x. Since H is twice continuously differentiable, $H''(x)$ is symmetric. Thus

$$\begin{aligned}\text{trace } (JH''(x)) &= \text{trace}((JH''(x))^T) = \text{trace } ((H''(x))^T J^T) \\ &= \text{trace } (H''(x)(-J)) = -\text{trace } (JH''(x)).\end{aligned}$$

Therefore trace $(JH''(x)) = 0$ and $\det(\phi_t'(x)) = 1$. □

From Lemma 2.1 and Theorem 2.2 it follows that a probability measure on the phase space Γ, i.e., an element of the set $\mathcal{P}(\Gamma, \mathcal{B}_\Gamma)$ of probability measure on Γ with Borel $\sigma-$algebra $\mathcal{B}_\Gamma$, whose Radon-Nikodym density with respect to the Lebesgue measure is a function of the Hamiltonian H alone is stationary with respect to the Hamiltonian flow $\Phi = \{\phi_t \colon t \in \mathbb{R}\}$.

Corollary 2.3 *Let* $\mu \in \mathcal{P}(\Gamma, \mathcal{B}_\Gamma)$ *with density* $\rho = F \circ H$ *for some function* $F \colon \mathbb{R} \to \mathbb{R}$ *be given, ie.,* $\mu(A) = \int_A \rho(x)\mathrm{d}x$ *for any* $A \in \mathcal{B}_\Gamma$. *Then*

$$\mu \circ \phi_t^{-1} = \mu \quad \textit{for any } t \in \mathbb{R}.$$

Proof. We have

$$\mu(A) = \int_\Gamma \mathbb{1}_A(x)\rho(x)\mathrm{d}x = \int_\Gamma \mathbb{1}_A(\phi_t(x))\rho(\phi_t(x))|\det \phi_t'(x)|\mathrm{d}x$$
$$= \int_\Gamma \mathbb{1}_{\phi_t^{-1}A}(x)\rho(x)\mathrm{d}x = \mu(\phi_t^{-1}A). \qquad \square$$

For such a stationary probability measure one gets a unitary group of time evolution operators in an appropriate Hilbert space as follows.

Theorem 2.4 (Koopman's Lemma:) *Let Γ_1 be a subset of the phase space Γ invariant under the flow Φ, i.e., $\phi_t\Gamma_1 \subset \Gamma_1$ for all $t \in \mathbb{R}$. Let $\mu \in \mathcal{P}(\Gamma_1, \mathcal{B}_{\Gamma_1})$ be a probability measure on Γ_1 stationary under the flow Φ that is $\mu \circ \phi_t^{-1} = \mu$ for all $t \in \mathbb{R}$. Define $U_t f = f \circ \phi_t$ for any $t \in \mathbb{R}$ and any function $f \in L^2(\Gamma_1, \mu)$, then $\{U_t \colon t \in \mathbb{R}\}$ is a unitary group of operators in the Hilbert space $L^2(\Gamma_1, \mu)$.*

Proof. Since $U_t U_{-t} = U_0 = I$, U_t is invertible and thus we have to prove only that U_t preserves inner products.

$$\langle U_t f, U_t g\rangle = \int \overline{(f \circ \phi_t)}(x)(g \circ \phi_t(x)\mu(\mathrm{d}x) = \int (\bar{f}g)(\phi_t(x))\mu(\mathrm{d}x)$$
$$= \int (\bar{f}g)(x)(\mu \circ \phi_t^{-1})(\mathrm{d}x) = \int (\bar{f}g)(x)\mu(\mathrm{d}x) = \langle f, g\rangle.$$

$\square$

Remark 2.5 (Boundary behaviour) *If the particles move inside a finite volume box $\Lambda \subset \mathbb{R}^d$ according to the equations* (2.3) *respectively* (2.4)*; these equations of motions do not hold when one of the particles reaches the boundary of Λ. Therefore it is necessary to add to theses equations some rules of reflection of the particles from the inner boundary of the domain Λ. For example, we can consider the elastic reflection condition: the angle of incidence is equal to the angle of reflection. Formally, such a rule can be specified by a boundary potential V_{bc}.*

We discuss briefly Boltzmann's Proposal for calculating measured values of **observables**. Observables are bounded continuous functions on the phase space. Let Γ_1 be a subset of phase space invariant under the flow Φ, i.e. $\phi_t\Gamma_1 \subset \Gamma_1$ for all $t \in \mathbb{R}$. Suppose that $f : \Gamma \to \mathbb{R}$ is an observable and suppose that the system is in Γ_1 so that it never leaves Γ_1. Boltzmann proposed that when we make a measurement it is not sharp in time but takes place over

a period of time which is long compared to say times between collisions. Therefore we can represent the observed value by

$$\bar{f}(x) = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t (f \circ \phi_t)(x).$$

Suppose that μ is a probability measure on Γ_1 invariant with respect to ϕ_t then

$$\begin{aligned}
\int_{\Gamma_1} \bar{f}(x)\mu(\mathrm{d}x) &= \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t \int_{\Gamma_1} (f \circ \phi_t)(x)\mu(\mathrm{d}x) \\
&= \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t \int_{\Gamma_1} f(x)(\mu \circ \phi_t^{-1})(\mathrm{d}x) \\
&= \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t \int_{\Gamma_1} f(x)\mu(\mathrm{d}x) \\
&= \int_{\Gamma_1} f(x)\mu(\mathrm{d}x).
\end{aligned}$$

Assume now that the observed value is independent of where the system is at $t = 0$ in Γ_1, i.e. if $\bar{f}(x) = \bar{f}$ for a constant $\bar{f}$, then

$$\int_{\Gamma_1} \bar{f}(x)\mu(\mathrm{d}x) = \int_{\Gamma_1} \bar{f}\mu(\mathrm{d}x) = \bar{f}.$$

Therefore

$$\bar{f} = \int_{\Gamma_1} f(x)\mu(\mathrm{d}x).$$

We have made two assumptions in this argument:

(1) $\lim_{T\to\infty} \frac{1}{T} \int_{-T}^{T} \mathrm{d}t (f \circ \phi_t)(x)$ exists.

(2) $\bar{f}(x)$ is constant on Γ_1.

Statement (1) has been proved by Birkhoff (Birkhoff's pointwise ergodic theorem (see section 2.3 below)): $\bar{f}(x)$ exists almost everywhere. We shall prove a weaker version of this, Von Neumann's ergodic theorem.
Statement (2) is more difficult and we shall discuss it later.

The continuity of the Hamiltonian flow entails that for each $f \in \mathcal{C}_{\mathrm{b}}(\mathbb{R}^d)$ and each $x \in \Gamma$ the function

$$f_x \colon \mathbb{R} \to \mathbb{R}, \mapsto f_x(t) = f(x(t)) \tag{2.5}$$

is a continuous function of the time t. For any time dependent function φ we define the following limit

$$\langle\overline{\varphi}\rangle := \lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\mathrm{d}t\varphi(t) \tag{2.6}$$

as the time average.

2.2 Boltzmann's heuristics and ergodic hypothesis

Boltzmann's argument (1896-1898) for the introduction of ensembles in statistical mechanics can be broken down into steps which were unfortunately entangled.

1. Step: Find a set of time dependent functions φ which admit an invariant mean $\langle\overline{\varphi}\rangle$ like (2.6).

2. Step: Find a reasonable set of observables, which ensure that the time average of each observable over an orbit in the phase space is independent of the orbit.

Let $\mathcal{C}_{\mathrm{b}}(\mathbb{R})$ be the set of all bounded continuous functions on the real line $\mathbb{R}$, equip it with the supremum norm $||\varphi||_\infty = \sup_{t\in\mathbb{R}}|\varphi(t)|$, and define

$$\mathcal{M} = \Big\{\varphi\in\mathcal{C}_{\mathrm{b}}(\mathbb{R})\colon \langle\overline{\varphi}\rangle = \lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\mathrm{d}t\varphi(t)\ \text{ exists }\Big\}. \tag{2.7}$$

Lemma 2.6 *There exist positive linear functionals $\lambda\colon\mathcal{C}_{\mathrm{b}}(\mathbb{R})\to\mathbb{R}$, normalised to 1, and invariant under time translations, i.e., such that*

(i) $\lambda(\varphi)\geq 0$ *for all* $\varphi\in\mathcal{M}$,

(ii) λ *linear,*

(iii) $\lambda(\mathbf{1}) = 1$,

(iv) $\lambda(\varphi_s) = \lambda(\varphi)$ *for all* $s\in\mathbb{R}$, *where* $\varphi_s(t) = \varphi(t-s), t, s\in\mathbb{R}$,

such that $\lambda(\varphi) = \lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\mathrm{d}t\varphi(t)$ *for all* $\varphi\in\mathcal{C}_{\mathrm{b}}(\mathbb{R})$ *where this limit exists.*

Our time evolution

$$(t,x)\in\mathbb{R}\times\Gamma\mapsto\phi_t(x) = x(t)$$

is continuous, and thus we can substitute f_x in (2.5) for φ in the above result. This allows to define averages on observables as follows.

Lemma 2.7 *For every $f \in \mathcal{C}_{\mathrm{b}}(\Gamma)$ and every $x \in \Gamma$, there exists a time-invariant mean λ_x given by*

$$\lambda_x \colon \mathcal{C}_{\mathrm{b}}(\Gamma) \to \mathbb{R}, f \mapsto \lambda_x(f) = \lambda(f_x),$$

with λ_x depending only on the orbit $\{x(t) \colon t \in \mathbb{R}, x(0) = x\}$.

For any $E \in \mathbb{R}_+$ let

$$\Sigma_E = \{(q,p) \in \Gamma \colon \ : H(q,p) = E\}$$

denote the **energy surface** for the energy value E for a given Hamiltonian H for the system of N particles.

The strict ergodicity hypothesis

The energy surface contains exactly one orbit, i.e. for every $x \in \Gamma$ and $E \geq 0$

$$\{x(t) \colon t \in \mathbb{R}, x(0) = x\} = \Sigma_E.$$

There is a more realistic mathematical version of this conjecture.

The ergodicity hypothesis

Each orbit in the phase space is dense on its energy surface, i.e. $\{x(t) \colon t \in \mathbb{R}, x(0) = x\}$ is a dense subset of Σ_E.

2.3 Formal Response: Birkhoff and von Neumann ergodic theories

We present in this section briefly the important results in the field of ergodic theory initiated by the ergodic hypothesis. For that we introduce the notion of a classical dynamical system.

Notation 2.8 (Classical dynamical system) *A classical dynamical system is a quadruple $(\Gamma, \mathcal{F}, \mu; \Phi)$ consisting of a probability space $(\Gamma, \mathcal{F}, \mu)$, where $\mathcal{F}$ is a $\sigma-$algebra on Γ, and a one-parameter (additive) group $\mathcal{T}$ ($\mathbb{R}$ or $\mathbb{Z}$) and a group Φ of actions, $\phi \colon \mathcal{T} \times \Gamma \to \Gamma, (t,x) \mapsto \phi_t(x)$, of the group $\mathcal{T}$ on the phase space Γ, such that the following holds.*

(a) $f_{\mathcal{T}} \colon \mathcal{T} \times \Gamma \to \mathbb{R}, (t,x) \mapsto f(\phi_t(x))$ *is measurable for any measurable* $f \colon \Gamma \to \mathbb{R}$,

(b) $\phi_t \circ \phi_s = \phi_{t+s}$ *for all* $s, t \in \mathcal{T}$,

(c) $\mu(\phi_t(A)) = \mu(A)$ *for all* $t \in \mathcal{T}$ *and* $A \in \mathcal{F}$.

Theorem 2.9 (Birkhoff) *Let* $(\Gamma, \mathcal{F}, \mu; \Phi)$ *be a classical dynamical system. For every* $f \in L^1(\Gamma, \mathcal{F}, \mu)$*, let*

$$\lambda_x^T(f) = \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t f(\phi_t(x)).$$

Then there exists an event $A_f \in \mathcal{F}$ *with* $\mu(A_f) = 1$ *such that*

(i) $\lambda_x(f) = \lim_{T\to\infty} \lambda_x^T(f)$ *exists for all* $x \in A_f$,

(ii) $\lambda_{\phi_t(x)}(f) = \lambda_x(f)$ *for all* $(t, x) \in \mathbb{R} \times A_f$,

(iii)

$$\int_\Gamma \mu(\mathrm{d}x)\lambda_x(f) = \int_\Gamma \mu(\mathrm{d}x) f(x).$$

Proof. [Bir31] or in the book [AA68]. □

Note that in Birkhoff's Theorem one has convergence almost surely. There exists a weaker version, the following ergodic theorem of von Neumann. We restrict in the following to classical dynamical system with $\mathcal{T} = \mathbb{R}$, the real time. Let $\mathcal{H} = L^2(\Gamma_1, \mathcal{F}, \mu)$ and define $U_t f = f \circ \phi_t$ for any $f \in \mathcal{H}$. Then by Koopman's lemma U_t is unitary for any $t \in \mathbb{R}$.

Theorem 2.10 (Von Neumann's Mean Ergodic Theorem) *Let*

$$\mathcal{M} = \{f \in \mathcal{H} \colon U_t f = f \quad \forall \quad t \in \mathbb{R}\},$$

then for any $g \in \mathcal{H}$,

$$g_T := \frac{1}{T} \int_0^T \mathrm{d}t U_t g$$

converges to Pg *as* $T \to \infty$*, where* P *is the orthogonal projection onto* $\mathcal{M}$.

For the proof of this theorem we need the following discrete version.

Theorem 2.11 *Let* $\mathcal{H}$ *be a Hilbert space and let* $U \colon \mathcal{H} \to \mathcal{H}$ *be an unitary operator. Let* $\mathcal{N} = \{f \in \mathcal{H} \colon Uf = f\} = \ker(U - I)$ *then*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N-1} U^n g = Qg$$

where Q *is the orthogonal projection onto* $\mathcal{N}$.

Proof of Theorem 2.10. Let $U = U_1$ and $g = \int_0^1 \mathrm{d}t U_t f$, then

$$U^n g = \int_0^1 \mathrm{d}t U_{n+t} f = \int_n^{n+1} \mathrm{d}t U_t f$$

and thus

$$\sum_{n=0}^{N-1} U^n g = \int_0^N \mathrm{d}t U_t f.$$

Therefore $\frac{1}{N}\int_0^N \mathrm{d}t U_t f$ converges as $N \to \infty$. For $T \in \mathbb{R}_+$, by writing $T = N + r$ where $0 \le r < 1$ and $N \in \mathbb{N}$, we deduce that $\frac{1}{T}\int_0^T \mathrm{d}t U_t f$ converges as $T \to \infty$. Define the operator $\tilde{P}$ by

$$\tilde{P} f = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t U_t f.$$

Note that $\tilde{P} f \in \mathcal{M}$ and

$$\tilde{P}^* f = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t U_{-t} f \in \mathcal{M}.$$

If $f \in \mathcal{M}$ then clearly $\tilde{P} f = f$, while if $f \in \mathcal{M}^\perp$ for all $g \in \mathcal{H}$, $\langle \tilde{P} f, g\rangle = \langle f, \tilde{P}^* g\rangle = 0$ since $\tilde{P}^* g \in \mathcal{M}$ and therefore $\tilde{P} f = 0$. Thus $\tilde{P} = P$. $\square$

Proof of the Discrete form, Theorem 2.11. We first check that

$$[\ker(I - U)]^\perp = \overline{\mathrm{Range}(I - U)}.$$

If $f \in \ker(I - U)$ and $g \in \mathrm{Range}(I - U)$, then for some h,

$$\begin{aligned}\langle f, g\rangle &= \langle f, (I - U)h\rangle = \langle (I - U^*)f, h\rangle \\ &= -\langle (I - U)f, Uh\rangle = 0.\end{aligned}$$

Thus $\mathrm{Range}(I - U) \subset [\ker(I - U)]^\perp$. Since $[\ker(I - U)]^\perp$ is closed,

$$\overline{\mathrm{Range}(I - U)} \subset [\ker\ (I - U)]^\perp.$$

If $f \in [\mathrm{Range}(I - U)]^\perp$, then for all g

$$0 = \langle f, (I - U)U^* g\rangle = \langle (I - U^*)f, U^* g\rangle = -\langle (I - U)f, g\rangle.$$

Therefore $(I - U)f = 0$, that is $f \in \ker(I - U)$. Thus

$$[\mathrm{Range}\ (I - U)]^\perp \subset \ker\ (I - U).$$

Then

$$[\ker\,(I-U)]^{\perp} \subset [\text{Range}\,(I-U)]^{\perp\perp} = \overline{\text{Range}\,(I-U)}.$$

If $g \in \text{Range}(I-U)$, then $g = (I-U)h$ for some h. Therefore

$$\begin{aligned}\frac{1}{N}\sum_{n=0}^{N-1} U^n g &= \frac{1}{N}\{h - Uh + Uh - U^2h + U^2h - U^3h + \ldots + U^{N-1}h - U^N h\} \\ &= \frac{1}{N}\{h - U^N h\}.\end{aligned}$$

Thus

$$\Big\|\frac{1}{N}\sum_{n=0}^{N-1} U^n g\Big\| \leq \frac{2\|h\|}{N} \to 0 \text{ as } N \to \infty.$$

Approximating elements of $\overline{\text{Range}(I-U)}$ by elements of $\text{Range}(I-U)$, we have that $\frac{1}{N}\sum_{n=0}^{N-1} U^n g \to 0 = Pg$ for all

$$g \in [\ker\,(I-U)]^{\perp} = \overline{\text{Range}(I-U)}.$$

If $g \in \ker\,(I-U)$, then

$$\frac{1}{N}\sum_{n=0}^{N-1} U^n g = g = Pg.$$

□

Definition 2.12 (Ergodicity) *Let $\Phi = (\phi_t)_{t\in\mathbb{R}}$ be a flow on Γ_1 and μ a probability measure on Γ_1 which is stationary with respect to Φ. Φ is said to be* **ergodic** *if for every measurable set $F \subset \Gamma_1$ such that $\phi_t(F) = F$ for all $t \in \mathbb{R}$, we have $\mu(F) = 0$ or $\mu(F) = 1$.*

Theorem 2.13 (Ergodic flows) *$\Phi = (\phi_t)_{t\in\mathbb{R}}$ is ergodic if and only if the only functions in $L^2(\Gamma_1, \mu)$ which satisfy $f \circ \phi_t = f$ are the constant functions.*

Proof. Below a.s.(almost surely) means that the statement is true except on a set of zero measure. Suppose that the only invariant functions are the constant functions. If $\phi_t(F) = F$ for all t then $\mathbb{1}_F$ is an invariant function and so $\mathbb{1}_F$ is constant a.s. which means that $\mathbb{1}_F(x) = 0$ a.s. or $\mathbb{1}_F(x) = 1$ a.s. Therefore $\mu(F) = 0$ or $\mu(F) = \mathbb{1}$.
Conversely suppose ϕ_t is ergodic and $f \circ \phi_t = f$. Let $F = \{x|\ f(x) < a\}$. Then $\phi_t F = F$ since

$$\phi_t(F) = \{\phi_t(x)|\ f(x) < a\} = \{\phi_t(x)|\ f(\phi_t(x) < a\} = F.$$

Therefore $\mu(F) = 0$ or $\mu(F) = 1$. Thus $f(x) < a$ a.s. or $f(x) \geq a$ a.s. for every $a \in \mathbb{R}$. Let

$$a_0 = \sup\{a|\ f(x) \geq a \ \text{ a.s.}\}.$$

Then, if $a > a_0$, $\mu(\{x|\ f(x) \geq a\}) = 0$, and if $a < a_0$, $\mu(\{x|\ f(x) < a\}) = 0$. Let (a_n) and (b_n) be sequences converging to a_0 such that $a_n > a_0 > b_n$. Then

$$\{x|\ f(x) \neq a_0\} = \cup_n \{x|\ f(x) \geq a_n\} \cup \{x|\ f(x) < b_n\}.$$

Thus

$$\mu(\{x|\ f(x) \neq a_0\}) \leq \sum_n (\mu(\{x|\ f(x) \geq a_n\}) + \mu(\{x|\ f(x) < b_n\})) = 0,$$

and so $f(x) = a_0$ a.s. □

If we can prove that a system is ergodic, then there is no problem in applying Boltzmann's prescription for the time average. For an ergodic system, by the above theorem, $\mathcal{M}$ is the one-dimensional space of constant functions so that

$$Pg = \langle 1, g\rangle 1 = \int_{\Gamma_1} g(x)\mu(\mathrm{d}x).$$

Therefore

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t U_t g = \int_{\Gamma_1} g(x)\mu(\mathrm{d}x).$$

Remark 2.14 *However proving ergodicity has turned out to be the most difficult part of the programme. There is only one example for which ergodicity has been claimed to be proved and that is for a system of hard rods (Sinai). This concerns finite systems. In the thermodynamic limit (see Chapter 5) ergodicity should hold, but we do not discuss this problem.*

2.4 Microcanonical measure

Suppose that we consider a system with Hamiltonian H and suppose also that we fix the energy of the system to be exactly E. We would like to devise a probability measure on the points of Γ with energy E such that the measure is stationary with respect to the Hamiltonian flow.
Note that the energy surface Σ_E is closed since $\Sigma_E = H^{-1}(\{E\})$ and H is assumed to be continuous. Clearly $\phi_t(\Sigma_E) = \Sigma_E$ since $H \circ \phi_t = H$. Let $\mathcal{A}(\Gamma)$ denote the algebra of continuous functions $\Gamma \to \mathbb{R}$ with compact support. The following Riesz-Markov theorem identifies positive linear functionals on $\mathcal{A}(\Gamma)$ with positive measures on Γ.

Theorem 2.15 (Riesz-Markov) *If $l\colon \mathcal{A}(\Gamma) \to \mathbb{R}$ is linear and for any positive $f \in \mathcal{A}(\Gamma)$ it holds $l(f) \geq 0$, then there is a unique Borel measure μ on Γ such that*

$$l(f) = \int_\Gamma f(x)\mu(\mathrm{d}x).$$

Now define a linear functional l_E on $\mathcal{A}(\Gamma)$ by

$$l_E(f) = \lim_{\delta \downarrow 0} \frac{1}{\delta} \int_{\Sigma_{[E,E+\delta]}} f(x)\mathrm{d}x,$$

where $\Sigma_{[E,E+\delta]} = \{x|\ H(x) \in [E, E+\delta]\}$ is the energy-shell of thickness δ. By the Riesz-Markov theorem there is a unique Borel measure μ'_E on Γ such that

$$l_E(f) = \int_\Gamma f(x)\mu'_E(\mathrm{d}x)$$

with the properties:

(i) μ'_E is concentrated on Σ_E.

If $\mathrm{supp} f \cap \Sigma_E = \emptyset$ then for δ small enough since $\mathrm{supp} f$ and $\Sigma_{[E,E+\delta]}$ are closed $\Sigma_{[E,E+\delta]} \cap \mathrm{supp} f = \emptyset$ and

$$\int_{\Sigma_{[E,E+\delta]}} f(x)\mathrm{d}x = \int f(x)\mathbb{1}_{\Sigma_{[E,E+\delta]}}(x)\mathrm{d}x = 0.$$

(ii) μ'_E is stationary with respect to ϕ_t.

Since the Lebesgue measure is stationary,

$$\begin{aligned} l_E(f \circ \phi_t) &= \lim_{\delta \downarrow 0} \frac{1}{\delta} \int_{\Sigma_{[E,E+\delta]}} (f \circ \phi_t)(x)\mathrm{d}x = \lim_{\delta \downarrow 0} \frac{1}{\delta} \int_{\phi_t(\Sigma_{[E,E+\delta]})} f(x)\mathrm{d}x \\ &= \lim_{\delta \downarrow 0} \frac{1}{\delta} \int_{\Sigma_{[E,E+\delta]}} f(x)\mathrm{d}x = l_E(f). \end{aligned}$$

Definition 2.16 (Microcanonical measure) *If $\omega(E) := \mu'_E(\Gamma) < \infty$ we can normalise μ'_E to obtain*

$$\mu_E := \mu'_E/\omega(E) \tag{2.8}$$

which is a probability measure on $(\Gamma, \mathcal{B}_\Gamma)$, concentrated of the energy shell Σ_E. The probability μ_E is called the **microcanonical measure** *or* **microcanonical ensemble**. *The normalisation $\omega(E)$ is also called the microcanonical partition function.*
The expression $S = k \log \omega(E)$ is called the **Boltzmann entropy** *or* **microcanonical entropy**, *where $k = 1,38 \times 10^{-23} Js$ is* **Boltzmann's constant**.

We now give an explicit expression for the microcanonical measure. First we briefly recall briefly facts on curvilinear coordinates.
Let $\zeta\colon \mathbb{R}^\nu \to A \subset \mathbb{R}^\nu$ be a bijection. Then we can use coordinates $t_1, t_2, \dots t_\nu$ where the point x corresponds to the point $t = \zeta(x)$ in the new coordinates. The coordinates are orthogonal if the level surfaces $t_i = \text{constant}$, $i = 1, \dots, \nu$ are orthogonal to each other, that is, for all $x \in \mathbb{R}^\nu$ if $i \neq j$,

$$\langle \nabla\zeta_i(x), \nabla\zeta_j(x)\rangle = 0.$$

Changing the variables of integration we then get

$$\begin{aligned}\int_{\mathbb{R}^\nu} f(x)\mathrm{d}x &= \int_A f(\zeta^{-1}(t))|\det(\zeta^{-1})'(t)|\mathrm{d}t = \int_A f(\zeta^{-1}(t))\frac{\mathrm{d}t}{|\det(\zeta'(\zeta^{-1}(t))|}\\ &= \int_A f(\zeta^{-1}(t))\frac{\mathrm{d}t}{\prod_{i=1}^\nu \|(\nabla\zeta_i)(\zeta^{-1}(t))\|}.\end{aligned}$$

Note that if A is an $n \times n$ matrix with rows $a_1, \dots, a_n$ where $\langle a_i, a_j\rangle = 0$ for $i \neq j$, then AA^T is a diagonal matrix with diagonal entries $\|a_1\|^2, \dots, \|a_n\|^2$. Therefore $\det(A) = \prod_{i=1}^n \|a_i\|$.
Let Σ_{t_1} be the level surface $\zeta_1(x) = t_1$ (constant). We define the element of surface area on Σ_{t_1} to be

$$\mathrm{d}\sigma_{t_1} = \frac{\mathrm{d}t_2 \dots \mathrm{d}t_\nu}{\prod_{i=2}^\nu \|(\nabla\zeta_i)(\zeta^{-1}(t))\|}.$$

Then

$$\mathrm{d}x = \frac{\mathrm{d}t_1}{\|\nabla\zeta_1\|}\mathrm{d}\sigma_{t_1}.$$

We apply this to the Microcanonical Measure.
Choose $\zeta\colon \mathbb{R}^{2n} \to A \subset \mathbb{R}^{2n}$ such that $\zeta_1 = H$ and so Σ_{t_1} is an energy surface. Then

$$\int_{\Sigma_{[E,E+\delta]}} f(x)\mathrm{d}x = \int_E^{E+\delta} \mathrm{d}t_1 \int_{\Sigma_{t_1}} \frac{f(\zeta^{-1}(t))}{\|\nabla H(\zeta^{-1}(t))\|}\mathrm{d}\sigma_{t_1}.$$

Therefore

$$\lim_{\delta\to 0}\frac{1}{\delta}\int_{\Sigma_{[E,E+\delta]}} f(x)\mathrm{d}x = \int_{\Sigma_E} \frac{f(\zeta^{-1}(E, t_2, \dots, t_{2n}))\mathrm{d}\sigma_E}{\|\nabla H(\zeta^{-1}(E, t_2 \dots, t_n))\|}.$$

Thus

$$\mu'_E(\mathrm{d}x) = \frac{\mathrm{d}\sigma_E}{\|\nabla H\|}.$$

In particular

$$\omega(E) = \int_{\Sigma_E} \frac{\mathrm{d}\sigma_E}{\|\nabla H\|}.$$

Note also that

$$\int_\Gamma g(H(x))f(x)\mathrm{d}x = \int \mathrm{d}t_1 g(t_1) \int_{\Sigma_{t_1}} \frac{f(\zeta^{-1}(t))}{\|\nabla H(\zeta^{-1}(t))\|}\mathrm{d}\sigma_{t_1}.$$

Notation 2.17 (Mircocanonical Gibbs ensemble) *Let $\Lambda \subset \mathbb{R}^d$ and $N \in \mathbb{N}$, and $H_\Lambda^{(N)}$ denotes the Hamiltonian for N particles in Λ with elastic boundary conditions. Then we denote the microcanonical measure on $(\Gamma_\Lambda, \mathcal{B}_\Lambda)$ by $\mu'_{E,\Lambda}$ and the partition function by*

$$\omega_\Lambda(E,N) = \frac{\mathrm{d}\sigma_E}{||H_\Lambda^{(N)}||}.$$

The microcanonical entropy is denoted by $S_\Lambda(E,N) = k \log \omega_\Lambda(E,N)$.

Remark 2.18 *Measure which are constructed like the microcanonical measure on hyperplanes are called Gelfand-Leray measures. In general one might imagine that there are several integrals of motions. For example the angular momentum is conserved. Then one has to consider intersections of several level surfaces. We will not discuss this in these lectures.*

3 Entropy

3.1 Probabilistic view on Boltzmann's entropy

We discuss briefly the famous Boltzmann formula $S = k \log W$ for the entropy and give here an elementary probabilistic interpretation. For that let Ω be a finite set (the state space) and let there be given a probability measure $\mu \in \mathcal{P}(\Omega)$ on Ω, where $\mathcal{P}(\Omega)$ denotes the set of probability measures on Ω with the σ-algebra being the set of all subsets of Ω. In the picture of Maxwell and Boltzmann, the set Ω is the set of all possible energy levels for a system of particles, and the probability measure μ corresponds to a specific histogram of energies describing some macrostate of the system. Assume that $\mu(x)$ is a multiple of $\frac{1}{n}$ for any $x \in \Omega$, $n \in \mathbb{N}$, i.e. μ is a histogram for n trials or a macrostate for a system of n particles. A microscopic state for the system of n particles is any configuration $\omega \in \Omega^n$.

Boltzmann's idea: The entropy of a macrostate $\mu \in \mathcal{P}(\Omega)$ corresponds to the degree of uncertainty about the actual microstate $\omega \in \Omega^n$ when only μ is known and thus can be measured by $\log N_n(\mu)$, the logarithmic number of microstates leading to μ.

The associate macrostate for a microstate $\omega \in \Omega^n$ is

$$L_n(\omega) = \frac{1}{n} \sum_{i=1}^{n} \delta_{\omega_i},$$

and $L_n(\omega)$ is called the *empirical distribution* or *histogram* of $\omega \in \Omega^n$. The number of microstates leading to a given $\mu \in \mathcal{P}(\Omega) \cap \frac{1}{n}[0,1]^\Omega$ is the number

$$N_n(\mu) = \Big|\{\omega \in \Omega^n \colon L_n(\omega) = \mu\}\Big| = \Big(\frac{n!}{\prod_{x\in\Omega}(n\mu(x))!}\Big).$$

We may approximate $\mu \in \mathcal{P}(\Omega)$ by a sequence $(\mu_n)_{n\in\mathbb{N}}$ of probability measures $\mu_n \in \mathcal{P}(\Omega)$ with $\mu_n \in \frac{1}{n}[0,1]^\Omega$. Then we define the uncertainty $H(\mu)$ of μ via Stirling's formula as the $n \to \infty$-limit of the mean-uncertainty of μ_n per particle.

Proposition 3.1 *Let $\mu \in \mathcal{P}(\Omega)$ and $\mu_n \in \mathcal{P}(\Omega) \cap \frac{1}{n}[0,1]^\Omega$ with $n \in \mathbb{N}$ and $\mu_n \to \mu$ as $n \to \infty$. Then the limit $\lim_{n\to\infty} \frac{1}{n} \log N_n(\mu_n)$ exists and equals*

$$\mathcal{H}(\mu) = -\sum_{x\in\Omega} \mu(x) \log \mu(x). \tag{3.9}$$

Proof. A proof with exact error bounds can be found in [CK81]. □

The entropy $\mathcal{H}(\mu)$ counts the number of possibilities to obtain the macrostate or histogram μ, and thus it describes the hidden multiplicity of the "true" microstates consistent with the observed μ. It is therefore a measure of the complexity inherent in μ.

3.2 Shannon's entropy

We give a brief view on the basic facts on Shannon's entropy, which was established by Shannon 1949 ([Sha48] and [SW49]). We base the specific form of the Shannon entropy functional on probability measures just on a couple of clear intuitive arguments. For that we start with a sequence of four axioms on a functional S that formalises the intuitive idea that entropy should measure the lack of information (or uncertainty) pertaining to a probability measure. For didactic reasons we limit ourselves to probability measures on a finite set $\Omega = \{\omega_1, \ldots, \omega_n\}$ of elementary events. Let $P \in \mathcal{P}(\Omega)$ be the probability measure with $P(\{\omega_i\}) = p_i \in [0,1], i = 1, \ldots, n$, and $\sum_{i=1}^n p_i = 1$. Now we formulate four axioms for a functional S acting on the set $\mathcal{P}(\Omega)$ of probability measures.

Axiom 1: To express the property that S is a function of $P \in \mathcal{P}(\Omega)$ alone and not of the order of the single entries, one imposes:

(a) For every permutation $\pi \in \mathfrak{S}_n$, where $\mathfrak{S}_n$ is the group of permutations of n elements, and any $P \in \mathcal{P}(\Omega)$ let $\pi P \in \mathcal{P}(\Omega)$ be defined as $\pi P(\{\omega_i\}) = p_{\pi(i)}$ for any $i = 1, \ldots, n$. Then

$$S(P) = S(\pi P).$$

(b) $S(P)$ is continuous in each of the entries $p_i = P(\{\omega_i\}), i = 1, \ldots, n$.

The next axiom expresses the intuitive fact that the outcome is most random for the uniform distribution.

Axiom 2: Let $P^{(\text{uniform})}(\{\omega_i\}) = \frac{1}{n}$ for $i = 1, \ldots, n$. Then

$$S(P) \leq S(P^{(\text{uniform})}) \quad \text{for any } P \in \mathcal{P}(\Omega).$$

The next axiom states that the entropy remains constant, whenever we extend our space of outcomes with vanishing probability.

Axiom 3: Let $P' \in \mathcal{P}(\Omega')$ where $\Omega' = \Omega \cup \{\omega_{n+1}\}$ and assume that $P'(\{\omega_{n+1}\}) = 0$. Then

$$S(P') = S(P)$$

for $P \in \mathcal{P}(\Omega)$ with $P(\{\omega_i\}) = P'(\{\omega_i\})$ for all $i = 1, \ldots, n$.

Finally we consider compositions.

Axiom 4: Let $P \in \mathcal{P}(\Omega)$ and $Q \in \mathcal{P}(\Omega')$ for some set $\Omega' = \{\omega'_1, \ldots, \omega'_m\}$ with $m \in \mathbb{N}$. Define the probability measure $P \vee Q \in \mathbb{P}(\Omega \times \Omega')$ as

$$P \vee Q(\{\omega_i, \omega'_l\}) = Q(\{\omega'_l\}|\{\omega_i\})P(\{\omega_i\})$$

for $i = 1, \ldots, n$, and $l = 1, \ldots, m$. Here $Q(\{\omega'_l\}|\{\omega_i\})$ is the conditional probability of the event $\{\omega'_l\} \in \Omega'$ conditioned that the event $\{\omega_i\} \in \Omega$ occurred. Then

$$S(P \vee Q) = S(P) + S(Q|P),$$

where $S(Q|P) = \sum_{i=1}^{n} p_i S_i(Q)$ is the expectation of

$$S_i(Q) = -\sum_{l=1}^{m} Q(\{\omega'_l\}|\{\omega_i\}) \log Q(\{\omega'_l\}|\{\omega_i\})$$

with respect to the probability measure P.

$S_i(Q)$ is the conditional entropy of Q given that event $\{\omega_i\} \in \Omega$ occurred. Note that when P and Q are independent one has $S(P \vee Q) = S(P) + S(Q)$.

Equipped with theses elementary assumptions we cite the following theorem which gives birth to the Shannon entropy.

Theorem 3.2 (Shannon entropy) *Let $\Omega = \{\omega_i, \ldots, \omega_n\}$ be a finite set. Any functional $S\colon \mathcal{P}(\Omega) \to \mathbb{R}$ satisfying Axioms (1) to (4) must be necessarily of the form*

$$S(P) = -k \sum_{i=1}^{n} p_i \log p_i \quad \textit{for } P \in \mathcal{P}(\Omega) \;\; \textit{with} \;\; P(\{\omega_i\}) = p_i, i = 1, \ldots, n,$$

and where $k \in \mathbb{R}_+$ is a positive constant.

Proof. The proof can be found in the original work by Shannon and Weaver [SW49] or in the book by Khinchin [Khi57]. □

Notation 3.3 (Entropy) *The functional*

$$\mathcal{H}(\mu) = -\sum_{\omega \in \Omega} \mu(\omega) \log \mu(\omega) \quad \textit{for } \mu \in \mathcal{P}(\Omega)$$

is called the **Shannon entropy** *of the probability measure μ.*

The connection with the previous Boltzmann entropy for the microcanonical ensemble is apparent from Axiom 2 above. Moreover, there are also connections to the Boltzmann-H-function not mentioned at all. The interested reader is referred to any of the following monographs [Bal91],[Bal92],[Gal99] and [EL02].

4 The Gibbs ensembles

In 1902 Gibbs proposed three Gibbs ensembles, the microcanonical, the canonical and the grandcanonical ensemble. The microcanonical ensemble was introduced in Section 2.4 as a probability measure on the energy surface, a hyperplane in the phase space. The microcanonical ensemble is most natural from the physical point of view. However, in practise mainly the canonical and the grandcanonical Gibbs ensembles are studied. The main reason is that these ensembles are defined as probability measures in the phase space with a density, the so-called **Boltzmann factor** $\mathrm{e}^{-\beta H}$, where $\beta > 0$ is the inverse temperature and H the Hamiltonian of the system. The mathematical justification to replace the microcanonical ensemble by the canonical or grandcanonical Gibbs ensemble goes under the name equivalence of ensembles, which we will discuss in Subsection 5.3. In this section we introduce first the canonical Gibbs ensemble. Then we study the so-called Gibbs paradox concerning the correct counting for a system of indistinguishable identical particles. It follows the definition of the grandcanonical Gibbs ensemble. In the last subsection we relate all the introduced Gibbs ensembles to classical thermodynamics. This leads to the orthodicity problem, namely the question whether the laws of thermodynamics are derived from the ensembles averages in the thermodynamic limit.

4.1 The canonical Gibbs ensemble

We define the canonical Gibbs ensemble for a finite volume box $\Lambda \subset \mathbb{R}^d$ and a fixed number $N \in \mathbb{N}$ of particles with Hamiltonian $H_\Lambda^{(N)}$ having appropriate boundary conditions (like elastic ones as for the microcanonical ensemble or periodic ones). In the following we denote the Borel-σ-algebra on the phase space Γ_Λ by $\mathcal{B}_\Lambda$. The universal **Boltzmann constant** is $k = k_\mathrm{B} = 1.3806505 \times 10^{-23}$ joule/kelvin. In the following T denotes temperature measured in Kelvin.

Definition 4.1 *Call the parameter $\beta = \frac{1}{kT} > 0$ the inverse temperature. The* **canonical Gibbs ensemble** *for parameter β is the probability measure $\gamma_{\Lambda,N}^\beta \in \mathcal{P}(\Gamma_\Lambda, \mathcal{B}_\Lambda)$ having the density*

$$\rho_{\Lambda,N}^\beta(x) = \frac{\mathrm{e}^{-\beta H_\Lambda^{(N)}(x)}}{Z_\Lambda(\beta, N)} \quad , x \in \Gamma_\Lambda, \tag{4.10}$$

with respect to the Lebesgue measure. Here

$$Z_\Lambda(\beta, N) = \int_{\Gamma_\Lambda} \mathrm{d}x \, \mathrm{e}^{-\beta H_\Lambda^{(N)}(x)} \tag{4.11}$$

is the normalisation and is called **partition function** *("Zustandsssume").*

Gibbs introduced this canonical measure as a matter of simplicity: he wanted the measure with density ρ to describe an equilibrium, i.e., to be invariant under the time evolution, so the most immediate candidates were to be functions of the energy. Moreover, he proposed that *"the most simple case conceivable"* is to take the $\log \rho$ linear in the energy. The following theorem was one of his justifications of the utility of the definition of the canonical ensemble.

Theorem 4.2 *Let $\Lambda_1, \Lambda_2 \subset \mathbb{R}^d$, $\Gamma_{\Lambda_1} \times \Gamma_{\Lambda_2}$ be an aggregate phase space Γ_{Λ_0} and $\gamma_0 \in \mathcal{P}(\Gamma_{\Lambda_0}, \mathcal{B}_0)$ with Lebesgue density ρ_0 be given. Define the reduced probability measures (or marginals) $\gamma_i \in \mathcal{P}(\Gamma_i, \mathcal{B}_i), i = 1, 2,$ as*

$$\gamma_1(A) = \int_{A \times \Gamma_2} \mathbb{1}_A(x_1)\rho_0(x_1, x_2)\mathrm{d}x_2 \quad \textit{for } A \in \mathcal{B}_1,$$
$$\gamma_2(B) = \int_{\Gamma_1 \times B} \mathbb{1}_A(x_2)\rho_0(x_1, x_2)\mathrm{d}x_1 \quad \textit{for } B \in \mathcal{B}_2$$

with the Lebesgue densities

$$\rho_1(x_1) = \int_{\Gamma_0} \rho_0(x_1, x_2)\mathrm{d}x_2 \quad \textit{and} \quad \rho_2(x_2) = \int_{\Gamma_0} \rho_0(x_1, x_2)\mathrm{d}x_1.$$

Then the entropies

$$S_i = -k \int_{\Gamma_i} \rho_i(x) \log \rho_i(x)\mathrm{d}x \quad \textit{with } \ i = 0, 1, 2,$$

satisfy the inequality

$$S_0 \leq S_1 + S_2$$

with equality $S_0 = S_1 + S_2$ if and only if $\rho_0 = \rho_1\rho_2$.

Proof. The proof is given with straightforward calculation and the use of Jensen's inequality for the convex function $f(x) = x \log x + 1 - x$. □

Gibbs himself recognised the condition for equality as a condition for independence. He claimed that with the notations of Theorem 4.2 in the special case ρ is the canonical ensemble density and the Hamiltonian is of the form $H_0 = H_1 + H_2$ with H_1 (respectively H_2) is independent of Γ_2 (respectively Γ_1), the reduced densities (marginal densities) ρ_1 and ρ_2 are independent, i.e., $\rho_0 = \rho_1\rho_2$, and are themselves canonical ensemble densities.
In [Gib02] he writes:

-a property which enormously simplifies the discussion, and is the foundation of extremely important relations to thermodynamics.

Indeed, it follows from this that the temperatures are all equal, i.e., $T_1 = T_2 = T_0$.

Remark 4.3 (Lagrange multipliers) *We note that the inverse temperature β in the canonical Gibbs ensemble can be seen as the Lagrange multiplicator for the extremum problem for the entropy under the constraint that the mean energy is fixed with a parameter like β, see further [Jay89], [Bal91], [Bal92], [EL02].*

Theorem 4.4 (Maximum Principle for the entropy) *Let $\beta > 0, \Lambda \subset$ and $N \in \mathbb{N}$ be given. The canonical Gibbs ensemble $\gamma^{\beta}_{\Lambda,N}$, where $\beta > 0$ is determined by $\int_{\Gamma_\Lambda} \mathrm{d}x \rho^{\beta}_{\Lambda,N}(x) = U$, maximises the entropy*

$$S(\gamma) = -k \int_{\Gamma_\Lambda} \rho(x) \log \rho(x) \mathrm{d}x$$

for any $\gamma \in \mathcal{P}(\Gamma_\Lambda, \mathcal{B}_\Lambda)$ having a Lebesgue density ρ subject to the constraint

$$U = \int_{\Gamma_\Lambda} \rho(x) H^{(N)}_{\Lambda}(x) \mathrm{d}x. \tag{4.12}$$

Moreover, the values of the temperature T and the partition function $Z_\Lambda(\beta, N)$ are uniquely determined from the condition

$$U = -\frac{\partial}{\partial \beta} \log Z_\Lambda(\beta, N) \quad \textit{with } \beta = \frac{1}{kT}.$$

Proof. We give only a rough sketch of the proof. We use that

$$a \log a - b \log b \leq (a - b)(1 + \log a) \quad a, b \in (0, \infty).$$

Let $\gamma \in \mathcal{P}(\Gamma_\Lambda, \mathcal{B}_\Lambda)$ with Lebesgue density ρ. Put $a = \rho^{\beta}_{\Lambda,N}(x)$ and $b = \rho(x)$ for any $x \in \Gamma_\Lambda$ and recall that $\rho^{\beta}_{\Lambda,N}$ is the density of the canonical Gibbs ensemble. Then

$$\begin{aligned} \rho^{\beta}_{\Lambda,N}(x) \log \rho^{\beta}_{\Lambda,N}(x) - \rho(x) \log \rho(x) \leq (\rho^{\beta}_{\Lambda,N}(x) - \rho(x))(1 - \log Z_\Lambda(\beta, N) \\ - \beta H^{(N)}_{\Lambda}(x)). \end{aligned}$$

Integrating with respect to Lebesgue we get

$$\begin{aligned}
S(\gamma^{\beta}_{\Lambda,N}) - S(\mu) \geq -k \Bigg\{ \int_{\Gamma_\Lambda} ((1 - \log Z_\Lambda(\beta, N) - \beta H^{(N)}_\Lambda(x))\rho^{\beta}_{\Lambda,N}(x)\mathrm{d}x \\
- \int_{\Gamma_\Lambda} (1 - \log Z_\Lambda(\beta, N) - \beta H^{(N)}_\Lambda(x))\rho(x))\mathrm{d}x \Bigg\} \\
= -k \left\{ (1 - \log Z_\Lambda(\beta, N) - \beta U) - (1 - \log Z_\Lambda(\beta, N) - \beta U) \right\} \\
= 0.
\end{aligned}$$

Therefore

$$S(\gamma^{\beta}_{\Lambda,N}) \geq S(\gamma).$$

Note that the entropy for the canonical ensemble is given by

$$\begin{aligned}
S(\gamma^{\beta}_{\Lambda,N}) &= k \int_{\Gamma_\Lambda} (\log Z_\Lambda(\beta, N) + \beta H^{(N)}_\Lambda(x))\rho^{\beta}_{\Lambda,N}(x)\mathrm{d}x \\
&= k \log Z_\Lambda(\beta, N) + k\beta \int_{\Gamma_\Lambda} H^{(N)}_\Lambda(x)\rho^{\beta}_{\Lambda,N}(x)\mathrm{d}x.
\end{aligned}$$

To prove the second assertion, note that

$$\begin{aligned}
\partial_\beta \log Z_\Lambda(\beta, N) &= -\int_{\Gamma_\Lambda} \rho^{\beta}_{\Lambda,N}(x) H^{(N)}_\Lambda(x)\mathrm{d}x, \\
\partial^2_\beta \log Z_\Lambda &= \int_{\Gamma_\Lambda} \rho^{\beta}_{\Lambda,N}(x) \Big(H^{(N)}_\Lambda(x) - \int_{\Gamma_\Lambda} \rho^{\beta}_{\Lambda,N}(x) H^{(N)}_\Lambda(x)\mathrm{d}x \Big)^2 \mathrm{d}x \geq 0.
\end{aligned}$$

□

Thermodynamic functions

For the canonical ensemble the relevant thermodynamical variables are the temperature T (or $\beta = (kT)^{-1}$) and the volume V of the region $\Lambda \subset \mathbb{R}$. We have already defined the entropy S of the canonical ensemble by

$$S_\Lambda(\beta, N) = k \log Z_\Lambda(\beta, N) + \frac{1}{T} \mathbb{E}_{\gamma^{\beta}_{\Lambda,N}}(H^{(N)}_\Lambda),$$

where $U = \mathbb{E}_{\gamma^{\beta}_{\Lambda,N}}(H^{(N)}_\Lambda) = \int_{\Gamma_\Lambda} H^{(N)}_\Lambda(x)\rho^{\beta}_{\Lambda,N}(x)\mathrm{d}x$, the expectation of H_Λ, sometimes denoted also by $\langle H^{(N)}_\Lambda \rangle$. We define the **Helmholtz Free Energy** by $A = U - TS$, and we shall call the Helmholtz Free Energy simply the **free energy** from now on. We have

$$\begin{aligned}
A = U - TS_\Lambda(\beta, N) &= \mathbb{E}_{\gamma^{\beta}_{\Lambda,N}}(H^{(N)}_\Lambda) - T(k \log Z_\Lambda(\beta, N) + \frac{1}{T} \mathbb{E}_{\gamma^{\beta}_{\Lambda,N}}(H^{(N)}_\Lambda)) \\
&= -\frac{1}{\beta} \log Z_\Lambda(\beta, N).
\end{aligned}$$

By analogy with Thermodynamics we define the absolute pressure P of the system by

$$P = -\left(\frac{\partial A}{\partial V}\right)_T.$$

The other thermodynamic functions can be defined as usual:
The Gibbs Potential, $G = U + PV - TS = A + PV$,
The Heat Capacity at Constant Volume, $C_V = \left(\frac{\partial U}{\partial T}\right)_V$.
Note that

$$S = -\left(\frac{\partial A}{\partial T}\right)_V$$

is also satisfied. The thermodynamic functions can all be calculated from A. Therefore all calculations in the canonical ensemble begin with the calculation of the partition function $Z_\Lambda(\beta, N)$.
To make the free energy density finite in the thermodynamic limit we redefine the **canonical partition function** by introducing **correct Boltzmann counting**

$$Z_\Lambda(\beta, N) = \frac{1}{(n/d)!}\int_{\Gamma_\Lambda} \mathrm{e}^{-\beta H_\Lambda^{(N)}(x)}\mathrm{d}x = \frac{1}{N!}\int_{\Gamma_\Lambda} \mathrm{e}^{-\beta H_\Lambda(x)}\mathrm{d}x, \tag{4.13}$$

see the following Subsection 4.2 for a justification of this correct Boltzmann counting.

Example 4.5 (The ideal gas in the canonical ensemble) *Consider a non-interacting gas of N identical particles of mass m in d dimensions, contained in a box $\Lambda \subset \mathbb{R}^d$ of volume V. The Hamiltonian for this system is*

$$H_\Lambda(x) = \frac{1}{2m}\sum_{i=1}^{N} p_i^2 \quad , x = (q, p) \in \Gamma_\Lambda.$$

We have for the partition function $Z_\Lambda(\beta, N)$

$$\begin{aligned} Z_\Lambda(\beta, N) &= \frac{1}{N!\ h^{Nd}}\int_{\Gamma_\Lambda} \mathrm{e}^{-\beta H_\Lambda(x)}\mathrm{d}x = \frac{1}{N!\ h^{Nd}} V^N \left(\int_{\mathbb{R}^d} \mathrm{e}^{-\frac{\beta p^2}{2m}}\mathrm{d}p\right)^N \\ &= \frac{1}{N!\ h^{Nd}} V^N \left(\int_{\mathbb{R}} \mathrm{e}^{-\frac{\beta p^2}{2m}}\mathrm{d}p\right)^{Nd} = \frac{1}{N!} V^N \left(\frac{2\pi m}{h^2\beta}\right)^{\frac{1}{2}Nd} \\ &= \frac{1}{N!}\left(\frac{V}{\lambda^d}\right)^N, \end{aligned} \tag{4.14}$$

where

$$\lambda = \left(\frac{h^2\beta}{2\pi m}\right)^{\frac{1}{2}}$$

is called the **thermal wavelength** *because it is of the order of the de Broglie wavelength of a particle of mass m with energy $\frac{1}{\beta}$. The* **free energy** $A_\Lambda(\beta, N)$ *is given by*

$$A_\Lambda(\beta, N) = -\frac{1}{\beta} \log Z_\Lambda(\beta, N) = \frac{1}{\beta} \left(\log N! + Nd \log \lambda - N \log V \right).$$

Thus the pressure is given by

$$P_\Lambda(\beta, N) = -\Big(\frac{\partial A_\Lambda(\beta, N)}{\partial V} \Big)_T = \frac{N}{\beta V} = \frac{kTN}{V}.$$

Let $a_N(\beta, v)$ be the free energy per particle considered as a function of the specific density v, that is,

$$a_N(\beta, v) = \frac{1}{N} A_{\Lambda_N}(\beta, N),$$

where Λ_N is a sequence of boxes with volume vN and let $p_N(\beta, v) = P_{\Lambda_N}(\beta, N)$ be the corresponding pressure. Then

$$p_N(\beta, v) = -\Big(\frac{\partial a_N(\beta, v)}{\partial v} \Big)_T.$$

For the ideal gas we get then

$$a_N(\beta, v) = \frac{1}{\beta} \left(\frac{1}{N} \log N! + d \log \lambda - \log v - \log N \right),$$

leading to

$$a(\beta, v) := \lim_{N \to \infty} a_N(\beta, v) = \frac{1}{\beta} \left(d \log \lambda - \log v - 1 \right),$$

since

$$\lim_{N \to \infty} \left(\frac{1}{N} \log N! - \log N \right) = -1.$$

If $p(\beta, v) := \lim_{N \to \infty} p_N(\beta, v)$, one gets

$$p(\beta, v) = -\Big(\frac{\partial a(\beta, v)}{\partial v} \Big)_T,$$

and thus $p(\beta, v) = \frac{1}{\beta v}$. We can also define the free energy density as a function of the particle density ρ, i.e.,

$$f_l(\beta, \rho) = \frac{1}{V_l} A_{\Lambda_l}(\beta, \rho V_l),$$

where Λ_l is a sequence of boxes with volume V_l with $\lim_{l\to\infty} V_l = \infty$ and

$$f(\beta,\rho) = \lim_{l\to\infty} f_l(\beta,\rho).$$

The pressure $p(\beta,\rho)$ then satisfies

$$p(\beta,\rho) = \rho\left(\frac{\partial f(\beta,\rho)}{\partial\rho}\right)_T - f(\beta,\rho).$$

Clearly $f(\beta,\rho) = \rho\, a(\beta,\frac{1}{\rho})$. For the ideal gas we get

$$f(\beta,\rho) = \frac{\rho}{\beta}\left(d\log\lambda + \log\rho - 1\right)$$

and therefore

$$p(\beta,\rho) = \frac{\rho}{\beta}.$$

Finally we want to check the relative dispersion of the energy in the canonical ensemble. Let $\langle H_\Lambda^{(N)}\rangle = \mathbb{E}_{\gamma^\beta_{\Lambda,N}}(H_\Lambda^{(N)})$. Then

$$\frac{\langle (H_\Lambda^{(N)} - \langle H_\Lambda^{(N)}\rangle)^2\rangle}{\langle H_\Lambda^{(N)}\rangle^2} = \frac{\partial_\beta^2 \log Z_\Lambda(\beta,N)}{(\partial_\beta \log Z_\Lambda(\beta,N))^2}.$$

This gives for the ideal gas

$$\frac{\sqrt{\langle (H_\Lambda^{(N)} - \langle H_\Lambda^{(N)}\rangle)^2\rangle}}{\langle H_\Lambda^{(N)}\rangle} = (\frac{1}{2}dN)^{-\frac{1}{2}} = O(N^{-\frac{1}{2}}).$$

4.2 The Gibbs paradox

The Gibbs paradox illustrates an essential correction of the counting within the microcanonical and the canonical ensemble. Gibbs 1902 was not aware of the fact that the partition function needed a re-definition, for instance a redefinition in (4.13) in case of the canonical ensemble. The ideal gas suffices to illustrate the main issue of that paradox. Recall the entropy of the ideal gas in the canonical ensemble

$$S_\Lambda(\beta,N) = kN\log(VT^{\frac{d}{2}}) + \frac{d}{2}kN(1+\log(2\pi m)) \quad ,\beta^{-1} = kT, \tag{4.15}$$

where $V = |\Lambda|$ is the volume of the box $\Lambda \subset \mathbb{R}^d$. Now, make the following "Gedanken"-experiment. Consider two vessels having volume V_i containing $N_i, i = 1,2$, particles separated by a thin wall. Suppose further that both

vessels are in equilibrium having the same temperature and pressure. Now imagine that the wall between the two vessels is gently removed. The aggregate vessel is now filled with a gas that is still in equilibrium at the same temperature and pressure. Denote by S_1 and S_2 the entropy on each side of the wall. Since the corresponding canonical Gibbs ensembles are independent of one another, the entropy S_{12} of the aggregate vessel - before the wall is removed - is exactly $S_1 + S_2$. However an easy calculation gives us

$$\begin{aligned} S_{12} - (S_1 + S_2) &= k((N_1 + N_2)\log(V_1 + V_2) - N_1 \log V_1 - N_2 \log V_2) \\ &= -k\Big(N_1 \log \frac{V_1}{V_1 + V_2} + N_2 \log \frac{V_2}{V_1 + V_2}\Big) > 0. \end{aligned} \tag{4.16}$$

This shows that the informational (Shannon) entropy has increased, while we expected the thermodynamic entropy to remain constant, since the wall between the two vessels is immaterial from a thermodynamical point of view. This is the **Gibbs paradox**.
We have indeed lost information in the course of removing the wall. Imagine the gas before removing the wall consists of yellow molecules in one vessel and of blue molecules in the other. After removal of the wall we get a uniform greenish mixture throughout the aggregate vessel. Before we knew with probability 1 that a blue molecule was initially in the vessel where we had put it, after removal of the wall we only know that it is in that part of the aggregate vessel with probability $\frac{N_1}{N_1 N_2}$.
The Gibbs paradox is resolved in classical statistical mechanics with an ad hoc ansatz. Namely, instead of the canonical partition function $Z_\Lambda(\beta, N)$ one takes $\frac{1}{N!} Z_\Lambda(\beta, N)$ and instead of the microcanonical partition function $\omega_\Lambda(E, N)$ one takes $\frac{1}{N!}\omega_\Lambda(E, N)$. This is called the correct **Boltzmann counting**. The appearance of the factorial can be justified in quantum mechanics. It has something to do with the in-distinguishability of identical particles. A state describing a system of identical particles should be invariant under any permutation of the labels identifying the single particle variables. However, this very interesting issue goes beyond the scope of this lecture, and we will therefore assume it from now on. In Subsection 5.1 we give another justification by computing the partition function and the entropy in the microcanonical ensemble.

4.3 The grandcanonical ensemble

We give a brief introduction to the grandcanonical Gibbs ensemble. One can argue that the canonical ensemble is more physical since in experiments we never consider an isolated system and we never measure the total energy

but we deal with systems with a given temperature. Similarly we like not to specify the number of particles but the average number of particles. In the grandcanonical ensemble the system can have any number of particles with the average number determined by external sources. The grandcanonical Gibbs ensemble is obtained if the canonical ensemble is put in a "particle-bath", meaning that the particle number is no longer fixed, only the mean of the particle number is determined by a parameter. This was similarly done in the canonical ensemble for the energy, where one considers a "heat-bath". The phase space for exactly N particles in box $\Lambda \subset \mathbb{R}^d$ can be written as

$$\Gamma_{\Lambda,N} = \{\omega \subset (\Lambda \times \mathbb{R}^d) \colon \omega = \{(q, p_q) \colon q \in \widehat{\omega}\}, \mathrm{Card}\,(\widehat{\omega}) = N\}, \tag{4.17}$$

where $\widehat{\omega}$, the set of positions occupied by the particles, is a locally finite subset of Λ, and p_q is the momentum of the particle at positions q. If the number of the particles is not fixed, then the phase space is

$$\Gamma_{\Lambda} = \{\omega \subset (\Lambda \times \mathbb{R}^d) \colon \omega = \{(q, p_q) \colon q \in \widehat{\omega}\}, \mathrm{Card}\,(\widehat{\omega}) \text{ finite}\}. \tag{4.18}$$

A counting variable on Γ_Λ is a random variable N_Δ on Γ_Λ for any Borel set $\Delta \subset \Lambda$ defined by $N_\Delta(\omega) = \mathrm{Card}\,(\widehat{\omega} \cap \Delta)$ for any $\omega \in \Gamma_\Lambda$.

Definition 4.6 (Grandcanonical ensemble) *Let $\Lambda \subset \mathbb{R}^d, \beta > 0$ and $\mu \in \mathbb{R}$. Define the phase space $\Gamma_\Lambda = \cup_{N=0}^{\infty} \Gamma_{\Lambda,N}$, where $\Gamma_{\Lambda,N} = (\Lambda \times \mathbb{R}^d)^{2N}$ is the phase space in Λ for N particles, and equip it with the σ-algebra $\mathcal{B}_\Lambda^\infty$ generated by the counting variables. The probability measure $\gamma_\Lambda^{\beta,\mu} \in \mathcal{P}(\Gamma_\Lambda, \mathcal{B}_\Lambda^\infty)$ such that the restrictions $\gamma_\Lambda^{\beta,\mu}\big|_{\Gamma_{\Lambda,N}}$ onto $\Gamma_{\Lambda,N}$ have the densities*

$$\rho_{\beta,\mu}^{(N)}(x) = Z_\Lambda(\beta,\mu)^{-1} \mathrm{e}^{-\beta(H_\Lambda^{(N)}(x) - \mu N)} \quad , N \in \mathbb{N},$$

where $H_\Lambda^{(N)}$ is the Hamiltonian for N particles in Λ, and partition function

$$Z_\Lambda(\beta,\mu) = \sum_{N=0}^{\infty} \int_{\Gamma_{\Lambda,N}} \mathrm{e}^{-\beta(H_\Lambda^{(N)}(x) - \mu N)} \mathrm{d}x \tag{4.19}$$

is called the **grandcanonical ensemble** *in Λ for the inverse temperature β and the* **chemical potential** *μ.*

Instead of the chemical potential μ sometimes the **fugacity** or **activity** $\mathrm{e}^{\beta\mu}$ is used for the grandcanonical ensemble. Observables are now sequences $f = (f_0, f_1, \ldots)$ with $f_0 \in \mathbb{R}$ and $f_N \colon \Gamma_{\Lambda,N} \to \mathbb{R}, N \in \mathbb{N}$, are functions on the N-particle phase spaces. Hence, the expectation in the grandcanonical ensemble is written as

$$\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(f) = \frac{1}{Z_\Lambda(\beta,\mu)} \sum_{N=0}^{\infty} \mathrm{e}^{\beta\mu N} Z_\Lambda(\beta, N) \int_{\Gamma_{\Lambda,N}} f_N(x) \rho_{\Lambda,N}^{\beta}(\mathrm{d}x). \tag{4.20}$$

If $\mathcal{N}$ denotes the particle number observable we get that

$$\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(\mathcal{N}) = \frac{1}{\beta}\frac{\partial}{\partial\mu}\log Z_\Lambda(\beta,\mu).$$

For the grandcanonical measure we have a *Principle of Maximum Entropy* very similar to those for the other two ensembles. We maximise the entropy subject to the constraint that the mean energy $\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(H_\Lambda)$ and the mean particle number $\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(\mathcal{N})$ are fixed, where $H_\Lambda = (H_\Lambda^{(0)}, H_\Lambda^{(1)}, \ldots)$ is the sequence of Hamiltonians for each possible number of particles.

Theorem 4.7 (Principle of Maximum Entropy) *Let P be a probability measure on Γ_Λ such that its restriction to $\Gamma_{\Lambda,N}$, denoted by P_N, is absolutely continuous with respect to the Lebesgue measure, that is*

$$P_N(A) = \int_A \rho_N(x)\mathrm{d}x \quad \textit{for any } A \in \mathcal{B}_\Lambda^{(N)}.$$

Define the entropy of the probability measure P to be

$$S(P) = -k\rho_0\log\rho_0 - k\sum_{N=1}^{\infty}\int_{\Gamma_{\Lambda,N}} \rho_N(x)\log(N!\rho_N(x))\mathrm{d}x.$$

Then the grandcanonical ensemble/measure $\gamma_\Lambda^{\beta,\mu}$, where β and μ are determined by $\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(H_\Lambda) = E$ and $\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(\mathcal{N}) = N_0$, $N_0 \in \mathbb{N}$, maximises the entropy among the absolutely continuous probability measures on Γ_Λ with mean energy E and mean particle number N_0.

Proof. As in the two previous cases we use $a\log a - b\log b \le (a-b)(1+\log a)$ and so

$$a\log ta - b\log tb \le (a-b)(1+\log a+\log t).$$

Let $\rho_N^{\beta,\mu}(x) = \dfrac{e^{\beta\mu N}e^{-\beta H_N(x)}}{N!Z_\Lambda(\beta,\mu)}$ and put $a = \rho_{\beta,\mu}^{(N)}(x)$, $b = \rho_N(x)$ and $t = N!$. Then, writing Z for $Z_\Lambda(\beta,\mu)$,

$$\begin{aligned}\rho_{\beta,\mu}^{(N)}(x)\log(N!\rho_{\beta,\mu}^{(N)}(x)) - \rho_N(x)\log(N!\rho_N(x))\\ \le (\rho_{\beta,\mu}^{(N)}(x) - \rho_N(x))(1 - \log Z - \beta H_\Lambda^{(N)}(x) + \beta\mu N).\end{aligned}$$

Integrating with respect to the Lebesgue measure on $\Gamma_{\Lambda,N}$ and summing over N we get

$$\begin{aligned}
S(\mu^{\beta,\mu}) - S(\mu) \geq -k\Big\{ &\sum_{N=1}^{\infty} \int_{\Gamma_{\Lambda,N}} (1 - \log Z - \beta H_\Lambda^{(N)}(x) + \beta\mu N)\rho_{\beta,\mu}^{(N)}(x)\mathrm{d}x \\
&+ (1 - \log Z)\rho_{\beta,\mu}^{(0)} - \sum_{N=1}^{\infty} \int_{\Gamma_{\Lambda,N}} (1 - \log Z - \beta H_\Lambda^{(N)}(x) + \beta\mu N)\rho_N(x))\mathrm{d}x \\
&- (1 - \log Z)\rho_0 \Big\} \\
&= -k\left\{(1 - \log Z - \beta E + \beta\mu N_0) - (1 - \log Z - \beta E + \beta\mu N_0)\right\} = 0.
\end{aligned}$$

Therefore

$$S(\mu^{\beta,\mu}) \geq S(\mu).$$

Note that the entropy for the grandcanonical ensemble is given by

$$S(\mu^{\beta,\mu}) = k \log Z_\Lambda(\beta,\mu) + k\beta\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(H_\Lambda) - k\beta\mu\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(\mathcal{N}).$$

□

Thermodynamic Functions:

We shall write Z for $Z_\Lambda(\beta,\mu)$ and we suppress for a while some obvious sub-indices and arguments. We have already defined the entropy S by

$$S = k \log Z + \frac{1}{T}(\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(H_\Lambda) - \mu\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(\mathcal{N})),$$

and as before we define the internal energy of the system U by $U = \mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(H_\Lambda)$. We then define the Helmholtz Free Energy as before by $A = U - TS$, and we shall call the Helmholtz Free Energy simply the free energy from now on. We have

$$\begin{aligned}
A =& U - TS = \mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(H_\Lambda) - T(k \log Z + \frac{1}{T}(\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(H_\Lambda) - \mu\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(\mathcal{N}))) \\
=& -\frac{1}{\beta}\left(\log Z - \mu\beta\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(\mathcal{N})\right).
\end{aligned}$$

In analogy with thermodynamics we should define the absolute **pressure** P of the system by

$$P = -\left(\frac{\partial A}{\partial V}\right)_T$$

with the constraint

$$\mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(\mathcal{N}) = \text{constant}.$$

This constraint means that μ is a function of V and β. Therefore

$$P = \frac{1}{\beta}\frac{\partial \mu}{\partial V}\frac{\partial}{\partial \mu}\left(\log Z - \mu\beta \mathbb{E}_{\gamma_\Lambda^{\beta,\mu}}(\mathcal{N})\right) + \frac{1}{\beta}\frac{\partial}{\partial V}\log Z = \frac{1}{\beta}\frac{\partial}{\partial V}\log Z.$$

It is argued that $\frac{1}{V}\log Z$ should be independent of V for large V and therefore we can write

$$\begin{aligned} P &= \frac{1}{\beta}\frac{\partial}{\partial V}\log Z = \frac{1}{\beta}\frac{\partial}{\partial V}\left(V\frac{1}{V}\log Z\right) = \frac{1}{\beta V}\log Z + \frac{V}{\beta}\frac{\partial}{\partial V}\left(\frac{1}{V}\log Z\right) \\ &\approx \frac{1}{\beta V}\log Z. \end{aligned}$$

Therefore we define the pressure by the equation

$$P = \frac{1}{\beta V}\log Z.$$

This definition can be justified *a posteriori* when we consider the equivalence of ensembles, see Subsection 5.3. The other thermodynamic functions can be defined as usual:
The **Gibbs Potential** $G = U + PV - TS = A + PV$,
The **heat capacity** at constant volume, $C_V = \left(\frac{\partial U}{\partial T}\right)_V$. Note

$$S = -\left(\frac{\partial A}{\partial T}\right)_V$$

is also satisfied.

All the thermodynamic functions can be calculated from $Z = Z_\Lambda(\beta, \mu)$. Therefore all calculations in the grandcanonical ensemble begin with the calculation of the partition function $Z = Z_\Lambda(\beta, \mu)$.

4.4 The "orthodicity problem"

We refer to one of the main aims of statistical mechanics, namely to derive the known laws of classical thermodynamics from the ensemble theory. The following question is called the **Orthodicity Problem**.

Which set $\mathcal{E}$ of statistical ensembles or probability measures has the property that, as an element $\mu \in \mathcal{E}$ changes infinitesimally within the set $\mathcal{E}$, the corresponding infinitesimal variations $\mathrm{d}U$ and $\mathrm{d}V$ of U and V are related to the pressure P and to the average kinetic energy per particle,

$$\overline{T_{\text{kin}}} = \frac{\mathbb{E}_\mu(T_{\text{kin}})}{N} \quad , T_{\text{kin}} = \frac{1}{2m}\sum_{i=1}^{N} p_i^2,$$

such that the differential

$$\frac{\mathrm{d}U + P\mathrm{d}V}{\overline{T_{\mathrm{kin}}}}$$

is an exact differential at least in the thermodynamic limit. This will then provide the second law of thermodynamics. Let us provide a heuristic check for the canonical ensemble. Here,

$$\mathbb{E}^{\beta}_{\gamma_{\Lambda,N}}(T_{\mathrm{kin}}) = \frac{1}{Z_\Lambda(\beta,N)} \int_{\Gamma_{\Lambda,N}} T_{\mathrm{kin}}(x) \mathrm{e}^{-\beta H^{(N)}_\Lambda(x)} \mathrm{d}x,$$

and $U = -\partial_\beta Z_\Lambda(\beta,N)$. The pressure in the canonical ensemble can be calculated as

$$P(\gamma^{\beta}_{\Lambda,N}) = \sum_Q \frac{N}{Z_\Lambda(\beta,N)} \int_{p>0} \mathrm{e}^{-\beta H^{(N)}_\Lambda(x)} \frac{1}{2m} p^2 \frac{a}{A} \frac{\mathrm{d}q_2 \cdots \mathrm{d}q_N \mathrm{d}p_1 \cdots \mathrm{d}p_N}{N!},$$

where the sum goes over all small cubes Q adjacent to the boundary of the box Λ with volume V by a side with area a while $A = \sum_Q a$ is the total area of the container surface and q_1 is the centre of Q. Let $n(Q,v)\mathrm{d}v$, where $v = \frac{1}{2m}p$ is the velocity, be the density of particles with normal velocity $-v$ that are about to collide with the external walls of Q. Particles will cede a momentum $2mv = p$ in normal direction to the wall at the moment of their collision ($-mv \to mv$ due to elastic boundary conditions). Then

$$\sum_Q \int_{v>0} \mathrm{d}v n(Q,v)(2mv)\frac{va}{A}$$

is the momentum transferred per unit time and surface area to the wall. Gaussian calculation gives then after a couple of steps that due to $F_\Lambda(\beta,N) = -\beta^{-1}\log Z_\Lambda(\beta,N)$ and $S_\Lambda(E;N) = (U - F_\Lambda(\beta,N))\beta$ we have that $T = (k\beta)^{-1} = \frac{2}{dk}\frac{\overline{T_{\mathrm{kin}}}}{N}$, and that

$$T\mathrm{d}S_\Lambda = \mathrm{d}(F_\Lambda + TS_\Lambda) + p\mathrm{d}V = \mathrm{d}U + p\mathrm{d}V,$$

with $p = \beta^{-1}\frac{\partial}{\partial V}\log Z_\Lambda(\beta,N)$. Details can be found in [Gal99], where also references are provided for rigorous proofs for the orthodicity in the canonical ensemble. The orthodicity problem is more difficult in the microcanonical ensemble. The heuristic approach goes similar. However, for a rigorous proof of the orthodicity one needs here a proof that the expectation of the kinetic energy in the microcanonical ensemble satisfies

$$\mathbb{E}(T^\alpha_{\mathrm{kin}}) = \mathbb{E}(T_{\mathrm{kin}})^\alpha(1+\theta_N) \quad ,\alpha > 0,$$

with $\theta_N \to 0$ as $N \to \infty$ (thermodynamic limit). The last requirement would be easy for independent velocity, but this is not the case here due to the microcanonical energy constraint, and therefore this refers not to an application of the usual law of large numbers. A rigorous proof concerning any fluctuations and moments of the kinetic energy in the microcanonical ensemble is in preparation [AL06].

5 The Thermodynamic limit

In this section we introduce the concept of taking the *thermodynamic limit*, give a simple example in the microcanonical ensemble and prove in Subsection 5.2 the existence of the thermodynamic limit for the specific free energy in the canonical Gibbs ensemble for a given class of interactions. In the last subsection we briefly discuss the equivalence of ensembles and the thermodynamic limit at the level of states/measures.

5.1 Definition

Let us call **state** of a physical system an expectation value functional on the observable quantities for this system. The averages, i.e., the expectation values with respect to the Gibbs ensembles, are such states. We shall say that the systems for which the expectation with respect to the Gibbs ensembles is taken are **finite systems** (e.g. finitely many particles in a region with finite volume), but we may also consider the corresponding **infinite systems** which contain an infinity of subsystems and extend throughout $\mathbb{R}^d$ or $\mathbb{Z}^d$ for lattice systems. Thus the discussion in the introduction leads us to assume that the ensemble expectation for finite systems approach in some sense states/measures of the corresponding infinite system. Besides the existence of such limit states/measures one is also interested in proving that these are independent on the choice of the ensemble leading to the question of **equivalence of ensembles**. One of the main problems of equilibrium statistical mechanics is to study the infinite systems equilibrium states/measures and their relation to the interactions which give rise to them. In Section 6 we introduce the mathematical concept of Gibbs measures which appear as natural candidates for equilibrium states/measures. We turn down one level in our study and consider the problem of determination of the thermodynamic functions from statistical mechanics in the *thermodynamic limit*. We introduced earlier for each Gibbs ensemble a partition function, which is the total mass of the measure defining the Gibbs ensemble. The logarithm of the partition function divided by the volume of the region Λ containing the system has a

limit when this systems becomes large ($\Lambda \uparrow \mathbb{R}^d$), and this limit is identified with a thermodynamic function. Any singularities for these thermodynamic functions in the thermodynamic limit may correspond to phase transitions (see [Min00],[Gal99] and [EL02] for details on theses singularities).

Taking the **thermodynamic limit** thus involves letting Λ tend to infinity, i.e., approaching $\mathbb{R}^d$ or $\mathbb{Z}^d$ respectively. We have to specify how Λ tends to infinity. Roughly speaking we consider the following notion.

Notation 5.1 (Thermodynamic limit) *A sequence $(\Lambda_n)_{n\in\mathbb{N}}$ of boxes $\Lambda_n \subset \mathbb{R}^d$ is a* **cofinal** *sequence approaching $\mathbb{R}^d$ if the following holds,*

(i) $\Lambda_n \uparrow \mathbb{R}^d$ *as* $n \to \infty$,

(ii) If $\Lambda_n^h = \{x \in \mathbb{R}^d \colon \mathrm{dist}(x, \partial\Lambda) \leq h\}$ *denotes the set of points with distance less or equal h to the boundary of Λ, the limit*

$$\lim_{n\to\infty} \frac{|\Lambda_n^h|}{|\Lambda|} = 0$$

exists.

The thermodynamic limit consists thus in letting $n \to \infty$ for a cofinal sequence $(\Lambda_n)_{n\in\mathbb{N}}$ of boxes with the following additional requirements for the microcanonical and the canonical ensemble:

Microcanonical ensemble: *There are energy densities $\varepsilon_n \in (0,\infty)$, given as $\varepsilon_n = \frac{E_n}{|\Lambda_n|}$ with $E_n \to \infty$ as $n \to \infty$, and particle densities $\rho_n \in (0,\infty)$, given as $\rho_n = \frac{N_n}{\Lambda_n}$ with $N_n \to \infty$ as $n \to \infty$, such that $\varepsilon_n \to \varepsilon$ and $\rho_n \to \rho \in (0,\infty)$ as $n \to \infty$.*

Canonical ensemble: *There are particle densities $\rho_n \in (0,\infty)$, given as $\rho_n = \frac{N_n}{\Lambda_n}$ with $N_n \to \infty$ as $n \to \infty$, such that $\rho_n \to \rho \in (0,\infty)$ as $n \to \infty$.*

In some models one needs more assumptions on the cofinal sequence of boxes, for details see [Rue69] and [Isr79].

We check the thermodynamic limit of the following simple model in the microcanonical ensemble, which will give also another justification of the correct Boltzmann counting.

Ideal gas in the microcanonical ensemble

Consider a non-interacting gas of N identical particles of mass m in d dimensions, contained in the box Λ of volume $V = |\Lambda|$. The gradient of the

Hamiltonian for this system is

$$\nabla H_\Lambda(x) = \nabla \frac{1}{2m}\sum_{i=1}^{n} p_i^2 = \frac{1}{m}(0,\ldots,0,p_1,\ldots,p_n) \quad , x \in \Gamma_\Lambda,$$

where as usual $n = Nd$. We have

$$|\nabla H(x)|^2 = \frac{1}{m^2}\sum_{i=1}^{n} p_i^2 = \frac{2}{m}H(x) \quad , x \in \Gamma_\Lambda,$$

where $|\cdot|$ denotes the norm in $\mathbb{R}^{2n}$. Therefore on the energy surface Σ_E, $|\nabla H| = (\frac{2E}{m})^{\frac{1}{2}}$. Let $S_\nu(r)$ be the hyper sphere of radius r in ν dimensions, that is $S_\nu(r) = \{x|\ x \in \mathbb{R}^\nu, |x| = r\}$. Let $\mathfrak{S}_\nu(r)$ be the surface area of $S_\nu(r)$. Then

$$\mathfrak{S}_\nu(r) = c_\nu r^{\nu-1} \quad \text{for some constant } \ c_\nu.$$

For the non-interacting gas, we have $\Sigma_E = \Lambda^N \times S_n((2mE)^{\frac{1}{2}})$ and

$$\begin{aligned}\omega(E) &= \left(\frac{m}{2E}\right)^{\frac{1}{2}} \int_{\Sigma_E} \mathrm{d}\sigma = \left(\frac{m}{2E}\right)^{\frac{1}{2}} V^N \mathfrak{S}_n((2mE)^{\frac{1}{2}}) \\ &= \left(\frac{m}{2E}\right)^{\frac{1}{2}} V^N c_{Nd}(2mE)^{\frac{1}{2}(Nd-1)} = mV^N c_{Nd}(2mE)^{\frac{1}{2}Nd-1}.\end{aligned}$$

The entropy S is given by

$$\exp(S/k) = \omega(E) = mV^N c_{Nd}(2mE)^{\frac{1}{2}Nd-1}$$

and therefore

$$(2mE)^{\frac{1}{2}Nd-1} = \frac{\exp(S/k)V^{-N}}{mc_{dN}}.$$

Thus, the internal energy follows as

$$U(S,V) = E = \frac{1}{2m}\frac{\exp\left(\frac{2S}{k(Nd-2)}\right)V^{-\frac{2N}{(Nd-2)}}}{(mc_{Nd})^{\frac{2}{(Nd-2)}}},$$

and the temperature as the partial derivative of the internal energy with respect to the entropy is

$$T = \left(\frac{\partial U}{\partial S}\right)_V = \frac{2}{k(Nd-2)}U = \frac{2U}{kNd(1-\frac{2}{Nd})} \approx \frac{2U}{kNd}$$

for large N. This gives for large N the following relations

$$U \approx \frac{d}{2}NkT,$$

$$C_V = \Big(\frac{\partial U}{\partial T}\Big)_V \approx \frac{d}{2}Nk.$$

$$P = -\Big(\frac{\partial U}{\partial V}\Big)_S = \frac{2}{d(1-\frac{2}{Nd})}\frac{U}{V} \approx \frac{2U}{dV} \approx \frac{NkT}{V}.$$

The previous relation is the empirical ideal gas law in which k is Boltzmann's constant. We can therefore identify k in the definition of the entropy with Boltzmann's constant.
We need to calculate c_ν. We have via a standard trick

$$\begin{aligned}\pi^{\frac{\nu}{2}} &= \Big(\int_{-\infty}^{\infty} \mathrm{e}^{-x^2}\mathrm{d}x\Big)^\nu = \int_{\mathbb{R}^\nu} \mathrm{e}^{-|x|^2}\mathrm{d}x = \int_0^\infty \mathcal{S}_\nu(r)\mathrm{e}^{-r^2}\mathrm{d}r \\ &= c_\nu \int_0^\infty r^{\nu-1}\mathrm{e}^{-r^2}\mathrm{d}r = \frac{c_\nu}{2}\int_0^\infty t^{\frac{\nu}{2}-1}\mathrm{e}^{-t}\mathrm{d}t = \frac{c_\nu}{2}\Gamma\Big(\frac{\nu}{2}\Big).\end{aligned}$$

This gives $c_\nu = \frac{2\pi^{\frac{\nu}{2}}}{\Gamma(\frac{\nu}{2})}$, where Γ is the Gamma-Function, defined as

$$\Gamma(x) = \int_0^\infty t^{x-1}\mathrm{e}^{-t}\mathrm{d}t.$$

Note that if $n \in \mathbb{N}$ then $\Gamma(n) = (n-1)!$. The behaviour of $\Gamma(x)$ for large positive x is given by Stirling's formula

$$\Gamma(x) \approx \sqrt{2\pi}x^{x-\frac{1}{2}}\mathrm{e}^{-x}.$$

This gives $\lim_{x\to\infty}(\frac{1}{x}\log\Gamma(x) - \log x) = -1$. We now have for the entropy of the non-interacting gas in a box Λ of volume V

$$S_\Lambda(E,N) = k\log\Big(mV^N\frac{2\pi^{\frac{Nd}{2}}}{\Gamma(\frac{Nd}{2})}(2mE)^{\frac{1}{2}Nd-1}\Big).$$

Let v be the *specific volume* and ε the *energy per particle*, that is

$$v = \frac{V}{N} \quad \text{and} \quad \varepsilon = \frac{E}{N}.$$

Let $s_N(\varepsilon, v)$ be the entropy per particle considered as a function of ε and v,

$$s_N(\varepsilon, v) = \frac{1}{N}S_{\Lambda_N}(\varepsilon N, N),$$

where Λ_N is a sequence of boxes with volume vN. Then

$$\begin{aligned}
s_N(\varepsilon, v) &= \frac{1}{N} k \log\Big(m v^N N^N \frac{2\pi^{\frac{Nd}{2}}}{\Gamma(\frac{Nd}{2})} (2m\varepsilon N)^{\frac{1}{2}Nd-1}\Big) \\
&\approx k\left(\log v + \frac{d+2}{2}\log N + \frac{d}{2}\log(4\pi m\varepsilon) - \frac{1}{N}\log\Gamma\Big(\frac{Nd}{2}\Big)\right) \\
&\approx k\left(\log v + \log N + \frac{d}{2}\log(4\pi m\varepsilon) + \frac{d}{2} - \frac{d}{2}\log(\frac{d}{2})\right) \\
&\approx k\log N.
\end{aligned}$$

We expect $s_N(\varepsilon, v)$ to be finite for large N. Gibbs (see Section 4.2) postulated that we have made an error in calculating $\omega(E)$, the number of states of the gas with energy E. We must divide $\omega(E)$ by $N!$. It is not possible to understand this classically since in classical mechanics particles are distinguishable. The reason is inherently quantum mechanical. In quantum mechanics particles are indistinguishable. We also divide $\omega(E)$ by h^{dN} where h is Planck's constant. This makes classical and quantum statistical mechanics compatible for high temperatures.
We therefore redefine the **microcanonical entropy** of the system to be

$$S_\Lambda(E, N) = k\log\Big(\frac{\omega_\Lambda(E,N)}{(n/d)!}\Big) = k\log\Big(\frac{\omega_\Lambda(E,N)}{N!}\Big), \tag{5.21}$$

where we put Planck's constant $h = 1$. Then

$$\begin{aligned}
s_N(\varepsilon, v) \approx k\Bigg(&\log v + \log N + \frac{d}{2}\log(4\pi m\varepsilon) + \frac{d}{2} - \frac{d}{2}\log(\frac{d}{2}) - d\log h \\
&-\frac{1}{N}\log(N!)\Bigg) \\
\to k&\left(\frac{d+2}{2} + \log v + \frac{d}{2}\log\varepsilon - \frac{d}{2}\log\Big(\frac{h}{\sqrt{4\pi m}}\Big) - \frac{d}{2}\log(\frac{d}{2})\right)
\end{aligned}$$

as $N \to \infty$.

5.2 Thermodynamic function: Free energy

We shall prove that the canonical free energy density exists in the thermodynamic limit for very general interactions. We consider a general interacting gas of N identical particles of mass m in d dimensions, contained in the box Λ of volume of V with elastic boundary conditions. The Hamiltonian for this system is

$$H_\Lambda^{(N)} = \frac{1}{2m}\sum_{i=1}^{N} p_i^2 + U(r_1, \ldots, r_N).$$

We have for the partition function $Z_\Lambda(\beta, N)$

$$Z_\Lambda(\beta, N) = \frac{1}{N!\ h^{Nd}} \int_\Gamma \mathrm{e}^{-\beta H_\Lambda^{(N)}(x)} \mathrm{d}x = \frac{1}{N!} \left(\int_{\mathbb{R}^d} \mathrm{e}^{-\frac{\beta p^2}{2m}} \mathrm{d}p \right)^N \int_{\Lambda^N} \mathrm{e}^{-\beta U(q)} \mathrm{d}q$$
$$= \frac{1}{N!} \left(\frac{2\pi m}{h^2 \beta} \right)^{\frac{1}{2}Nd} \int_{\Lambda^N} \mathrm{e}^{-\beta U(q)} \mathrm{d}q = \frac{1}{N!} \frac{1}{\lambda^{dN}} \int_{\Lambda^N} \mathrm{e}^{-\beta U(q)} \mathrm{d}q.$$

We shall assume that the interaction potential is given by a **pair interaction potential** $\phi\colon \mathbb{R} \to \mathbb{R}$, that is

$$U(q_1, \ldots, q_N) = \sum_{1 \le i < j \le N} \phi(|q_i - q_j|) \quad , (q_1, \ldots, q_N) \in \mathbb{R}^{dN},$$

where $|x|$ denotes the norm for a the vector $x \in \mathbb{R}^d$.

Definition 5.2 *Let the pair potential function $\phi\colon \mathbb{R} \to \mathbb{R}$ be given.*

(i) The pair potential ϕ is **tempered** *if there exists $R > 0$ such that $\phi(|q|) \le 0$ if $|q| > R, q \in \mathbb{R}^d$.*

(ii) The pair potential ϕ is **stable** *if there exists $B \ge 0$ such that for all $q_1, r_2, \ldots, q_N$ in $\mathbb{R}^d$*

$$\sum_{1 \le i < j \le N} \phi(|q_i - q_j|) \ge -NB.$$

(iii) If the pair potential ϕ is not stable then it is said to be **catastrophic**.

Recall that the free energy in a box $\Lambda \subset \mathbb{R}^d$ for an inverse temperature β and particle number N is given by

$$A_\Lambda(\beta, N) = -\frac{1}{\beta} \log Z_\Lambda(\beta, N).$$

Theorem 5.3 (Fisher-Ruelle) *Let ϕ be a stable and tempered pair potential. Let R be as above in Definition 5.2 and for $\rho \in (0, \infty)$ let L_0 be such that $\rho(L_0 + R)^d \in \mathbb{N}$. Let $L_n = 2^n(L_0 + R) - R$ and let Λ_n be the cube centred at the origin with side L_n and volume $V_n = |\Lambda_n| = L_n^d$. Let $N_n = \rho(L_0 + R)^d 2^{dn}$. If*

$$f_n(\beta, \rho) = \frac{1}{V_n} A_{\Lambda_n}(\beta, N_n),$$

then $\lim_{n\to\infty} f_n(\beta, \rho)$ exists.

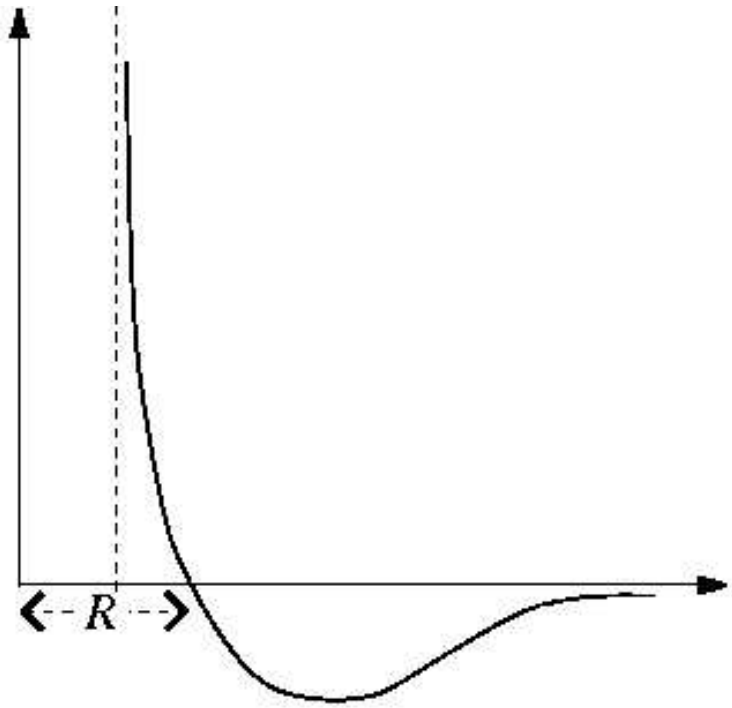

Figure 1: typical form of ϕ

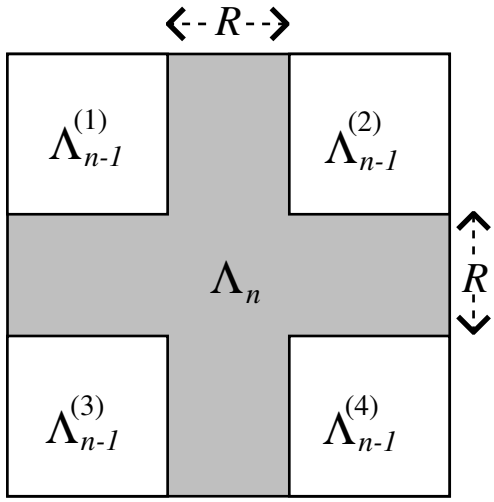

Figure 2: Λ_n contains 4 cubes of side length L_{n-1}

Proof. Note that $\lim_{n\to\infty} N_n/V_n = \rho$. Note also that $N_n = 2^d N_{n-1}$ and $L_n = 2L_{n-1} + R$. Because of the last equation Λ_n contains 2^d cubes of side L_{n-1} with a corridor of width R between them. Denote these by $\Lambda^{(i)}_{n-1}, i = 1, \ldots, 2^d$ and let

$$U_N(q_1, \ldots, q_N) = \sum_{1\le i<j\le N} \phi(|q_i - q_j|).$$

Let $Z_n = Z_{\Lambda_n}(\beta, N_n)$ and $g_n = \frac{1}{N_n} \log Z_n$. It is sufficient to prove that g_n converges.

$$Z_n = \frac{1}{N_n! \lambda^{dN_n}} \int_{\Lambda_n^{N_n}} \mathrm{d}q_1 \ldots \mathrm{d}q_{N_n} \mathrm{e}^{-\beta U_{N_n}(q_1,\ldots,q_{N_n})}.$$

Let

$$\Omega_n = \{(r_1, \ldots r_{N_n}) \in \Lambda_n^{N_n} |\ \text{ each } \ \Lambda^{(i)}_{n-1} \ \text{ contains } N_{n-1}\ r_k\text{'s}\}.$$

Note that for $(q_1, \ldots q_{N_n}) \in \Omega_n$ there are no r_k's in the corridor between the $\Lambda^{(i)}_{n-1}$.

Let

$$\tilde{\Omega}_n = \{(q_1, \ldots q_{N_n}) \in \Lambda_n^{N_n} \colon q_1, \ldots, q_{N_{n-1}} \in \Lambda^{(1)}_{n-1}, q_{N_{n-1}+1}, \ldots, q_{2N_{n-1}} \in \Lambda^{(2)}_{n-1}, \\ \ldots, q_{(2^d-1)N_{n-1}+1}, \ldots q_{2^d N_{n-1}} \in \Lambda^{(2^d)}_{n-1}\}.$$

Since $\Omega_n \subset \Lambda_n^{N_n}$

$$\begin{aligned} Z_n &\geq \frac{1}{N_n!\lambda^{dN_n}} \int_{\Omega_n} \mathrm{d}q_1 \dots \mathrm{d}q_{N_n} \mathrm{e}^{-\beta U_{N_n}(q_1,\dots,q_{N_n})} \\ &= \frac{N_n!}{(N_{n-1}!)^{2^d}} \frac{1}{N_n!} \frac{1}{\lambda^{dN_n}} \int_{\tilde{\Omega}_n} \mathrm{d}q_1 \dots \mathrm{d}q_{N_n} \mathrm{e}^{-\beta U_{N_n}(q_1,\dots q_{N_n})}. \end{aligned}$$

Since ϕ is tempered, we get for $q_1, \dots, q_{N_n} \in \tilde{\Omega}_n$

$$\begin{aligned} U_{N_n}(q_1, \dots, q_{N_n}) \leq & U_{N_{n-1}}(q_1, \dots, q_{N_{n-1}}) \dots \\ & + U_{N_{n-1}}(q_{(2^d-1)N_{n-1}+1}, \dots, q_{2^d N_{n-1}}). \end{aligned}$$

Thus

$$\begin{aligned} Z_n &\geq \frac{1}{(N_{n-1}!))^{2^d}} \frac{1}{\lambda^{dN_n}} \left(\int_{\Lambda_{n-1}^{N_{n-1}}} \mathrm{d}q_1 \dots \mathrm{d}q_{N_{n-1}} \mathrm{e}^{-\beta U_{N_{n-1}}(q_1,\dots,q_{N_{n-1}})} \right)^{2^d} \\ &= (Z_{n-1})^{2^d}. \end{aligned}$$

Therefore

$$g_n = \frac{1}{N_n} \log Z_n = \frac{1}{2^d N_{n-1}} \log Z_n \geq \frac{1}{2^d N_{n-1}} \log (Z_{n-1})^{2^d} = g_{n-1}.$$

The sequence $(g_n)_{n\in\mathbb{N}}$ is increasing. To prove that g_n converges it is sufficient to show that g_n is bounded from above. Since the pair potential ϕ is stable we have

$$U_{N_n}(q_1, \dots, q_{N_n}) \geq -BN_n$$

and therefore

$$\begin{aligned} Z_n &= \frac{1}{N_n!\lambda^{dN_n}} \int_{\Lambda_n^{N_n}} \mathrm{d}q_1 \dots \mathrm{d}q_{N_n} \mathrm{e}^{-\beta U_{N_n}(q_1,\dots,q_{N_n})} \\ &\leq \frac{1}{N_n!\lambda^{dN_n}} \int_{\Lambda_n^{N_n}} \mathrm{d}q_1 \dots \mathrm{d}q_{N_n} \mathrm{e}^{\beta B N_n} \leq \frac{{V_n}^{N_n}}{N_n!\lambda^{dN_n}} \mathrm{e}^{\beta B N_n}. \end{aligned}$$

Thus

$$\begin{aligned} g_n &\leq \log V_n - \frac{1}{N_n} \log N_n! - d \log \lambda + \beta B = -\log \left(\frac{N_n}{V_n} \right) + \log N_n \\ &\quad - \frac{1}{N_n} \log N_n! - d \log \lambda + \beta B \\ &\leq -\log \rho + 2 - d \log \lambda + \beta B \end{aligned}$$

for large n since

$$\lim_{n\to\infty} \frac{N_n}{V_n} = \rho \text{ and } \lim_{n\to\infty} \left(\log N_n - \frac{1}{N_n} \log N_n! \right) = 1.$$

□

5.3 Equivalence of ensembles

The equivalence of the Gibbs ensemble is the key problem of equilibrium statistical mechanics. It goes back to Gibbs 1902, who conjectured that both the canonical and the grandcanonical Gibbs ensemble are equivalent with the microcanonical ensemble. The main difficulty to answer the question of equivalence lies in the precise definition of the notion equivalence. Nowadays the term can have three different meanings, each on a different level of information. We briefly introduce these concepts, but refer for details to one of the following research articles ([Ada01], [Geo95], [Geo93]).

Equivalence at the level of thermodynamic functions

Under general assumptions on the interaction potential, e.g. stability and temperedness as in Subsection 5.2, one is able to prove the following thermodynamic limits of the thermodynamic functions given by the three Gibbs ensembles. Let $(\Lambda_n)_{n\in\mathbb{N}}$ be any cofinal sequence of boxes with corresponding sequences of energy densities $(\varepsilon_n)_{n\in\mathbb{N}}$ and particle densities $(\rho_n)_{n\in\mathbb{N}}$. Then there is a closed packing density $\rho^{(\mathrm{cp})} \in (0,\infty)$ and an energy density $\varepsilon(\rho) \in (0,\infty)$ such that the following limits exist under some additional requirements (details are in [Rue69]) depending on the specific model chosen.

Grandcanonical Gibbs ensemble Let $\beta > 0$ be the inverse temperature and $\mu \in \mathbb{R}$ the chemical potential. Then the function $p(\beta,\mu)$, defined by

$$\beta p(\beta,\mu) = \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \log Z_{\Lambda_n}(\beta,\mu),$$

is called the **pressure**.

Canonical Gibbs ensemble Let $\beta > 0$ be the inverse temperature and $(\rho_n)_{n\in\mathbb{N}}$ with $\rho_n \to \rho \in (0,\rho^{(\mathrm{cp})})$ a sequence of particle densities $\rho_n = \frac{N_n}{|\Lambda_n|}$. Then the function $f(\beta,\rho)$, defined by

$$-\beta f(\beta,\rho) = \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \log Z_{\Lambda_n}(\beta,\rho_n|\Lambda_n|),$$

is called the **free energy**.

Microcanonical Gibbs ensemble Let $(\rho_n)_{n\in\mathbb{N}}$ with $\rho_n \to \rho \in (0,\rho^{(\mathrm{cp})})$ be a sequence of particle densities $\rho_n = \frac{N_n}{|\Lambda_n|}$, and let $(\varepsilon_n)_{n\in\mathbb{N}}$ with $\varepsilon_n \to \varepsilon \in (\varepsilon(\rho),\infty)$ be a sequence of energy densities $\varepsilon_n = \frac{E_n}{|\Lambda_n|}$. Then the function

$$s(\varepsilon,\rho) = \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \log \omega_{\Lambda_n}(\varepsilon_n|\Lambda_n|),\rho_n|\Lambda_n|) \quad \text{is called } \textbf{entropy}.$$

Now equivalence at the level of thermodynamic functions is given if all three thermodynamic functions in the thermodynamic limit are related to each other by a Legendre-Fenchel transform for specific regions of parameter regions of ε, ρ, β and μ. Roughly speaking this kind of equivalence is mainly given in absence of phase transitions, i.e., only for those parameters where there are no singularities. For details see the monograph [Rue69], where the following transforms are established.

$$\begin{aligned}
\beta p(\beta,\mu) &= \sup_{\rho\le\rho^{(\mathrm{cp})},\varepsilon>\varepsilon(\rho)} \{s(\varepsilon,\rho)-\beta\varepsilon-\rho\mu\} \\
f(\beta,\rho) &= \inf_{\varepsilon>\varepsilon(\rho)} \{\varepsilon-\beta^{-1}s(\varepsilon,\rho)\} \\
p(\beta,\mu) &= \sup_{\rho\le\rho^{(\mathrm{cp})}} \{\rho\mu-f(\beta,\rho)\}.
\end{aligned}$$

Equivalence at the level of canonical and microcanonical Gibbs measures

In Section 6 we introduce the concept of Gibbs measures. A similar concept can be formulated for canonical Gibbs measures (see [Geo79] for details) as well as for microcanonical Gibbs measures (see [Tho74] and [AGL78] for details). The idea behind these concepts is roughly speaking to condition outside any finite region on particle density and energy density events.
Equivalence at the level of canonical and microcanonical Gibbs measures is then given if the microcanonical and canonical Gibbs measures are certain convex combinations of Gibbs measures (see details in [Tho74], [AGL78] and [Geo79]).

Equivalence at the level of states/measures

At the level of states/measures one is interested in any weak (in the sense of probability measures, i.e., weak-$*$-topology) limit points (accumulation points) of the Gibbs ensembles. To define a consistent limiting procedure we need an appropriate phase or configuration space for the infinite systems in the thermodynamic limit. We consider here only continuous systems whose phase space (configuration space) for any finite region Λ and finitely many particles is Γ_Λ. In Section 6 we introduce the corresponding configuration space for lattice systems. Define

$$\Gamma = \{\omega \subset (\mathbb{R}^d \times \mathbb{R}^d) \colon \omega = \{(q,p_q) \colon q \in \hat{\omega}\}\},$$

where $\hat{\omega}$, the set of occupied positions, is a locally finite subset of $\mathbb{R}^d$, and p_q is the momentum of the particle at position q. Let $\mathcal{B}$ denote the σ-algebra of

this set generated by counting variables (see [Geo95] for details). Then each Gibbs ensemble can be extended trivially to a probability on $(\Gamma, \mathcal{B})$ just by putting the whole mass on a subset. Therefore it makes sense to consider all weak limit points in the thermodynamic limit. If the limit points are not unique, i.e., there are several accumulation points, one considers the whole set of accumulation points closed appropriately as the set of equilibrium states/measure or Gibbs measures.
Equivalence at the level of states/measures is given if all accumulation points of the different Gibbs ensembles belong to the same set of equilibrium points or the same set of Gibbs measure ([Geo93],[Geo95],[Ada01]).

In the next section we develop the mathematical theory for Gibbs measures without any limiting procedure.

6 Gibbs measures

In this section we introduce the mathematical concept of Gibbs measures, which are natural candidates to be the equilibrium measures for infinite systems, i.e., for systems after taking the thermodynamic limit. We will restrict our study from now on to lattice systems, i.e., the phase space is given as the set of functions (configurations) on some countable discrete set with values in a finite set, called the state space.

6.1 Definition

Let $\mathbb{Z}^d$ the square lattice for dimensions $d \geq 1$ and let E be any finite set. Define $\Omega := E^{\mathbb{Z}^d} = \{\omega = (\omega_i)_{i\in\mathbb{Z}^d} \colon \omega_i \in E\}$ the set of configurations with values in the state space E. Let $\mathcal{E}$ be the power set of E, and define the $\sigma-$algebra $\mathcal{F} = \mathcal{E}^{\mathbb{Z}^d}$ such that $(\Omega, \mathcal{F})$ is a measurable space. Denote the set of all probability measures on $(\Omega, \mathcal{F})$ by $\mathcal{P}(\Omega, \mathcal{F})$.

Definition 6.1 (Random field) *Let $\mu \in \mathcal{P}(\Omega, \mathcal{F})$. Any family $(\sigma_i)_{i\in\mathbb{Z}^d}$ of random variables which is defined on the probability space $(\Omega, \mathcal{F}, \mu)$ and which takes values in $(E, \mathcal{E})$ is called a* **random field**.

If one considers the canonical setup, where $\sigma_i \colon \Omega \to E$ are the projections for any $i \in \mathbb{Z}^d$, a random field is synonymous with a probability measure $\mu \in \mathcal{P}(\Omega, \mathcal{F})$. Let $\mathcal{S} = \{\Lambda \subset \mathbb{Z}^d \colon |\Lambda| < \infty\}$ be the set of finite volume subsets of the square lattice $\mathbb{Z}^d$. Cylinder events are defined as $\{\sigma_\Lambda \in A\}$ for any $A \in \mathcal{E}^\Lambda$ and any projection $\sigma_\Lambda \colon \Omega \to E^\Lambda$ for $\Lambda \in \mathcal{S}$. Then $\mathcal{F}$ is the smallest σ- algebra containing all cylinder events. If $\Lambda \in \mathcal{S}$ the $\sigma-$ algebra $\mathcal{F}_\Lambda$ on Ω contains all cylinder events $\{\sigma_{\Lambda'0} \in A\}$ for all $A \in \mathcal{E}$ and $\Lambda' \subset \Lambda$.

If we return to our physical intuition we are interested in random fields for which the so-called spin variables σ_i exhibit a particular type of dependence. We employ a similar dependence structure as for Markov chains, where the dependence is expressed as a condition on past events. This approach was introduced by Dobrushin ([Dob68a],[Dob68b],[Dob68c]) and Lanford and Ruelle ([LR69]). Here, we condition on the complement of any finite set $\Lambda \subset \mathbb{Z}^d$. To prescribe these conditional distributions of all finite collections of variables we define the σ-algebras

$$\mathcal{T}_\Lambda = \mathcal{F}_{\mathbb{Z}^d \setminus \Lambda} \quad \text{for any } \Lambda \in \mathcal{S}. \tag{6.22}$$

The intersection of all these σ-algebras is denoted by $\mathcal{T} = \cap_{\Lambda \in \mathcal{S}} \mathcal{T}_\Lambda$ and called the **tail-σ-algebra** or **tail-field**.
The dependence structure will be described by some functions linking the random variables and expressing the energy for a given dependence structure.

Definition 6.2 *An* **interaction potential** *is a family $\Phi = (\phi_A)_{A \in \mathcal{S}}$ of functions $\phi_A \colon \Omega \to \mathbb{R}$ such that the following holds.*

(i) ϕ_A is $\mathcal{F}_A$-measurable for all $A \in \mathcal{S}$,

(ii) For any $\Lambda \in \mathcal{S}$ and any configuration $\omega \in \Omega$ the expression

$$H_\Lambda(\omega) = \sum_{A \in \mathcal{S}, A \cap \Lambda \neq \emptyset} \phi_A(\omega) \tag{6.23}$$

exists. The term $\exp(-\beta H_\Lambda(\omega))$ is called the **Boltzmann factor** *for some parameter $\beta > 0$, where β is the inverse temperature.*

Example 6.3 (Pair potential) *Let $\phi_A = 0$ whenever $|A| > 2$ and let $J \colon \mathbb{Z}^d \times \mathbb{Z}^d \to \mathbb{R}$, $\varphi \colon E \times E \to \mathbb{R}$ and $\psi \colon E \to \mathbb{R}$ symmetric and measurable. Then a general pair interaction potential is given by*

$$\phi_A(\omega) = \begin{cases} J(i,j)\varphi(\omega_i, \omega_j) & \text{if } A = \{i,j\}, i \neq j, \\ J(i,i)\psi(\omega_i) & \text{if } A = \{i\}, \\ 0 & \text{if } |A| > 2 \end{cases} \qquad \text{for } \omega \in \Omega.$$

We combine configurations outside and inside of any finite set of random variable as follows. Let $\omega \in \Omega$ and $\xi \in \Omega_\Lambda, \Lambda \in \mathcal{S}$, be given. Then $\xi\omega_{\mathbb{Z}^d \setminus \Lambda} \in \Omega$ with $\sigma_\Lambda(\xi\omega_{\mathbb{Z}^d \setminus \Lambda}) = \xi$ and $\sigma_{\mathbb{Z}^d \setminus \Lambda}(\xi\omega_{\mathbb{Z}^d \setminus \Lambda}) = \omega_{\mathbb{Z}^d \setminus \Lambda}$. With this notation we can define a nearest-neighbour Hamiltonian with given boundary condition.

Example 6.4 (Hamiltonian with boundary) *Let $\Lambda \in \mathcal{S}$ and $\eta \in \Omega$ and the functions J, φ and ψ as in Example 6.3 be given. Then*

$$H_\Lambda^\eta(\omega) = \frac{1}{2} \sum_{i,j\in\Lambda,\langle i-j\rangle=1} J(i,j)\varphi(\omega_i,\omega_j) + \sum_{\substack{i\in\Lambda, j\in\Lambda^c,\\ \langle i-j\rangle=1}} \varphi(\omega_i,\eta_j) + \sum_{i\in\Lambda} J(i,i)\psi(\omega_i)$$

denotes a Hamiltonian in Λ with nearest-neighbour interaction and with configurational boundary condition $\eta \in \Omega$, where $\langle x, y\rangle = \max_{i\in\{1,\dots,d\}} |x_i - y_i|$ for $x, y \in \mathbb{Z}^d$. Instead of a given configurational boundary condition one can model the free boundary condition and the periodic boundary condition as well.

In the following we fix a probability measure $\lambda \in \mathcal{P}(E, \mathcal{E})$ on the state space and call it the **reference** or **a priori measure**. Later we may also consider the Lebesgue measure as reference measure. Choosing a probability measure as a reference measure for finite sets Λ gives just a constant from normalisation.

Definition 6.5 (Gibbs measure)

(i) Let $\eta \in \Omega, \Lambda \in \mathcal{S}$, $\beta > 0$ the inverse temperature and Φ be an interaction potential. Define for any event $A \in \mathcal{F}$

$$\gamma_\Lambda^\Phi(A|\eta) = Z_\Lambda(\eta)^{-1} \int_{\Omega_\Lambda} \lambda^\Lambda(\mathrm{d}\omega) \mathbb{1}_A(\omega\eta_{\mathbb{Z}^d\setminus\Lambda}) \exp\Big(-\beta H_\Lambda(\omega\eta_{\mathbb{Z}^d\setminus\Lambda})\Big) \tag{6.24}$$

with normalisation or **partition function**

$$Z_\Lambda(\eta) = \int_{\Omega_\Lambda} \lambda^\Lambda(\mathrm{d}\omega) \exp\Big(-\beta H_\Lambda(\omega\eta_{\mathbb{Z}^d\setminus\Lambda})\Big).$$

Then $\gamma_\Lambda^\Phi(\cdot|\eta)$ is called the **Gibbs distribution** *in Λ with boundary condition $\eta_{\mathbb{Z}^d\setminus\Lambda}$, with interaction potential Φ, inverse temperature β and reference measure λ.*

(ii) A probability measure $\mu \in \mathcal{P}(\Omega, \mathcal{F})$ is a **Gibbs measure** *for the interaction potential Φ and inverse temperature β if*

$$\mu(A|\mathcal{F}_\Lambda) = \gamma_\Lambda^\Phi(A|\cdot) \quad \mu \text{ a.s. for all } A \in \mathcal{F}, \Lambda \in \mathcal{S}, \tag{6.25}$$

where γ_Λ^Φ is the Gibbs distribution for the parameter β (6.24). The set of Gibbs measures for inverse temperature β with interaction potential Φ is denoted by $\mathcal{G}(\Phi, \beta)$.

(iii) An interaction potential Φ is said to exhibit a first-order phase transition if $|\mathcal{G}(\Phi, \beta)| > 1$ for some $\beta > 0$.

If the interaction potential Φ is known we may skip the explicit appearance of the interaction potential and write instead $\mathcal{G}(\beta)$ for the set of Gibbs measure with inverse temperature β. However, the parameter β can ever be incorporated in the interaction potential Φ.

Remark 6.6

(i) $\gamma_\Lambda^\Phi(A|\cdot)$ is $\mathcal{T}_\Lambda$-measurable for any event $A \in \mathcal{F}$.

(ii) The equation (6.25) *is called the* **DLR-equation** *or* **DLR-condition** *in honour of R. Dobrushin, O. Lanford and D. Ruelle.*

6.2 The one-dimensional Ising model

In this subsection we study the one-dimensional Ising model. If the state space E is finite, then one can show a one-to-one correspondence between the set of all positive transition matrices and a suitable class of nearest-neighbour interaction potentials such that the set $\mathcal{G}(\Phi)$ of Gibbs measures is the singleton with the Markov chain distribution. This is essentially for a geometric reason in dimension one, the condition on the boundary is a two-sided Markov chain, for details see [Geo88]. A simple one-dimensional model which shows this equivalence was suggested 1920 by W. Lenz ([Len20]), and its investigation by E. Ising ([Isi24]) was a first and important step towards a mathematical theory of phase transitions. Ising discovered that this model fails to exhibit a phase transition and he conjectured that this will hold also in the multidimensional case. Nowadays we know that this is not true. In Subsection 6.4 we discuss the multidimensional case.

Let $E = \{-1, +1\}$ be the state space and consider the lattice $\mathbb{Z}$. At each site the spin can be *downwards*, i.e., -1, or be *upwards*, i.e., $+1$. The nearest-neighbour interaction is modelled by a constant J, called the *coupling* constant, through the expression $J\omega_i\omega_j$ for any $i, j \in \mathbb{Z}$ with $|i - j| = 1$:

$J > 0$: Any two adjacent spins have minimal energy if and only if they are aligned in that they have the same sign. This interaction is therefore **ferromagnetic**.

$J < 0$: Any two adjacent spins prefer to point in opposite directions. Thus this is a model of an **antiferromagnet**.

$h \in \mathbb{R}$: A constant h describes the action of an external field (directed upwards when $h > 0$).
Hence the nearest-neighbour interaction potential $\Phi^{J,h} = (\phi_A^{J,h})_{A\in\mathcal{S}}$ reads

$$\phi_A^{J,h}(\omega) = \begin{cases} -J\omega_i\omega_{i+1}\ , & \text{if } \ A = \{i, i+1\}, \\ -h\omega\ , & \text{if } \ A = \{i\}, \\ 0\ , & \text{else} \end{cases} \qquad \text{for } \ \omega \in \Omega. \tag{6.26}$$

We employ periodic boundary conditions, i.e., for $\Lambda \subset \mathbb{Z}$ finite and with $\Lambda = \{1, \ldots, |\Lambda|\}$ we set $\omega_{|\Lambda|+1} = \omega_1$ for any $\omega \in \Omega$. The Hamiltonian in Λ with periodic boundary conditions reads

$$H_\Lambda^{(\mathrm{per})}(\omega) = -J \sum_{i=1}^{|\Lambda|} \omega_i\omega_{i+1} - h \sum_{i=1}^{|\Lambda|} \omega_i. \tag{6.27}$$

The partition function depends on the inverse temperature $\beta > 0$, the coupling constant J and the external field $h \in \mathbb{R}$, and is given by

$$Z_\Lambda(\beta, J, h) = \sum_{\omega_1=\pm1} \cdots \sum_{\omega_{|\Lambda|}=\pm1} \exp\Big(-\beta H_\Lambda^{(\mathrm{per})}(\omega)\Big). \tag{6.28}$$

We compute this by the one-dimensional version of *transfer matrix formalism* introduced by [KW41] for the two-dimensional Ising model. More details about this formalism and further investigations on lattice systems can be found in [BL99a] and [BL99b]. Crucial is the identity

$$Z_\Lambda(\beta, J, h) = \sum_{\omega_1=\pm1} \cdots \sum_{\omega_{|\Lambda|}=\pm1} V_{\omega_1,\omega_2} V_{\omega_2,\omega_3} \cdots V_{\omega_{|\Lambda|-1},|\Lambda|} V_{\omega_{|\Lambda|},\omega_1}$$

with

$$V_{\omega_i\omega_{i+1}} = \exp\Big(\frac{1}{2}\beta h\omega_i + \beta J\omega_i\omega_{i+1} + \frac{1}{2}\beta h\omega_{i+1}\Big)$$

for any $\omega \in \Omega$ and $i = 1, \ldots, |\Lambda|$. Hence, $Z_\Lambda(\beta, J, h) = \mathrm{Trace}\, \mathbb{V}^{|\Lambda|}$ with the symmetric matrix

$$\mathbb{V} = \begin{pmatrix} \mathrm{e}^{\beta(J+h)} & \mathrm{e}^{-\beta J} \\ \mathrm{e}^{-\beta J} & \mathrm{e}^{\beta(J-h)} \end{pmatrix}$$

that has the eigenvalues

$$\lambda_\pm = \mathrm{e}^{\beta J}\cosh(\beta h) \pm \Big(\mathrm{e}^{2\beta J}\sinh^2(\beta h) + \mathrm{e}^{-2\beta J}\Big)^{\frac{1}{2}}. \tag{6.29}$$

This gives finally

$$Z_\Lambda(\beta, J, h) = \lambda_+^{|\Lambda|} + \lambda_-^{|\Lambda|}. \tag{6.30}$$

This is a smooth expression in the external field parameter h and the inverse temperature β; it rules out the appearance of a discontinuous isothermal magnetisation: so far, *no* phase transition. The thermodynamic limit of the free energy per volume is

$$f(\beta, J, h) = \lim_{\Lambda \uparrow \mathbb{Z}} \frac{1}{\beta|\Lambda|} \log Z_\Lambda(\beta, J, h) = -\frac{1}{\beta} \log \lambda_+, \tag{6.31}$$

because $|\Lambda|^{-1} \log Z_\Lambda(\beta, J, h) = -\log \lambda_+ - \frac{1}{|\Lambda|}\Big(1 + (\frac{\lambda_-}{\lambda_+})^{|\Lambda|}\Big)$. The magnetisation in the canonical ensemble is given as the partial derivative of the specific free energy per volume,

$$m(\beta, J, h) = -\partial_h f(\beta, J, h) = \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + \mathrm{e}^{-4\beta J}}}.$$

This is symmetric, $m(\beta, J, 0) = 0$ and $\lim_{h \to \pm\infty} m(\beta, J, h) = \pm 1$ and for all $h \neq 0$ we have $|m(\beta, J, h)| > |m(\beta, 0, h)|$ saying that the absolute value of the magnetisation is increased by the non-vanishing coupling constant J. The set $\mathcal{G}(\Phi, \beta)$ of Gibbs measures contains only one element, called $\mu^\beta_{J,h}$, see [Geo88] for the explicit construction of this measure as the corresponding Markov chain distribution, here we outline only the main steps.
1.) The nearest-neighbour interaction $\Phi^{J,h}$ in (6.26) defines in the usual way the Gibbs distributions $\gamma^{J,h}_\Lambda(\cdot|\omega)$ for any finite $\Lambda \subset \mathbb{Z}$ and any boundary condition $\omega \in \Omega$. Define the function $g\colon E^3 \to (0, \infty)$ by

$$\gamma^{J,h}_{\{i\}}(\sigma_i = y|\omega) = g(\omega_{i-1}, y, \omega_{i+1}), \quad y \in E, i \in \mathbb{Z}, \omega \in \Omega. \tag{6.32}$$

We compute

$$g(x, y, z) = \mathrm{e}^{\beta y(h + Jx + Jz)}/2\cosh(\beta(h + Jx + Jz)) \quad \text{for } x, y, z \in E. \tag{6.33}$$

Fix any $a \in E$. Then the matrix

$$Q = \left(\frac{g(a, x, y)}{g(a, a, y)}\right)_{x,y \in E} \tag{6.34}$$

is positive. By the well-known theorem of Perron and Frobenius we have a unique positive eigenvalue q such that there is a strictly positive right eigenvector r corresponding to q.
2.) The matrix $P_{J,h}$, defined as

$$P_{J,h} = \left(\frac{Q(x, y)r(y)}{qr(x)}\right)_{x,y \in E} \tag{6.35}$$

is uniquely determined by the matrix Q and therefore by g in (6.33). Clearly, $P_{J,h}$ is stochastic. We then let $\mu^{\beta}_{J,h} \in \mathcal{P}(\Omega)$ denote (the distribution of) the unique stationary Markov chain with transition matrix $P_{J,h}$. It is uniquely defined by

$$\mu^{\beta}_{J,h}(\sigma_i = x_0, \sigma_{i+1} = x_1, \ldots, \sigma_{i+n} = x_n) = \alpha_{P_{J,h}}(x_0) \prod_{i=1}^{n} P_{J,h}(x_{i-1}, x_i), \quad (6.36)$$

where $i \in \mathbb{Z}, n \in N, x_0, \ldots, x_n \in E$, and $\alpha_{P_{J,h}}$ satisfies $\alpha_{P_{J,h}} P_{J,h} = \alpha_{P_{J,h}}$.

The expectation at each site is given by

$$\mathbb{E}_{\mu_{J,h}}(\sigma_i) = \left(\mathrm{e}^{-4\beta J} + \sinh^2(\beta h)\right)^{-\frac{1}{2}} \sinh(\beta h) \quad , i \in \mathbb{Z}.$$

In the *low temperature limit* one is interested in the behaviour of the set $\mathcal{G}(\Phi, \beta)$ of Gibbs measures as $\beta \to \infty$. A configuration $\omega \in \Omega$ is called a **ground state** of the interaction potential Φ if for each site $i \in \mathbb{Z}$ the pair (ω_i, ω_{i+1}) is a minimal point of the function

$$\psi \colon \{-1, +1\}^2 \to \mathbb{R}; (x, y) \mapsto \psi(x, y) = -Jxy + \frac{1}{2}h(x + y).$$

Note that the interaction potential $\Psi = (\psi_A)_{A \in \mathcal{S}}$ with

$$\psi_A = \begin{cases} \psi(\sigma_i, \sigma_{i+1}) \ , & \text{if } A = \{i, i+1\} \\ 0 \ , & \text{otherwise} \end{cases}$$

is equivalent to the given nearest neighbour interaction potential Φ. We denote the constant configuration with only upward-spins by ω_+ (respectively the constant configuration with only downward-spins by ω_-). The Dirac measure on these constant configurations is denoted by δ_+ respectively δ_-. Then, for $h > 0$, we get that

$$\mu^{\beta}_{J,h} \to \delta_+ \quad \text{weakly in sense of probability measures as } \beta \to \infty,$$

and hence ω_+ is the unique ground state of the nearest-neighbour interaction potential Φ. Similarly, for $h < 0$, we get that

$$\mu^{\beta}_{J,h} \to \delta_- \quad \text{weakly in sense of probability measures as } \beta \to \infty,$$

and hence ω_- is the unique ground state of the nearest-neighbour interaction potential Φ. In the case $h = 0$ the nearest neighbour interaction potential Φ has precisely two ground states, namely ω_+ and ω_-, and hence we get

$$\mu^{\beta}_{J,0} \to \frac{1}{2}\delta_+ + \frac{1}{2}\delta_- \quad \text{weakly in sense of probability measures as } \beta \to \infty.$$

6.3 Symmetry and symmetry breaking

Before we study the two-dimensional Ising model, we briefly discuss the role of symmetries for Gibbs measures and their connections with phase transitions. As is seen by the spontaneous magnetisation below the Curie temperature, the spin system takes one of several possible equilibrium states each of which is characterised by a well-defined direction of magnetisation. In particular, these equilibrium states fail to be preserved by the spin reversal (**spin-flip**) transformation. Thus breaking of symmetries has some connection with the occurrence of phase transitions.
Let T denote the set of transformations

$$\tau\colon \Omega \to \Omega, \omega \mapsto (\tau_i \omega_{\tau_*^{-1} i})_{i\in\mathbb{Z}^d},$$

where $\tau_*\colon \mathbb{Z}^d \to \mathbb{Z}^d$ is any bijection of the lattice $\mathbb{Z}^d$, and the $\tau_i\colon E \to E, i \in \mathbb{Z}^d$, are invertible measurable transformations of E with measurable inverses. Each $\tau \in T$ is a composition of a spatial transformation τ_* and the spin transformations $\tau_i, i \in \mathbb{Z}^d$, which act separately at distinct sites of the square lattice $\mathbb{Z}^d$.

Example 6.7 (Spatial shifts) *Denote by* $\Theta = (\theta_i)_{i\in\mathbb{Z}^d}$ *the group of all* **spatial transformations** *or* **spatial shifts** *or* **shift transformations** $\theta_j\colon \Omega \to \Omega, (\omega_i)_{i\in\mathbb{Z}^d} \mapsto (\omega_{i-j})_{i\in\mathbb{Z}^d}$.

Example 6.8 (Spin-flip transformation) *Let the state space E be a symmetric Borel set of $\mathbb{R}$ and define the* **spin-flip** *transformation*

$$\tau\colon \Omega \to \Omega, (\omega)_{i\in\mathbb{Z}^d} \mapsto (-\omega_i)_{i\in\mathbb{Z}^d}.$$

Notation 6.9 *The set of all translation invariant probability measures on Ω is denoted by $\mathcal{P}_\Theta(\Omega, \mathcal{F}) = \{\mu \in \mathcal{P}(\Omega, \mathcal{F})\colon \mu = \mu \circ \theta_i^{-1} \text{ for any } i \in \mathbb{Z}^d\}$.*

The set of all translation invariant Gibbs measures for the interaction potential Φ and inverse temperature β is denoted by $\mathcal{G}_\Theta(\Phi, \beta) = \{\mu \in \mathcal{G}(\Phi, \beta)\colon \mu = \mu \circ \theta_i^{-1} \text{ for any } i \in \mathbb{Z}^d\}$.

Definition 6.10 (Symmetry breaking) *A symmetry $\tau \in T$ is said to be broken if there exists some $\mu \in \mathcal{G}(\Phi, \beta)$ such that $\tau(\mu) \neq \mu$ for some β.*

A direct consequence of symmetry breaking is that $|\mathcal{G}(\Phi, \beta)| > 1$, i.e., when there is a symmetry breaking the interaction potential exhibit a phase transition. There are models where all possible symmetries are broken as well as models where only a subset of symmetries is broken. A first example is the one-dimensional inhomogeneous Ising model, which is probably the

simplest model showing symmetry breaking. The one-dimensional inhomogeneous Ising model on the lattice $\mathbb{N}$ has the inhomogeneous nearest-neighbour interaction potential $\Phi = (\phi_A)_{A\in\mathcal{S}}$ defined for a sequence $(J_n)_{n\in\mathbb{N}}$ of real numbers $J_n > 0$ for all $n \in \mathbb{N}$ such that $\sum_{n\in\mathbb{N}} \mathrm{e}^{-2J_n} < \infty$, as follows

$$\phi_A = \begin{cases} -J_n\sigma_n\sigma_{n+1}\ , & \text{if } A = \{n, n+1\}, \\ 0 \text{ otherwise}\ , & \end{cases} .$$

This model is spatial inhomogeneous, the potential Φ is invariant under the spin-flip transformation τ, but some Gibbs measures are not invariant under this spin-flip transformation (for details see [Geo88]) for $\beta > 0$. The simplest spatial shift invariant model which exhibits a phase transition is the two-dimensional Ising model, which we will study in the next subsection 6.4. This model breaks the spin-flip symmetry while the shift-invariance is preserved. Another example of symmetry breaking is the discrete two-dimensional Gaussian model by Shlosman ([Shl83]). Here the spatial shift invariance is broken. More information can be found in [Geo88] or [GHM00].

6.4 The Ising ferromagnet in two dimensions

Let $E = \{-1, 1\}$ be the state space and define the nearest-neighbour interaction potential $\Phi = (\phi_A)_{A\in\mathcal{S}}$ as

$$\phi_A = \begin{cases} -\sigma_i\sigma_j\ , & \text{if } A = \{i, j\}, |i-j| = 1 \\ 0\ , & \text{otherwise} \end{cases} .$$

The interaction potential Φ is invariant under the spin flip transformation τ and the shift-transformations $\theta_i, i \in \mathbb{Z}^d$. Let δ_+, δ_- be the Dirac measures for the constant configurations $\omega_+ \in \Omega$ and $\omega_- \in \Omega$. The interaction potential takes its minimum at ω_+ and ω_-, hence ω_+ and ω_- are ground states for the system. The ground state generacy implies a phase transition if ω_+, ω_- are stable in the sense that the set of Gibbs measure $\mathcal{G}(\Phi, \beta)$ is attracted by each of the measures δ_+ and δ_- for $\beta \to \infty$. Let d denote the Lévy metric compatible with weak convergence in the sense of probability measures.

Theorem 6.11 (Phase transition) *Under the above assumptions it holds*

$$\lim_{\beta\to\infty} \mathrm{d}(\mathcal{G}_\Theta(\Phi, \beta), \delta_+) = \lim_{\beta\to\infty} \mathrm{d}(\mathcal{G}_\Theta(\Phi, \beta), \delta_-) = 0.$$

For sufficiently large β there exist two shift-invariant Gibbs measure $\mu_+^\beta, \mu_-^\beta \in \mathcal{G}_\Theta(\Phi, \beta)$ with $\tau(\mu_+^\beta) = \mu_-^\beta$ and

$$\mu_-^\beta(\omega_0) = \mathbb{E}_{\mu_-^\beta}(\omega_0) < 0 < \mu_+^\beta(\omega_0) = \mathbb{E}_{\mu_+^\beta}(\omega_0).$$

Remark 6.12

(i) $\mu_+^\beta(\omega_0)$ *is the mean magnetisation. Thus: The two-dimensional Ising ferromagnet admits an equilibrium state/measure of positive magnetisation although there is no action of an external field. This phenomenon is called* **spontaneous magnetisation**.

(ii) $\left|\mathcal{G}_\Theta(\Phi,\beta)\right| > 1 \Leftrightarrow \mu_+^\beta(\omega_0) > 0$ *goes back to [LL72]. Moreover, the Griffith's inequality implies that the magnetisation* $\mu_+^\beta(\omega_0)$ *is a non-negative non-decreasing function of* β*. Moreover there is a critical inverse temperature* β_c *such that* $\left|\mathcal{G}_\Theta(\Phi,\beta)\right| = 1$ *when* $\beta < \beta_c$ *and* $\left|\mathcal{G}_\Theta(\Phi,\beta)\right| > 1$ *when* $\beta > \beta_c$*. The value of* β_c *is*

$$\beta_c = \frac{1}{2}\sinh^{-1} 1 = \frac{1}{2}\log\left(1+\sqrt{2}\right)$$

and the magnetisation for $\beta \geq \beta_c$ *is*

$$\mu_+^\beta(\omega_0) = \left(1 - (\sinh 2\beta)^{-4}\right)^{\frac{1}{8}}.$$

(iii) For the same model in three dimensions one has again $\mu_+^\beta, \mu_-^\beta \in \mathcal{G}_\Theta(\Phi,\beta)$*, but there also exist non-shift-invariant Gibbs measures ([Dob73]).*

Proof of Theorem 6.11. Let $\Lambda \subset \mathbb{Z}^2$ be a centred cube. Denote by

$$\mathbb{B}_\Lambda = \{\{i,j\} \subset \mathbb{Z}^2 \colon |i-j| = 1, \{i,j\} \cap \Lambda \neq \emptyset\}$$

the set of all nearest-neighbour *bonds* which emanate from sites in Λ. Each bond $b = \{i,j\} \in \mathbb{B}_\Lambda$ should be visualised as a line segment between i and j. This line segment crosses a unique "dual" line segment between two nearest-neighbour sites u, v in the dual cube Λ^* (shift by $\frac{1}{2}$ in the canonical directions). The associate set $b^* = \{u,v\}$ is called the *dual bond* of b, and we write

$$\mathbb{B}_\Lambda^* = \{b^* \colon b \in \mathbb{B}_\Lambda\} = \{\{u,v\} \subset \Lambda^* \colon |u-v| = 1\}$$

for the set of all dual bonds. Note

$$b^* = \{u \in \Lambda^+ \colon |u - (i+j)/2| = \frac{1}{2}\}.$$

A set $c \subset \mathbb{B}_\Lambda^*$ is called a circuit of length l if $c = \{\{u^{(k-1)}, u^{(k)}\} \colon 1 \leq k \leq l\}$ for some $(u^{(0)}, \ldots, u^{(l)})$ with $u^{(l)} = u^{(0)}$, $|\{u^{(1)}, \ldots, u^{(l)}\}| = l$ and $\{u^{(k-1)}, u^{(k)}\} \in \mathbb{B}_\Lambda^*, 1 \leq k \leq l$. A circuit c surrounds a site $a \in \Lambda$ if for all paths $(i^{(0)}, \ldots, i^{(n)})$ in $\mathbb{Z}^2$ with $i^{(0)} = a$ and $i^{(n)} \notin \Lambda$ and $\{i^{(m-1)}, i^{(m)}\} \in \mathbb{B}_\Lambda$ for all $1 \leq m \leq n$ there exits a $m \in \mathbb{N}$ with $\{i^{(m-1)}, i^{(m)}\}^* \in c$. We denote the set of circuits which surround a by C_a. We need a first lemma.

Lemma 6.13 *For all $a \in \Lambda$ and $l \geq 1$ we have*

$$\big|\{c \in C_a \colon |c| = l\}\big| \leq l3^{l-1}.$$

Proof. Each $c \in C_a$ of length l contains at least one of the l dual bonds

$$\{a + (k-1, 0), a + (k, 0)\}^* \quad k = 1, \ldots, l,$$

which cross the horizontal half-axis from a to the right for example. The remaining $l - 1$ dual bonds are successively added, at each step there are at most 3 possible choices. $\square$

The ingenious idea of Peierls ([Pei36]) was to look at circuits which occur in a configuration. For each $\omega \in \Omega$ we let

$$\mathbb{B}^*_\Lambda(\omega) = \{b^* \colon b = \{i, j\} \in \mathbb{B}_\Lambda, \omega_i \neq \omega_j\}$$

denote the set of all dual bonds in $\mathbb{B}^*$ which cross a bond between spins of opposite sign. A circuit c with $c \subset \mathbb{B}^*_\Lambda(\omega)$ is called a **contour** for ω. We let ω outside of Λ be constant. As in Figure 3 we put outside + -spins. If a site $a \in \Lambda$ is occupied by a minus spin then a is surrounded by a contour for ω.

The idea for the proof of Theorem 6.11 is as follows. Fix ω_+ boundary condition outside of Λ. Then the minus spins in Λ form (with high probability) small islands in an ocean of plus spins. Then in the limit $\Lambda \uparrow \mathbb{Z}^2$ one obtains a $\mu^\beta_+ \in \mathcal{G}(\beta\Phi)$ which is close to the delta measure δ_+ for β sufficiently large. As δ_+ and δ_- are distinct, so are μ^β_+ and μ^β_- when β is large. Hence $\big|\mathcal{G}(\beta\Phi)\big| > 1$ when β is large. We turn to the details. The next lemma just ensures the existence of a contour for positive boundary conditions and one minus spin in Λ. We just cite it without any proof.

Lemma 6.14 *Let $\omega \in \Omega$ with $\omega_i = +1$ for all $i \in \Lambda^{\mathrm{c}}$ and $\omega_a = -1$ for some $a \in \Lambda$. Then there exists a contour for ω which surrounds a.*

Now we are at the heart of the Peierls argument, which is formulated in the next lemma.

Lemma 6.15 *Suppose $c \subset \mathbb{B}^*_\Lambda$ is a circuit. Then*

$$\gamma^{\beta\Phi}_\Lambda(c \subset \mathbb{B}^*_\Lambda(\cdot)|\omega) \leq \mathrm{e}^{-2\beta|c|}$$

for all $\beta > 0$ and for all $\omega \in \Omega$.

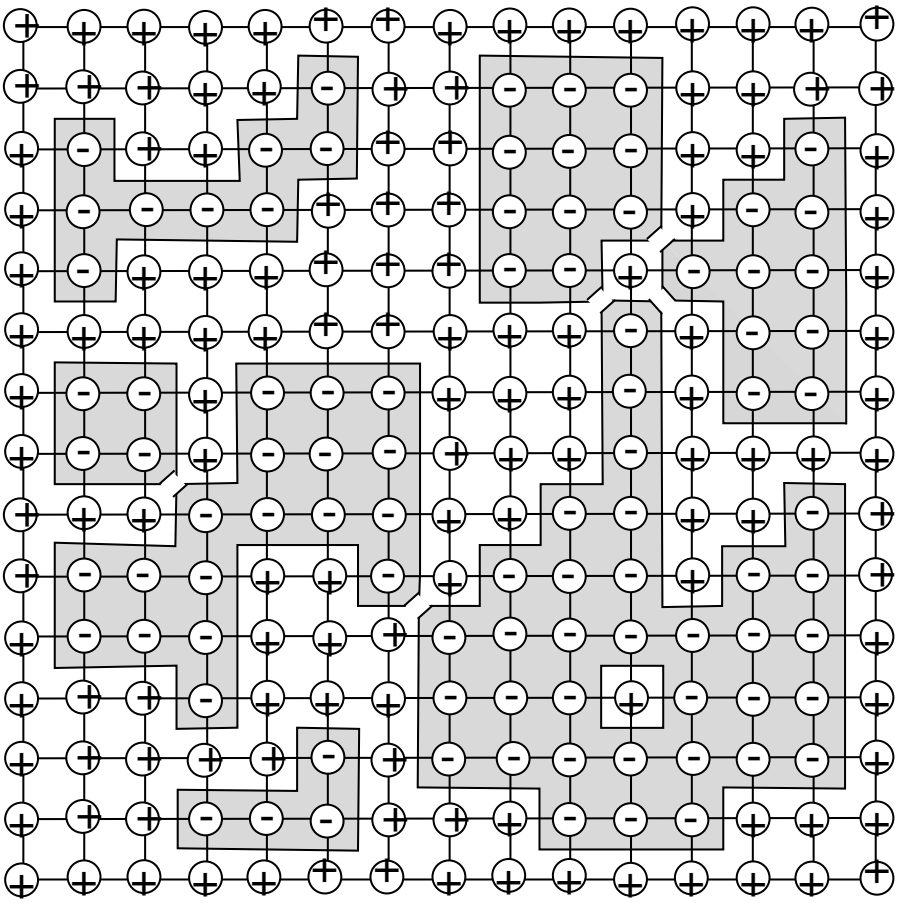

Figure 3: a contour for + boundary condition

Proof. Note that for all $\xi \in \Omega$ we have

$$\begin{aligned}-H_\Lambda(\xi) &= \sum_{\{i,j\}\in\mathbb{B}_\Lambda} \xi_i\xi_j = |\mathbb{B}_\Lambda| - \sum_{\{i,j\}\in\mathbb{B}_\Lambda} (1-\xi_i\xi_j) \\ &= |\mathbb{B}_\Lambda| - 2|\{\{i,j\}\in\mathbb{B}_\Lambda \colon \xi \neq \xi_j\}| = |\mathbb{B}_\Lambda| - 2|\mathbb{B}^*_\Lambda|.\end{aligned}$$

Now we define two disjoint sets of configurations which we need later for an estimation.

$$\begin{aligned}A_1 &= \{\xi\in\Omega \colon \xi_{\mathbb{Z}^d\setminus\Lambda} = \omega_{\mathbb{Z}^d\setminus\Lambda}, c\subset \mathbb{B}^*_\Lambda(\xi)\} \\ A_2 &= \{\xi\in\Omega \colon \xi_{\mathbb{Z}^d\setminus\Lambda} = \omega_{\mathbb{Z}^d\setminus\Lambda}, c\cap \mathbb{B}^*_\Lambda(\xi) = \emptyset\}.\end{aligned}$$

There is a mapping $\tau_c \colon \Omega \to \Omega$ with

$$(\tau_c\xi)_i = \begin{cases} -\xi\ , & \text{if } i \text{ is surrounded by } c, \\ \xi\ , & \text{otherwise} \end{cases},$$

which flips all spins in the interior of the circuit c. Moreover, for all $\{i,j\} \in \mathbb{B}_\Lambda$ we have

$$(\tau_c\xi)_i(\tau_c\xi)_j = \begin{cases} \xi_i\xi_j\ , & \text{if } \{i,j\}^* \notin c \\ -\xi_i\xi_j\ , & \text{if } \{i,j\}^* \in c \end{cases},$$

resulting in $\mathbb{B}^*_\Lambda(\tau_c\xi)\triangle\mathbb{B}^*_\Lambda(\xi) = c$ (this was the motivation behind the definition of mappings), where $\triangle$ denotes the symmetric difference of sets. In particular we get that τ_c is a bijection from A_2 to A_1, and we have

$$H_\Lambda(\xi) - H_\Lambda(\tau_c\xi) = 2|\mathbb{B}^*_\Lambda(\xi)| - 2|\mathbb{B}^*_\Lambda(\tau_c\xi)| = -2|c|.$$

Now we can estimate with the help of the set of events A_1, A_2

$$\begin{aligned}\gamma_\Lambda(c\subset\mathbb{B}^*_\Lambda(\cdot)|\omega) &\le \frac{\sum_{\xi\in A_1}\exp(-\beta H_\Lambda(\xi))}{\sum_{\xi\in A_2}\exp(-\beta H_\Lambda(\xi))} = \frac{\sum_{\xi\in A_2}\exp(-\beta H_\Lambda(\tau_c\xi))}{\sum_{\xi\in A_2}\exp(-\beta H_\Lambda(\xi))} \\ &= \exp(-2\beta|c|).\end{aligned}$$

□

Now we finish our proof of Theorem 6.11. For $\beta > 0$ define

$$r(\beta) = 1 \wedge \sum_{l\ge 1} l(3\mathrm{e}^{-2\beta})^l,$$

where $\wedge$ denotes the minimum, and note that $r(\beta) \to 0$ as $\beta \to \infty$. The preceding lemmas yield

$$\gamma_\Lambda(\omega_a|\omega^+) \le \sum_{c\in C_a} \gamma_\Lambda(c\subset\mathbb{B}^*_\Lambda(\cdot)|\omega^+) \le \sum_{c\in C_a} \mathrm{e}^{-2\beta|c|} \le \sum_{l\ge 1} l3^{l-2\beta l},$$

and thus $\gamma_\Lambda(\omega_a|\omega^+) \leq r(\beta)$ for all $a \in \mathbb{Z}^2, \beta > 0$ and $\Lambda \subset \mathbb{Z}^2$. Choose $\Lambda_N = [-N, N]^2 \cap \mathbb{Z}^2$ and define the approximating measures

$$\nu_N^+ = \frac{1}{|\Lambda_N|} \sum_{i \in \Lambda_N} \gamma_{\Lambda_N + i}(\cdot|\omega^+).$$

As $\mathcal{P}(\Omega, \mathcal{F})$ is compact, the sequence $(\nu_N^+)_{N \in \mathbb{N}}$ has a cluster point μ_+^β and one can even show that $\mu_+^\beta \in \mathcal{G}_\Theta(\Phi, \beta)$ ([Geo88]). Our estimation above gives then $\mu_+^\beta(\omega_a = -1) \leq r(\beta)$, and in particular one can show that

$$\lim_{\beta \to \infty} \mu_+^\beta = \delta_+ \quad \text{and} \quad \lim_{\beta \to \infty} \mathrm{d}(\mathcal{G}_\Theta(\beta\Phi), \delta_+) = 0.$$

Note $\mu_-^\beta = \tau(\mu_+^\beta)$. Hence,

$$\mu_+^\beta(\omega_0 = -1|\omega^+) = \mu_-^\beta(\omega_0 = +1|\omega^-).$$

If β is so large that $\mu_+^\beta(\omega_0 = -1) \leq r(\beta) < \frac{1}{3}$, then

$$\mu_+^\beta(\omega_0 = -1) = \mu_-^\beta(\omega_0 = +1) < \frac{1}{3}.$$

But $\{\omega_0 = -1\} \cup \{\omega_0 = +1\} = \Omega$, and hence

$$\mu_+^\beta(\omega_0 = +1) = 1 - \mu_+^\beta(\omega_0 = -1) \geq \frac{2}{3}.$$

□

6.5 Extreme Gibbs measures

The set $\mathcal{G}(\Phi, \beta)$ of Gibbs measures for some interaction potential Φ and inverse temperature $\beta > 0$ is a convex set, i.e., if $\mu, \nu \in \mathcal{G}(\Phi, \beta)$ and $0 < s < 1$ then $s\mu + (1-s)\nu \in \mathcal{G}(\Phi, \beta)$. An extreme Gibbs measure (or in physics: a pure state) is an extreme element μ of the convex set $\mathcal{G}(\Phi, \beta)$. The set of all extreme Gibbs measures is denoted by $\operatorname{ex}\mathcal{G}(\Phi, \beta)$. Below we give a characterisation of extreme Gibbs measures. But first we briefly discuss **microscopic** and **macroscopic** quantities. A real function $f\colon \Omega \to \mathbb{R}$ is said to describe a **macroscopic** observable if f is measurable with respect to the tail-σ-algebra $\mathcal{T}$. The $\mathcal{T}$-measurability of a function f means that the value of f is not affected by the behaviour of any finite set of spins. For example, the event

$$\left\{ \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \sum_{i \in \Lambda_n} \omega_i \ \text{ exists and belongs to } \ B \right\} \quad B \in \mathcal{B}_\mathbb{R},$$

is a tail event in $\mathcal{T}$ for any cofinal sequence $(\Lambda_n)_{n\in\mathbb{N}}$ with $\Lambda_n \uparrow \mathbb{Z}^d$ as $n \to \infty$. A function f describes a **microscopic** observable if it depends only on finitely many spins. A function $f\colon \Omega \to \mathbb{R}$ is called **cylinder function** or **local function** if it is $\mathcal{F}_\Lambda$-measurable for some $\Lambda \in \mathcal{S}$. The function f is called **quasi-local** if it can be approximated in supremum norm by local functions. The following theorem gives a characterisation of extreme Gibbs measures. It was invented by Lanford and Ruelle [LR69] and but was introduced earlier in a weaker form by Dobrushin [Dob68a],[Dob68b].

Theorem 6.16 (Extreme Gibbs measures) *A Gibbs measure $\mu \in \mathcal{G}(\Phi)$ is extreme if and only if μ is trivial on the tail-σ-algebra $\mathcal{T}$, i.e. if $\mu(A) = 0$ or $\mu(A) = 1$ for any $A \in \mathcal{T}$.*

Microscopic quantities are subject to rapid fluctuations in contrast to macroscopic quantities. A probability measure $\mu \in \mathcal{P}(\Omega, \mathcal{F})$ describing the equilibrium state of a given system is consistent with the observed empirical distributions of microscopic variables when it is a Gibbs measure. The second requirement even gives that macroscopic quantities are constant with probability one, and with Theorem 6.16 it follows that only extreme Gibbs measures are an appropriate description of equilibrium states. For this reason, an extreme Gibbs measure is often called a *phase*. However this term should not be confused with the physical concept of a pure phase. Note that the stable coexistence of distinct pure phases in separated regions of space will also be represented by an extreme Gibbs measure (see Figure 4, which was taken from [Aiz80]). This can be seen quite nicely in the three-dimensional Ising model ([Dob73]), where a Gibbs measure is constructed via Gibbs distributions whose boundary is on one half-space given by upward-spins and on the other half-space given by downward-spins. It is a tempting misunderstanding to believe that the coexistence of two pure phases was described by a mixture like $\frac{1}{2}(\mu_1 + \mu_2), \mu_1, \mu_2 \in \mathcal{G}(\Phi, \beta)$. Such a mixture rather corresponds to an uncertainty about the true phase of the system. See the Figure 4 for an illustration of this fact.

6.6 Uniqueness

In this subsection we give a short intermezzo about the question of uniqueness of Gibbs measures, i.e., the situation when there is a most one Gibbs measure possible for the given interaction potential. One might guess that this question has something to due with the dependence structure introduced from the interaction potential. One is therefore led to check the dependence structure of the conditional Gibbs distributions at one given lattice site. For

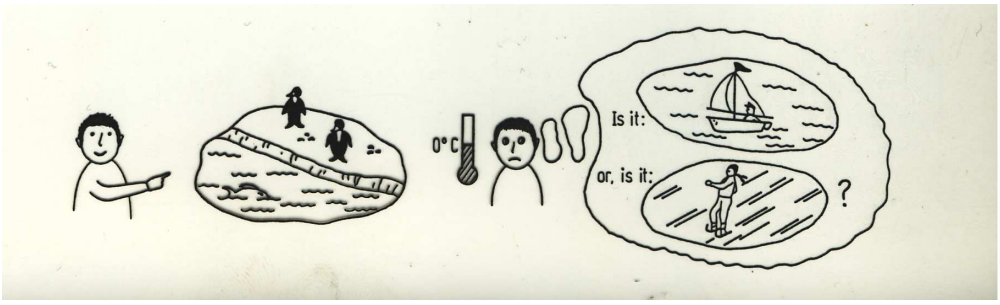

Figure 4: An extreme $\mu^{(\text{coexistence})}$ and mixture $\frac{1}{2}(\mu^{(\text{water})} + \mu^{(\text{ice})})$

that, fix any $i \in \mathbb{Z}^d$ and consider the ω_j-dependence of the Gibbs distribution $\gamma^{\Phi}_{\{i\}}(\cdot|\omega)$ for each $j \in \mathbb{Z}^d$ and $\omega \in \Omega$ for a given interaction potential Φ. Introduce the matrix elements

$$C_{i,j}(\Phi) = \sup_{\substack{\xi,\eta\in\Omega,\\ \xi_{\mathbb{Z}^d\setminus\{j\}}=\eta_{\mathbb{Z}^d\setminus\{j\}}}} ||\gamma^{\Phi}_{\{i\}}(\cdot|\xi) - \gamma^{\Phi}_{\{i\}}(\cdot|\eta)||,$$

where $||\cdot||$ denotes the uniform distance of probability measures on E, which is one half of the total variation distance. Note that $\gamma^{\Phi}_{\{i\}}(\cdot|\xi) \in \mathcal{P}(E, \mathcal{E})$ for any $\xi \in \Omega$. The matrix $(C_{i,j})_{i,j\in\mathbb{Z}^d}$ is called *Dobrushin's interdependence matrix.* A first guess describing the dependence structure would be to consider the sum

$$\sum_{j\in\mathbb{Z}^d} C_{i,j}(\Phi),$$

however this tells us nothing about the behaviour of the configuration $\omega \in \Omega$ at infinity.

Definition 6.17 *An interaction potential Φ is said to satisfy Dobrushin's uniqueness condition if*

$$C(\Phi) = \sup_{i\in\mathbb{Z}^d} \sum_{j\in\mathbb{Z}^d} C_{i,j}(\Phi) < 1. \tag{6.37}$$

To provide a sufficient condition for Dobrushin's condition to hold, define the oscillation of any function $f\colon \Omega \to \mathbb{R}$ as

$$\delta(f) = \sup_{\xi,\eta\in\Omega} |f(\xi) - f(\eta)|.$$

Theorem 6.18 *Let Φ be an interaction potential and $d \geq 1$.*

(i) If Dobrushin's uniqueness condition (6.37) *is satisfied, then $|\mathcal{G}(\Phi)| \leq 1$.*

(ii) If

$$\sup_{i\in\mathbb{Z}^d}\sum_{A\ni i}(|A|-1)\delta(\phi_A)<2,$$

then Dobrushin's uniqueness condition (6.37) *is satisfied.*

Proof. See [Geo88] and references therein. □

Example 6.19 (Lattice gas) *Let $E=\{0,1\}$ and let the reference measure be the counting measure. Let $K\colon \mathcal{S}\to\mathbb{R}$ be any function on the set of all finite subsets of $\mathbb{Z}^d$ and define for $\omega\in\Omega$ the interaction potential Φ by*

$$\phi_A(\omega)=\begin{cases} K(A)\ , & \text{if } \omega_A=\prod_{i\in A}\omega_i=1\\ 0\ , & \text{otherwise}\end{cases}$$

for any $A\in\mathcal{S}$. Note that $\delta(\phi_A)=|K(A)|$. Thus uniqueness is given whenever

$$\sup_{i\in\mathbb{Z}^d}\sum_{A\ni i}(|A|-1)|K(A)|<4.$$

Example 6.20 (One-dimensional systems) *Let Φ be a shift-invariant interaction potential and $d=1$. Then there is at most one Gibbs measure whenever*

$$\sum_{\substack{A\in\mathcal{S},\\ \min A=0}}\operatorname{diam}(A)\delta(\phi_A)<\infty.$$

6.7 Ergodicity

We look at the convex set $\mathcal{P}_\Theta(\Omega,\mathcal{F})$ of all shift-invariant random fields on $\mathbb{Z}^d$. $\mathcal{P}_\Theta(\Omega,\mathcal{F})$ is always non-empty. We also consider the σ-algebra

$$\mathcal{I}=\{A\in\mathcal{F}\colon \theta_iA=A \text{ for all } i\in\mathbb{Z}^d\} \tag{6.38}$$

of all shift-invariant events. A $\mathcal{F}$-measurable function $f\colon\Omega\to\mathbb{R}$ is $\mathcal{I}$-measurable if and only if f is invariant, in that $f\circ\theta_i=f$ for all $i\in\mathbb{Z}^d$. A standard result in ergodic theory is the following theorem.

Theorem 6.21 *(i) A probability measure $\mu\in\mathcal{P}_\Theta(\Omega,\mathcal{F})$ is extreme in $\mathcal{P}_\Theta(\Omega,\mathcal{F})$ if and only if μ is trivial on the invariant σ-algebra.*

(ii) Each $\mu\in\mathcal{P}_\Theta(\Omega,\mathcal{F})$ is uniquely determined (within $\mathcal{P}_\Theta(\Omega,\mathcal{F})$) by its restriction to $\mathcal{I}$.

(iii) Distinct probability measures $\mu, \nu \in \operatorname{ex} \mathcal{P}_\Theta(\Omega, \mathcal{F})$ are mutually singular on $\mathcal{I}$ in that there exists an $A \in \mathcal{I}$ such that $\mu(A) = 1$ and $\nu(A) = 0$.

Proof. Standard textbooks of ergodic theory or [Geo88]. □

Definition 6.22 (Ergodic measure) *A probability measure $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ is said to be* **ergodic** *(with respect to the shift-transformation group Θ) if μ is trivial on the σ-algebra $\mathcal{I}$ of all shift-invariant events. In mathematical physics such a μ is often called a* **pure state**.

Proposition 6.23 (Characterisation of ergodic measures)
Let μ be a probability measure $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ and $(\Lambda_N)_{N\in\mathbb{N}}$ any sequence of cubes with $\Lambda_N \uparrow \mathbb{Z}^d$ as $N \to \infty$. Then the following statements are equivalent.

(i) μ is ergodic.

(ii) For all events $A \in \mathcal{F}$,

$$\lim_{N\to\infty} \sup_{B\in\mathcal{F}} \Big| \frac{1}{|\Lambda_N|} \sum_{i\in\Lambda_N} \mu(A \cap \theta_i B) - \mu(A)\mu(B) \Big| = 0.$$

(iii) For arbitrary cylinder events A and B,

$$\lim_{N\to\infty} \frac{1}{|\Lambda_N|} \sum_{i\in\Lambda_N} \mu(A \cap \theta_i B) = \mu(A)\mu(B).$$

One can show that each extreme measure is a limit of finite volume Gibbs distributions with suitable boundary conditions. Now, what about ergodic Gibbs measures? The ergodic Theorem 6.24 below gives an answer: If $\mu \in \operatorname{ex} \mathcal{P}_\Theta(\Omega, \mathcal{F})$ and $(\Lambda_N)_{N\in\mathbb{N}}$ a sequence of cubes with $\Lambda_N \uparrow \mathbb{Z}^d$ as $N \to \infty$ one gets

$$\mu(f) = \lim_{N\to\infty} \frac{1}{|\Lambda_N|} \sum_{i\in\Lambda_N} f(\theta_i \omega)$$

for μ-almost all $\omega \in \Omega$ and bounded measurable function $f\colon \Omega \to \mathbb{R}$. Thus

$$\mu = \lim_{N\to\infty} \frac{1}{|\Lambda_N|} \sum_{i\in\Lambda_N} \delta_{\theta_i \omega} \quad \text{for } \mu - \text{a.a. } \omega \in \Omega$$

in any topology which is generated by countably many evaluation mappings $\nu \mapsto \nu(f)$. For E finite, the weak topology (of probability measures) has this property.

For any given measurable function $f\colon \Omega \to \mathbb{R}$ define

$$R_N f = \frac{1}{|\Lambda_N|} \sum_{i \in \Lambda_N} f \circ \theta_i \quad N \in \mathbb{N}. \tag{6.39}$$

The *multidimensional ergodic theorem* says something about the limiting behaviour of $R_N f$ as $N \to \infty$. Let $(\Lambda_N)_{N \in \mathbb{N}}$ be a cofinal sequence of boxes with $\Lambda_N \uparrow \mathbb{Z}^d$ as $N \to \infty$.

Theorem 6.24 (Multidimensional Ergodic Theorem) *Let a probability measure $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ be given. For any measurable $f\colon \Omega \to \mathbb{R}$ with $\mu(|f|) < \infty$,*

$$\lim_{N \to \infty} R_N f = \mu(f|\mathcal{I}) \quad \mu - a.s.$$

7 A variational characterisation of Gibbs measures

In this section we give a variational characterisation for translation invariant Gibbs measures. This characterisation will prove useful in the study of Gibbs measures and it has a close connection to the physical intuition, namely that an equilibrium state minimises the free energy. This will be proved rigorously in this section. Let us start with some heuristics and assume for this purpose only that the set Ω of configurations is finite. Denote by $\nu(\omega) = Z^{-1} \exp(-H(\omega))$ a Gibbs measure with suitable normalisation Z and Hamiltonian H. The mean energy for any probability measure $\mu \in \mathcal{P}(\Omega)$ is

$$\mathbb{E}_\mu(H) = \mu(H) = \sum_{\omega \in \Omega} \mu(\omega) H(\omega),$$

and its entropy is given by

$$\mathcal{H}(\mu) = -\sum_{\omega \in \Omega} \mu(\omega) \log \mu(\omega).$$

Now $\mu(H) - \mathcal{H}(\mu) = F(\mu)$ is called the *free energy* of μ, and for any $\mu \in \mathcal{P}(\Omega)$ we have

$$F(\mu) \geq -\log Z \quad \text{ and } F(\mu) = -\log Z \quad \text{ if and only if } \mu = \nu.$$

To see this, apply Jensen's inequality for the convex function $\varphi(x) = x \log x$ and conclude by simple calculation

$$\begin{aligned} \mu(H) - \mathcal{H}(\mu) + \log Z &= \sum_{\omega \in \Omega} \mu(\omega) \log\Big(\frac{\mu(\omega)}{\nu(\omega)}\Big) = \sum_{\omega \in \Omega} \nu(\omega) \varphi\Big(\frac{\mu(\omega)}{\nu(\omega)}\Big) \\ &\geq \varphi\Big(\sum_{\omega \in \Omega} \nu(\omega) \frac{\mu(\omega)}{\nu(\omega)}\Big) = \varphi(1) = 0, \end{aligned}$$

and as φ is strictly convex there is equality if and only if $\frac{\mu(\omega)}{\nu(\omega)}$ is a constant. As Ω is finite one gets that $\mu = \nu$. If Ω is not finite one has to employ quite some mathematical theory which we present briefly in the rest of this section.

Definition 7.1 (Relative entropy) *Let $\mathcal{A} \subset \mathcal{F}$ be a sub-σ-algebra of $\mathcal{F}$ and $\mu, \nu \in \mathcal{P}(\Omega, \mathcal{F})$ be two probability measures. Then*

$$\mathcal{H}_{\mathcal{A}}(\mu|\nu) = \begin{cases} \nu(f_{\mathcal{A}} \log f_{\mathcal{A}}) = \int_\Omega f_{\mathcal{A}}(\omega) \log f_{\mathcal{A}}(\omega) \nu(\mathrm{d}\omega) \ , & \text{if } \mu \ll \nu \text{ on } \mathcal{A} \\ \infty \ , & \text{otherwise} \end{cases} ,$$

where $f_{\mathcal{A}}$ is the Radon-Nikodym density of $\mu|_{\mathcal{A}}$ relative to $\nu|_{\mathcal{A}}$ ($\mu|_{\mathcal{A}}$ and $\nu|_{\mathcal{A}}$ are the restrictions of the measures to the sub-σ-algebra $\mathcal{A}$), is called the **relative entropy** *or* **Kullback-Leibler information** *or* **information divergence** *of μ relative to ν on $\mathcal{A}$.*

If $\mathcal{A} = \mathcal{F}_\Lambda$ for some $\Lambda \in \mathcal{S}$ one writes

$$\mathcal{H}_{\Lambda}(\mu|\nu) = \begin{cases} \nu(f_{\Lambda} \log f_{\Lambda}) = \int_{\Omega_\Lambda} f_{\Lambda}(\omega) \log f_{\Lambda}(\omega) \nu(\mathrm{d}\omega) \ , & \text{if } \mu \ll \nu \text{ on } \Lambda \\ \infty \ , & \text{otherwise} \end{cases} ,$$

where $f_\Lambda = \left(\frac{\mathrm{d}\mu_\Lambda}{\mathrm{d}\nu_\Lambda}\right)$ is the Radon-Nikodym density and μ_Λ and ν_Λ are the marginals of μ and ν on Λ for the projection map $\sigma_\Lambda \colon \Omega \to \Omega_\Lambda$.

We collect the most important properties of the relative entropy in the following proposition.

Proposition 7.2 *Let $\mathcal{A} \subset \mathcal{F}$ a sub-σ-algebra of $\mathcal{F}$ and $\mu, \nu \in \mathcal{P}(\Omega, \mathcal{F})$ any two probability measures. Then*

(a) $\mathcal{H}_{\mathcal{A}}(\mu|\nu) \geq 0$,

(b) $\mathcal{H}_{\mathcal{A}}(\mu|\nu) = 0$ *if and only if* $\mu = \nu$ *on* $\mathcal{A}$,

(c) $\mathcal{H}_{\mathcal{A}}$ *is an increasing function of* $\mathcal{A}$,

(d) $\mathcal{H}(\cdot|\cdot)$ *is convex.*

We now connect the relative entropy to our previous definition of the entropy functional in Section 3. For this let any finite signed a priori measure λ on $(E, \mathcal{E})$ be given. Note that the a priori or reference measure need not be normalised to one (probability measure), and the following notion depends on the choice of this reference measure. Recall that λ^Λ denotes the product measure on $\Omega_\Lambda = (E^\Lambda, \mathcal{E}^\Lambda)$.

Notation 7.3 *Let $\mu \in \mathcal{P}(\Omega, \mathcal{F})$. The function*

$$S_\Lambda = -\mathcal{H}_\Lambda(\mu|\sigma_\Lambda^{-1}(\lambda^\Lambda))$$

is called the **entropy** *of μ in Λ relative to the reference/a priori measure λ.*

If the reference measure λ is the counting measure we get back Shannon's formula

$$\mathcal{H}_\Lambda(\mu) = -\sum_{\xi \in \Omega_\Lambda} \mu(\sigma_\Lambda = \xi) \log \mu(\sigma_\Lambda = \xi) \geq 0$$

for the entropy. We wish to show that the thermodynamic limit of the entropy exists, i.e.wish to show that

$$h(\mu) = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \mathcal{H}_{\Lambda_n}(\mu)$$

exists for any cofinal sequence $(\Lambda_n)_{n \in \mathbb{N}}$ of finite volume boxes in $\mathcal{S}$. Essential device for the proof of the existence of this limit is the following sub-additivity property.

Proposition 7.4 (Strong Sub-additivity) *Let $\Lambda, \Delta \in \mathcal{S}$ and $\mu \in \mathcal{P}(\Omega, \mathcal{F})$ be given. Then*

$$\mathcal{H}_\Lambda(\mu) + \mathcal{H}_\Delta(\mu) \geq \mathcal{H}_{\Lambda \cap \Delta}(\mu) + \mathcal{H}_{\Lambda \cup \Delta}(\mu). \tag{7.40}$$

Proof. A proof is given in [Rue69],[Isr79] and in [Geo88]. □

Equipped with this inequality we go further and assume $\Lambda \cap \Delta = \emptyset$ (note $\mathcal{H}_\emptyset(\mu) = 0$) and observe that for a translation invariant probability measure $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ we get that

$$\mathcal{H}_{\Lambda+i}(\mu) = \mathcal{H}_\Lambda(\mu) \quad \text{for any } \Lambda \in \mathcal{S} \text{ and any } i \in \mathbb{Z}^d.$$

Denote by $\mathcal{S}_{\text{r.B.}}$ the set of all rectangular boxes in $\mathbb{Z}^d$.

Lemma 7.5 *Suppose that the function $a\colon \mathcal{S}_{\text{r.B.}} \to [-\infty, \infty)$ satisfies*

(i) $a(\Lambda + i) = a(\Lambda)$ *for all* $\Lambda \in \mathcal{S}_{\text{r.B.}}, i \in \mathbb{Z}^d$,

(ii) $a(\Lambda) + a(\Delta) \geq a(\Lambda \cup \Delta)$ *for* $\Lambda, \Delta \in \mathcal{S}_{\text{r.B.}}, \Lambda \cap \Delta = \emptyset$,

$(\Lambda_n)_{n \in \mathbb{N}}$ *a cofinal sequence of cubes with* $\Lambda_n \uparrow \mathbb{Z}^d$ *as* $n \to \infty$. *Then the limit*

$$\lim_{n \to \infty} \frac{1}{|\Lambda_n|} a(\Lambda_n) = \inf_{\Delta \in \mathcal{S}_{\text{r.B.}}} \frac{1}{|\Delta|} a(\Delta) \tag{7.41}$$

exists in $[-\infty, \infty)$.

Proof. Choose

$$c > \alpha := \inf_{\Delta \in \mathcal{S}_{\text{r.B.}}} \frac{1}{|\Delta|} a(\Delta)$$

and let $\Delta \in \mathcal{S}_{\text{r.B.}}$ be such that $\frac{1}{|\Delta|} a(\Delta) < c$. Denote by N_n the number of disjoint translates of Δ contained in Λ_n. Then Λ_n is split into N_n translates of Δ and a remainder in the boundary layer. Choose N_n as large as possible. Then $\lim_{n\to\infty} \frac{|\Lambda_n|}{N_n|\Delta|} = 1$. The sub-additivity gives

$$a(\Lambda_n) \leq N_n a(\Delta) + (|\Lambda_n| - N_n|\Delta|) a(\{0\}).$$

Hence,

$$\begin{aligned} \alpha &\leq \limsup_{n\to\infty} \frac{1}{|\Lambda_n|} a(\Lambda_n) = \limsup_{n\to\infty} N_n^{-1} |\Delta|^{-1} a(\Lambda_n) \\ &< |\Delta|^{-1} a(\Delta) < c. \end{aligned}$$

Letting c tend to α gives the proof of the lemma. □

Now, both Proposition 7.4 and Lemma 7.5 provide the main steps of the proof of the following theorem.

Theorem 7.6 (Specific entropy) *Fix a finite signed reference measure λ on the measurable state space $(E, \mathcal{E})$. Let $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ be a translation invariant probability measure and $(\Lambda_n)_{n\in\mathbb{N}}$ a cofinal sequence of boxes with $\Lambda_n \uparrow \mathbb{Z}^d$ as $n \to \infty$. Then,*

(a)

$$h(\mu) = \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \mathcal{H}_{\Lambda_n}(\mu)$$

exists in $[-\infty, \lambda(E)]$.

(b) $h\colon \mathcal{P}_\Theta(\Omega, \mathcal{F}) \to \mathbb{R}, \mu \mapsto h(\mu)$, is affine and upper semi-continuous. The level sets $\{h \geq c\}, c \in \mathbb{R}$, are compact with respect to the weak topology of probability measures.

Notation 7.7 *$h(\mu)$ is called the* **specific entropy per site** *of $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ relative to the reference measure λ.*

Proof of Theorem 7.6. The existence of the specific entropy was proved first by Shannon ([Sha48]) for the case $d = 1, |E| < \infty$ and λ the counting measure. Extensions are due to McMillan ([McM53]) and Breiman ([Bre57]). The multidimensional version of Shannon's result is due to Robinson and Ruelle ([RR67]). The first two assertions of (b) can already be found in [RR67], an explicit proof of this can be found in [Isr79]. □

Now the following question arises. What happens if we take instead of the reference measure any Gibbs measure and evaluate the relative entropy? We analyse this question in the following. To define the specific energy of a translation invariant probability measure it proves useful to introduce the following function. Let $\Phi = (\phi_A)_{A\in\mathcal{S}}$ be a translation invariant interaction potential. Define the function $f_\Phi \colon \Omega \to \mathbb{R}$ as

$$f_\Phi = \sum_{A\ni 0} |A|^{-1}\phi_A. \tag{7.42}$$

In the following theorem we prove the existence of the specific energy. To derive an expression which is independent of any chosen boundary condition, we formulate the theorem for an arbitrary sequence of boundary conditions, which applies also to the case of periodic and free boundary conditions.

Theorem 7.8 (Specific energy) *Let $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$, Φ be a translation invariant interaction potential, $(\Lambda_n)_{n\in\mathbb{N}}$ be a cofinal sequence of boxes with $\Lambda_n \uparrow \mathbb{Z}^d$ as $n \to \infty$ and $(\omega_n)_{n\in\mathbb{N}}$ be a sequence of configurations $\omega_n \in \Omega$. Then the specific energy*

$$\mathbb{E}_\mu(f_\Phi) = \mu(f_\Phi) = \lim_{n\to\infty} \frac{1}{|\Lambda_n|}\mu(H_{\Lambda_n}^{\omega_n}) \tag{7.43}$$

exists.

Notation 7.9 (Specific free energy) *$\mathbb{E}_\mu(f_\Phi)$ or $\mu(f_\Phi)$ is called the* **specific** *(internal)* **energy** *per site of μ relative to Φ. The quantity $f(\mu) = \mu(f_\Phi) - h(\mu)$ is called the* **specific free energy** *of μ for Φ.*

Proof of Theorem 7.8. For the proof see any of the books [Geo88],[Rue69] or [Isr79]. The proof goes back to Dobrushin [Dob68b] and Ruelle [Rue69]. □

We continue our investigations with the previously occurred question of the relative entropy with respect to a given Gibbs measure.

Theorem 7.10 (Pressure) *Let $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ and $\gamma \in \mathcal{G}_\Theta(\Phi, \beta)$, $\beta > 0$, Φ be a translation invariant interaction potential, $(\Lambda_n)_{n\in\mathbb{N}}$ be a cofinal sequence of boxes with $\Lambda_n \uparrow \mathbb{Z}^d$ as $n \to \infty$ and $(\omega_n)_{n\in\mathbb{N}}$ be a sequence of configurations $\omega_n \in \Omega$. Then,*

(a) $P(\Phi) = \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \log Z_{\Lambda_n}(\omega_n)$ *exists.*

(b) The limit $\lim_{n\to\infty} \frac{1}{|\Lambda_n|}\mathcal{H}_{\Lambda_n}(\mu|\gamma)$ *exists and equals*

$$h(\mu|\Phi) = P(\Phi) + \mu(f_\Phi) - h(\mu) = P(\Phi) + f(\mu). \tag{7.44}$$

Notation 7.11 $P = P(\Phi)$ *is called the* **pressure** *and* **specific Gibbs free energy**.

Proof of Theorem 7.10. We just give the main idea of the proof. Details can be found in [Isr79],[Geo88] and go back to [GM67]. Let $\Lambda \in \mathcal{S}$ and $\omega \in \Omega$ fixed. Recall that the marginal of μ on Λ is a probability measure on $(\Omega_\Lambda, \mathcal{F}_\Lambda)$ as well as the conditional Gibbs distribution $\gamma_\Lambda(\cdot|\omega)$ for any given configuration $\omega \in \Omega$. Then compute

$$\begin{aligned}
\mathcal{H}_\Lambda(\mu|\gamma_\Lambda(\cdot|\omega)) &= \int_{\Omega_\Lambda} \mu_\Lambda(\mathrm{d}\xi) \log \frac{\mathrm{d}\mu_\Lambda}{\mathrm{d}\gamma_\Lambda}(\xi) = \int_{\Omega_\Lambda} \mu_\Lambda(\mathrm{d}\xi) \log \frac{\mathrm{d}\mu_\Lambda}{\mathrm{d}\lambda^\Lambda}(\xi) \\
&\quad - \int_{\Omega_\Lambda} \mu_\Lambda(\mathrm{d}\xi) \log \frac{\mathrm{d}\lambda^\Lambda}{\mathrm{d}\gamma_\Lambda}(\xi) \\
&= -\mathcal{H}_\Lambda(\mu) + \int_{\Omega_\Lambda} \mu_\Lambda(\mathrm{d}\xi) H_\Lambda(\xi\omega_{\mathbb{Z}^d\setminus\Lambda}) + \log Z_\Lambda(\omega).
\end{aligned}$$

We can draw an easy corollary, which is the first part of the variational principle for Gibbs measures.

Corollary 7.12 (First part variational principle) *For a translation invariant interaction potential* Φ *and* $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ *we have* $h(\mu|\phi) \geq 0$. *If moreover* $\mu \in \mathcal{G}_\Theta(\Phi, \beta)$ *then* $h(\mu|\Phi) = 0$.

Proof. The assertions are due to Dobrushin ([Dob68a]) and Lanford and Ruelle ([LR69]). □

The next theorem gives the reversed direction and a summary of the whole variational principle.

Theorem 7.13 (Variational principle) *Let* Φ *be a translation invariant interaction potential,* $(\Lambda_n)_{n\in\mathbb{N}}$ *a cofinal sequence of boxes with* $\Lambda_n \uparrow \mathbb{Z}^d$ *as* $n \to \infty$ *and* $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$. *Then,*

(a) Let $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ *be such that* $\liminf_{n\to\infty} \frac{1}{|\Lambda_n|}\mathcal{H}_{\Lambda_n}(\mu|\nu) = 0$. *Then* $\mu \in \mathcal{G}_\Theta(\Phi, \beta)$.

(b) $h(\mu|\Phi) \geq 0$ *and* $h(\mu|\Phi) = 0$ *if and only if* $\mu \in \mathcal{G}_\Theta(\Phi, \beta)$.

(c) $h(\cdot|\Phi)\colon \mathcal{P}_\Theta(\Omega,\mathcal{F}) \to [0,\infty]$ *is an affine lower semi continuous functional which attains its minimum* 0 *on the set* $\mathcal{G}_\Theta(\Phi,\beta)$. *Equivalently,* $\mathcal{G}_\Theta(\Phi)$ *is the set on which the specific free energy functional*

$$f\colon \mathcal{P}_\Theta(\Omega,\mathcal{F}) \to [0,\infty]$$

attains its minimum $-P(\Phi)$.

Proof. This variational principle is due to Lanford and Ruelle ([LR69]). A transparent proof which reveals the significance of the relative entropy is due to Föllmer ([Föl73]). □

8 Large deviations theory

In this section we give a short view on large deviations theory. We motivate this by the simple coin tossing model. We finish with some recent large deviations results for Gibbs measures, which we can only discuss briefly.

8.1 Motivation

Consider the coin tossing experiment. The microstates are elements of the configuration space $\Omega = \{0,1\}^{\mathbb{N}}$ equipped with the product measure $\mathbb{P}_\nu$, where $\nu \in \mathcal{P}(\{0,1\})$ is given as $\nu = \rho_0\delta_0 + \rho_1\delta_1$ with $\rho_0+\rho_1 = 1$. If $\rho_0 = \rho_1 = \frac{1}{2}$ we have a "fair" coin. Recall the projections $\sigma_j\colon \Omega \to \{0,1\}, j \in \mathbb{N}$, and consider the mean

$$S_N(\omega) = \frac{1}{N}\sum_{j=1}^{N} \sigma_j(\omega) \quad \text{for } \omega \in \Omega.$$

If m_ν denotes the mean ($m_\nu = \frac{1}{2}$ for a fair coin), the *weak law of large numbers* (WLLN) tells us that for $\varepsilon > 0$

$$\mathbb{P}_\nu(S_N \in (m_\nu - \varepsilon, m_\nu + \varepsilon)) \to 1 \quad \text{as } N \to \infty,$$

and for $\varepsilon >$ small enough and $z \neq m_\nu$

$$\mathbb{P}_\nu(S_N \in (z - \varepsilon, z + \varepsilon)) \to 0 \quad \text{as } N \to \infty.$$

In particular one can even prove exponential decay of the latter probability, which we sketch briefly. The problem of decay of probabilities of rare events

is the main task of large deviations theory. For simplicity we assume now that $m_\nu = \frac{1}{2}$. Then

$$\begin{aligned} F(z,\varepsilon) &= -\lim_{N\to\infty} \frac{1}{N} \log \mathbb{P}_\nu(S_N \in (z-\varepsilon, z+\varepsilon)) \\ &= \inf_{x\in(z-\varepsilon,z+\varepsilon)} I(x), \end{aligned}$$

where the function I is defined as

$$I(x) = \begin{cases} x\log 2x + (1-x)\log 2(1-x) \ , \ x \in [0,1] \\ \qquad\qquad\qquad\qquad\qquad\qquad \infty \ , \ x \notin [0,1] \end{cases},$$

where as usual $0 \log 0 = 0$. Since $F(z,\varepsilon) \to I(z)$ as $\varepsilon \to 0$, we may (heuristically) write

$$\mathbb{P}_\nu(S_N \in (z-\varepsilon, z+\varepsilon)) \approx \exp(-NI(z))$$

for N large and ε small. The term $I(z)$ measures the randomness of z and $z = \frac{1}{2} = m_\nu$ is the macrostate which is compatible with the most microstates ($I(\frac{1}{2}) = 0$). The mean S_N gives only very limited information. If we want to know more about the whole random process we might go over to the **empirical measure**

$$L_N(\omega) = \frac{1}{N} \sum_{j=1}^{N} \delta_{\sigma_j(\omega)} \ \in \mathcal{P}(\{0,1\}) \quad \text{for any } \ \omega \in \Omega;$$

or even to the **empirical field**

$$R_N(\omega) = \frac{1}{N} \sum_{k=0}^{N-1} \delta_{T^k\omega^{(N)}} \ \in \mathcal{P}(\Omega),$$

where $T^0 = \mathrm{id}$ and $(T\omega)_j = \omega_{j+1}$ is the shift and $\omega^{(N)}$ is the periodic continuation of the restriction of ω to Λ_N.

The latter example can be connected to our experience with Gibbs measures and distributions as follows. Let $\Lambda_N = [-N,N]^d \cap \mathbb{Z}^d$, $N \in \mathbb{N}$, and define the **periodic empirical field** as

$$R_N^{(\mathrm{per})}(\omega) = \frac{1}{|\Lambda_N|} \sum_{k\in\Lambda_N} \delta_{\theta_k\omega^{(N)}} \ \in \mathcal{P}_\Theta(\Omega,\mathcal{F}) \quad \text{for all } \ \omega \in \Omega,$$

where $\omega^{(N)} \in \Omega$ is the periodic continuation of the restriction of ω onto Λ_N to the whole lattice $\mathbb{Z}^d$. Here, the periodic continuation ensures that the

periodic empirical field is translation invariant. The LLN is not available in general, it is then replaced by some ergodic theorem. For example if $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ is an ergodic measure, then $R_N^{(\mathrm{per})} \Rightarrow \mu$ μ-a.s. as $N \to \infty$. Going back to the coin tossing example the distributions of S_N, L_N and R_N under the product measure $\mathbb{P}_\nu$ are the following probability measures

$$\begin{aligned}
&\mathbb{P}_\nu \circ S_N^{-1} \in \mathcal{P}([0,1]) \\
&\mathbb{P}_\nu \circ L_N^{-1} \in \mathcal{P}(\mathcal{P}([0,1])) \\
&\mathbb{P}_\nu \circ R_N^{-1} \in \mathcal{P}(\mathcal{P}(\Omega)).
\end{aligned}$$

The WLLN implies for all of these probabilities exponential decay of the rare events given by a function I as the rate in N. This will be generalised in the next subsection, where such functions I are called rate functions.

8.2 Definition

In the following we consider the general setup, i.e. we let X denote a Polish space and equip it with the corresponding Borel-σ-algebra $\mathcal{B}_X$.

Definition 8.1 (Rate function) *A function $I\colon X \to [0,\infty]$ is called a* **rate function** *if*

(1) $I \neq \infty$,

(2) I is lower semi continuous,

(3) I has compact level sets.

Definition 8.2 (Large deviations principle) *A sequence $(P_N)_{N\in\mathbb{N}}$ of probability measures $P_N \in \mathcal{P}(X, \mathcal{B}_X)$ on X is said to satisfy the large deviations principle with rate (speed) N and rate function I if the following upper and lower bound hold,*

$$\begin{aligned}
\limsup_{N\to\infty} \frac{1}{N} \log P_N(C) &\leq -\inf_{x\in C} I(x) \qquad \textit{for } C \subset X \textit{ closed}, \\
\liminf_{N\to\infty} \frac{1}{N} \log P_N(O) &\geq -\inf_{x\in O} I(x) \qquad \textit{for } O \subset X \textit{ open}.
\end{aligned} \tag{8.45}$$

Let us consider the following situation. Let $(X_i)_{i\in\mathbb{N}}$ be i.i.d. real-valued random variables, i.e., there is a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ such that each random variable has the distribution $\mu = \mathbb{P} \circ X_1^{-1} \in \mathcal{P}(\mathbb{R}, \mathcal{B}_\mathbb{R})$. Denote the distribution of the mean S_N by $\mu_N = \mathbb{P}^N \circ S_N^{-1} \in \mathcal{P}(\mathbb{R}, \mathcal{B}_\mathbb{R})$. For this situation there is the following theorem about a large deviations principle

for the sequence $(\mu_N)_{N\in\mathbb{N}}$. Before we formulate that theorem we need some further definitions. For $\mu \in \mathcal{P}(\mathbb{R}, \mathcal{B}_{\mathbb{R}})$ let

$$\Lambda_\mu(\lambda) = \log\Big(\int_{\mathbb{R}} \exp(\lambda x)\mu(\mathrm{d}x)\Big) \quad \lambda \in \mathbb{R},$$

be the logarithmic moment generating function. It is known that Λ_μ is lower semi continuous and $\Lambda_\mu(\lambda) \in (-\infty, \infty], \lambda \in \mathbb{R}$. The Legendre-Fenchel transform Λ_μ^* of Λ_μ is given by

$$\Lambda_\mu^*(x) = \sup_{\lambda\in\mathbb{R}}\{\lambda x - \Lambda_\mu(\lambda)\} \quad x \in \mathbb{R}.$$

Theorem 8.3 (Cramér's Theorem) *Let $(X_i)_{i\in\mathbb{N}}$ be i.i.d. real-valued random variables with distribution $\mu \in \mathcal{P}(\mathbb{R}, \mathcal{B}_{\mathbb{R}})$ and let μ_N denote the distribution of the mean S_N. Assume further that $\Lambda_\mu(\lambda) < \infty$ for all $\lambda \in \mathbb{R}$. Then the sequence $(\mu_N)_{N\in\mathbb{N}}$ satisfies a large deviations principle with rate function given by the limit of the Legendre-Fenchel transform Λ_μ^* of the logarithmic moment generating function Λ_{μ_N}, i.e., for any measurable $\Gamma \in \mathcal{B}_{\mathbb{R}}$*

$$\begin{aligned} \limsup_{N\to\infty} \frac{1}{N}\log\mu_N(\Gamma) &\le -\inf_{x\in\overline{\Gamma}} \Lambda_\mu^*(x) \\ \liminf_{N\to\infty} \frac{1}{N}\log\mu_N(\Gamma) &\ge -\inf_{x\in\Gamma^\circ} \Lambda_\mu^*(x). \end{aligned} \tag{8.46}$$

Proof. See [DZ98] or [Dor99]. □

An important tool in proving large deviations principle is the following alternative version of the well-known Varadhan Lemma ([DZ98]).

Theorem 8.4 (Tilted LDP) *Let the sequence $(P_N)_{N\in\mathbb{N}}$ of probability measures $P_N \in \mathcal{P}(X, \mathcal{B}_X)$ satisfy a large deviations principle with rate (speed) N and rate function I. Let $F\colon X \to \mathbb{R}$ be a continuous function that is bounded from above. Define*

$$J_N(S) = \int_S \mathrm{e}^{NF(x)} P_N(\mathrm{d}x) \quad , \ S \in \mathcal{B}_X.$$

Then the sequence $(P_N^F)_{N\in\mathbb{N}}$ of probability measures $P_N^F \in \mathcal{P}(X, \mathcal{B}_X)$ defined by

$$P_N^F(S) = \frac{J_N(S)}{J_N(X)} \quad , \ S \in \mathcal{B}_X$$

satisfies a large deviations principle on X with rate N and rate function

$$I^F(x) = \sup_{y\in X}\{F(y) - I(y)\} - (F(x) - I(x)).$$

Proof. See [dH00] or [DZ98] for the original version of Varadhan's Lemma and [Ell85] or [Dor99] for a version as in the theorem.

□

8.3 Some results for Gibbs measures

We present some results on large deviations principles for Gibbs measures. We assume the set-up of Section 6 and Section 7. Let Φ an interaction potential and note that the expectation of the interaction potential with the periodic empirical field is given by

$$\langle R_N^{(\mathrm{per})}(\omega), \Phi\rangle = |\Lambda_N|^{-1} H_{\Lambda_N}^{(\mathrm{per})}(\omega) \quad , \omega \in \Omega, \tag{8.47}$$

where $H_{\Lambda_N}^{(\mathrm{per})}$ is the Hamiltonian in Λ_N with interaction potential Φ and periodic boundary conditions. Recall that $\gamma_{\Lambda_N}^{\Phi,\omega}$ denotes the Gibbs distribution in Λ_N with configurational boundary condition $\omega \in \Omega$ and $\gamma_{\Lambda_N}^{\Phi,\mathrm{per}}$ the Gibbs distribution in Λ_N with periodic boundary condition. Further, if $\mu \in \mathcal{G}_\Theta(\Phi, \beta)$ is a Gibbs measure, $h(\cdot|\mu) = h(\cdot|\Phi)$ denotes the specific relative entropy with respect to the Gibbs measure μ with respect to the given interaction potential Φ. Denote by $\mathfrak{e}(\Omega)$ the evaluation σ-algebra for the probability measures on Ω. Note that the mean energy $\langle \cdot, \Phi\rangle$ can be identified as a linear form on a vector space of finite range interaction potentials. In particular we define

$$\tau_{\Lambda_N}^{\Psi}(\omega) = \langle R_N^{(\mathrm{per})}(\omega), \Psi\rangle \quad \omega \in \Omega$$

for any interaction potential Ψ with finite range. In the limit $N \to \infty$ one gets a linear functional τ on the vector space V of all interaction potentials with finite range (see [Isr79] and[Geo88] for details on this vector space).

Theorem 8.5 (LDP for Gibbs measures) *Let $\Lambda_N = [-N, N]^d \cap \mathbb{Z}^d$, $\beta > 0$ and Φ be an interaction potential with finite range. Then the following assertions hold.*

(a) Let $\mu \in \mathcal{G}_\Theta(\Phi, \beta)$ be given. Then the sequence $(\mu \circ (R_N^{(\mathrm{per})})^{-1})_{N\in\mathbb{N}}$ of probability measures $\mu \circ (R_N^{(\mathrm{per})})^{-1} \in \mathcal{P}(\mathcal{P}(\Omega, \mathcal{F}), \mathfrak{e}(\Omega))$ satisfies a large deviations principle with rate (speed) $|\Lambda_N|$ and rate function $h(\cdot|\mu)$.

(b) Let $\gamma_{\Lambda_N}^{\Phi,\omega}$ be the Gibbs distribution in Λ_N with boundary condition $\omega \in \Omega$. Then for any closed set $F \subset \mathcal{P}(\Omega, \mathcal{F})$ and any open set $G \subset \mathcal{P}(\Omega, \mathcal{F})$,

$$\begin{aligned}
\limsup_{N\to\infty} \frac{1}{|\Lambda_N|} \log \sup_{\omega\in\Omega} \gamma_{\Lambda_N}^{\Phi,\omega}(R_N^{(\mathrm{per})} \in F) &\le -\inf_{\nu\in F}\{h(\nu) + \langle \nu, \Phi\rangle + P(\Phi)\}, \\
\liminf_{N\to\infty} \frac{1}{|\Lambda_N|} \log \sup_{\omega\in\Omega} \gamma_{\Lambda_N}^{\Phi,\omega}(R_N^{(\mathrm{per})} \in G) &\ge -\inf_{\nu\in G}\{h(\nu) + \langle \nu, \Phi\rangle + P(\Phi)\}.
\end{aligned} \tag{8.48}$$

(c) Let $K \subset$ in V^* be a measurable subset. Then

$$\begin{aligned} \limsup_{N\to\infty} \frac{1}{|\Lambda_N|} \log \sup_{\omega\in\Omega} \gamma^{\Phi,\omega}_{\Lambda_N}(\tau_{\Lambda_N} \in K) &\leq -\inf_{\tau\in\overline{K}} \{J^{\Phi}_V(\tau)\} \\ \liminf_{N\to\infty} \frac{1}{|\Lambda_N|} \log \sup_{\omega\in\Omega} \gamma^{\Phi,\omega}_{\Lambda_N}(\tau_{\Lambda_N} \in K) &\geq -\inf_{\tau\in K^\circ} \{J^{\Phi}_V(\tau)\}, \end{aligned} \tag{8.49}$$

with $J^{\Phi}_V(\tau) = P(\Phi) + \inf_{\Psi\in V}\{\tau(\Psi) + P(\Psi + \Phi)\}$.

Proof. The part (a) can be found in [Geo88] and in [FO88] or alternatively in [Oll88], all for the case that the state space E is finite. If E is an arbitrary measurable space, see [Geo93]. Part (b) is in [Geo93] and [Oll88], and part (c) in [Geo93]. Note that the restrictions on the interaction potential can even be relaxed, see [Geo93]. The corresponding theorems for continuous systems can be found in [Geo95]. □

A last remark to part (c) of the Theorem 8.5.

Theorem 8.6 (Equivalence of ensembles) *Let $\Lambda_N = [-N, N]^d \cap \mathbb{Z}^d$ and Φ be an interaction potential with finite range. Let $K \subset \mathbb{R}$ be a measurable set of energy densities. Then there is an interaction potential $\Psi \in V$ such that $\Psi + \Phi \in V$ and it holds.*

$$\mathsf{acc}_{N\to\infty}\big\{\gamma^{\Phi,\mathrm{per}}_{\Lambda_N}(\cdot|\tau^{\Phi}_{\Lambda_N} \in K)\big\} \subset \mathcal{G}_{\Theta}(\Phi + \Psi). \tag{8.50}$$

Proof. See [Geo93] and [Geo95] and [LPS95]. Observe that the periodic boundary conditions are crucial for this result (they ensure the translation invariance). Translation invariance provides, as we know from Section 7, a variational characterisation for Gibbs measures. There exists no proof for configurational boundary conditions for dimension $d \geq 2$. For the case $d = 1$ see [Ada01]. □

9 Models

We present here some important models in statistical mechanics. For more models for lattice systems see [BL99a] and [BL99b]. The last example in this section is the continuous Ising model which is an effective model for interfaces and plays an important role for many investigations.

9.1 Lattice Gases

We consider here a system of particles occupying a set $\Lambda \subset \mathbb{Z}^d$ with $|\Lambda| = V$. Here $|\Lambda|$ denotes the number of sites in Λ. At each point of Λ there is at most one particle. For $i \in \Lambda$ we set $\omega_i = 1$ if there is a particle at the site i and set $\omega_i = 0$ otherwise. Any $\omega \in \Omega := \{0,1\}^\Lambda$ is called a *configuration*. For a configuration ω we have the Hamiltonian $H_\Lambda(\omega)$. The canonical partition function is

$$Z_\Lambda(\beta, N) = \sum_{\substack{\omega\in\Omega,\\ \sum_{i\in\Lambda}\omega_i = N}} \mathrm{e}^{-\beta H_\Lambda(\omega)}.$$

Note that there is no need here for $N!$ since the particles are indistinguishable. The thermal wavelength λ is put equal to 1. The grandcanonical partition function is then

$$\begin{aligned} Z_\Lambda(\beta,\mu) &= \sum_{N=0}^{V} \mathrm{e}^{\beta N\mu} \sum_{\substack{\omega\in\Omega,\\ \sum_{i\in\Lambda}\omega_i = N}} \mathrm{e}^{-\beta H_\Lambda(\omega)} = \sum_{N=0}^{V} \sum_{\substack{\omega\in\Omega,\\ \sum_{i\in\Lambda}\omega_i = N}} \mathrm{e}^{-\beta(H_\Lambda(\omega) - \mu\sum_{i\in\Lambda}\omega_i)} \\ &= \sum_{\omega\in\Omega} \mathrm{e}^{-\beta(H_\Lambda(\omega) - \mu\sum_{i\in\Lambda}\omega_i)}. \end{aligned}$$

The thermodynamic functions are defined in the usual way. The probability for a configuration $\omega \in \{0,1\}^\Lambda$ is

$$\frac{\mathrm{e}^{-\beta(H_\Lambda(\omega) - \mu\sum_{i\in\Lambda}\omega_i)}}{Z_\Lambda(\beta,\mu)}.$$

The Hamiltonian is of the form

$$H_\Lambda(\omega) = \sum_{i,j\in\Lambda,\ i\neq j} \omega_i\omega_j\phi(q_i - q_j),$$

where q_i is the position vector of the site $i \in \Lambda$. However this is too difficult to solve in general. We consider two simplifications of the potential energy:

Mean-field Models: ϕ is taken to be a constant. Therefore

$$H_\Lambda(\omega) = -\lambda \sum_{i,j\in\Lambda,\ i\neq j} \omega_i\omega_j.$$

Take $\lambda > 0$, otherwise the interaction potential is not tempered. When $\omega_i = 1$ for all $i \in \Lambda$, $H_\Lambda(\omega) = -\lambda\frac{V(V-1)}{2}$ and therefore H_Λ is not stable. For H_Λ to be stable we must take $\lambda = \frac{\gamma}{V}$ with $\gamma > 0$. Thus

$$H_\Lambda(\omega) = -\frac{\gamma}{V} \sum_{i,j\in\Lambda,\ i\neq j} \omega_i\omega_j.$$

Note that for Mean-field models the lattice structure is not important since the interaction does not depend on the location of the lattice sites and therefore we can take $\Lambda = \{1, 2, \ldots, V\}$.

Nearest-neighbour Models: In these models we take

$$\phi(q_i - q_j) = \begin{cases} -J\ , & \text{if } |q_i - q_j| = 1 \\ 0\ , & \text{if } |q_i - q_j| > 1 \end{cases},$$

that is the interaction is only between nearest neighbours and is then equal to $-J, J \in \mathbb{R}$. If we denote a pair of neighbouring sites i and j by $\langle i, j\rangle$ we have

$$H_\Lambda(\omega) = -J \sum_{\langle i,j\rangle} \omega_i \omega_j.$$

Note that J can be negative or positive.

9.2 Magnetic Models

In magnetic models at each site of Λ there is a dipole or spin. This spin could be pointing upwards or downwards, that is, along the direction of the external magnetic field or in the opposite direction. For $i \in \Lambda$ we set $\sigma_i = 1$ if the spin at the site i is pointing upwards and $\sigma_i = -1$ if it is pointing downwards. The term $\sigma \in \{-1, 1\}^\Lambda$ is called a configuration. For a configuration σ we have an energy $\mathcal{E}(\sigma)$ and an interaction with an external magnetic field of strength h, $-h \sum_{i\in\Lambda} \sigma_i$. The partition function is then

$$Z_\Lambda(\beta, h) = \sum_{\sigma\in\{-1,1\}^\Lambda} \mathrm{e}^{-\beta(\mathcal{E}(\sigma) - h \sum_{i\in\Lambda} \sigma_i)}.$$

The free energy per lattice site is

$$f_\Lambda(\beta, h) = -\frac{1}{\beta V} \log Z_\Lambda(\beta, h).$$

The probability for a configuration $\sigma \in \{-1, 1\}^\Lambda$ is

$$\frac{\mathrm{e}^{-\beta(\mathcal{E}(\sigma) - h \sum_{i\in\Lambda} \sigma_i)}}{Z_\Lambda(\beta, h)}.$$

The total magnetic moment is the random variable

$$M_\Lambda(\sigma) = \sum_{i\in\Lambda} \sigma_i$$

and therefore

$$\mathbb{E}(M_\Lambda) = \frac{\sum_{\sigma\in\{-1,1\}^\Lambda}(\sum_{i\in\Lambda}\sigma_i)\mathrm{e}^{-\beta(\mathcal{E}(\sigma)-h\sum_{i\in\Lambda}\sigma_i)}}{Z_\Lambda(\beta,h)} = \frac{1}{\beta}\frac{\partial}{\partial h}\log Z_\Lambda(\beta,h).$$

Then if $m_\Lambda(\beta,h)$ denotes the mean magnetisation per lattice site we have

$$m_\Lambda(\beta,h) = \frac{\mathbb{E}(M_\Lambda)}{V} = -\frac{\partial}{\partial h}f_\Lambda(\beta,h).$$

Note that

$$\frac{\partial^2}{\partial h^2}f_\Lambda(\beta,h) = -\frac{\beta}{V}\mathbb{E}(M_\Lambda - \mathbb{E}(M_\Lambda))^2 \leq 0.$$

Therefore $h \mapsto f_\Lambda(\beta,h)$ is *concave*. If $\mathcal{E}(\sigma) = \mathcal{E}(-\sigma)$, then

$$f_\Lambda(\beta,-h) = f_\Lambda(\beta,h).$$

If Λ_l is a sequence of regions tending to infinity and if

$$\lim_{l\to\infty} f_{\Lambda_l}(\beta,h) = f(\beta,h),$$

then $h \mapsto f(\beta,h)$ is also concave and if it is differentiable

$$m(\beta,h) := \lim_{l\to\infty} m_{\Lambda_l}(\beta,h) = -\frac{\partial}{\partial h}f(\beta,h).$$

Relation between Lattice Gas and Magnetic Models

We can relate the Lattice Gas to a Magnetic Model and vice versa by the transformation

$$\omega_i = (\sigma_i + 1)/2$$

or

$$\sigma_i = 2\omega_i - 1.$$

This gives

$$H_\Lambda(\omega) - \mu\sum_{i\in\Lambda}\sigma_i = \mathcal{E}(\sigma) - (a + \frac{1}{2}\mu)\sum_{i\in\Lambda}\sigma_i - (b + \frac{1}{2}\mu)V,$$

where a and b are constants. Therefore

$$\pi_\Lambda(\beta,\mu) = (b + \frac{1}{2}\mu) - f_\Lambda(\beta, a + \frac{1}{2}\mu)$$

and

$$\rho_\Lambda(\beta,\mu) = \frac{1}{2}(1 + m_\Lambda(\beta, a + \frac{1}{2}\mu)).$$

9.3 Curie-Weiss model

We study here the Curie-Weiss Model, which is a mean-field model given by the interaction energy

$$\mathcal{E}(\sigma) = -\frac{\alpha}{V} \sum_{i \le i < j \le V} \sigma_i \sigma_j = -\frac{\alpha}{2V} \left(\sum_{i=1}^{V} \sigma_i \right)^2 + \frac{\alpha}{2} \quad , \sigma \in \{-1,1\}^{\Lambda},$$

where $\alpha > 0$ and Λ is any finite set with $|\Lambda| = V$. We sketch here only some explicit calculations, more on the model can be found in the books [Ell85],[Dor99], [Rei98], and [TKS92]. The partition function is given by

$$Z_\Lambda(\beta, h) = \sum_{\sigma \in \{-1,1\}^V} \mathrm{e}^{-\beta(\mathcal{E}(\sigma) - h \sum_{i=1}^{V} \sigma_i)}.$$

For $\nu = \beta\alpha$ this becomes

$$Z_\Lambda(\beta, h) = \mathrm{e}^{-\frac{\nu}{2}} \sum_{\sigma \in \{-1,1\}^V} \exp\left[\frac{\nu}{2V} \left(\sum_{i=1}^{V} \sigma_i \right)^2 + \beta h \sum_{i=1}^{V} \sigma_i \right].$$

Note that $Z_\Lambda(\beta, -h) = Z_\Lambda(\beta, h)$. In the identity

$$\int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}y^2} \mathrm{d}y = \sqrt{2\pi},$$

put $y = x - a$. This gives

$$\int_{-\infty}^{\infty} \mathrm{e}^{(-\frac{1}{2}x^2 + ax)} \mathrm{d}x = \sqrt{2\pi} \mathrm{e}^{\frac{1}{2}a^2}$$

or

$$\mathrm{e}^{\frac{1}{2}a^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{(-\frac{1}{2}x^2 + ax)} \mathrm{d}x.$$

Using this identity with $a = \sqrt{\frac{\nu}{V}} \left(\sum_{i=1}^{V} \sigma_i \right)$ we get

$$\begin{aligned} Z_\Lambda(\beta, h) &= \mathrm{e}^{-\frac{\nu}{2}} \sum_{\sigma \in \{-1,1\}^V} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{2}x^2 + \left(x\sqrt{\frac{\nu}{V}} + \beta h \right) \sum_{i=1}^{V} \sigma_i \right] \mathrm{d}x \\ &= \mathrm{e}^{-\frac{\nu}{2}} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}x^2} \sum_{\sigma \in \{-1,1\}^V} \exp\left[\left(x\sqrt{\frac{\nu}{V}} + \beta h \right) \sum_{i=1}^{V} \sigma_i \right] \mathrm{d}x. \end{aligned}$$

Now

$$\sum_{\sigma\in\{-1,1\}^V} \exp(\kappa \sum_{i=1}^{V} \sigma_i) = (2\cosh\kappa)^V.$$

Therefore

$$Z_\Lambda(\beta,h) = \mathrm{e}^{-\frac{\nu}{2}} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}x^2} \left[2\cosh\left(x\sqrt{\frac{2}{V}} + \beta h\right)\right]^V \mathrm{d}x.$$

Putting $\eta = \frac{x}{\sqrt{\nu V}}$, we get

$$\begin{aligned} Z_\Lambda(\beta,h) &= \mathrm{e}^{-\frac{\nu}{2}} 2^V \left(\frac{\nu V}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \left[\exp(-\frac{\nu\eta^2}{2})\cosh(\nu\eta+\beta h)\right]^V \mathrm{d}\eta \\ &= \mathrm{e}^{-\frac{\nu}{2}} 2^V \left(\frac{\nu V}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{VG(h,\eta)} \mathrm{d}\eta, \end{aligned}$$

where

$$G(h,\eta) = -\frac{1}{2}\nu\eta^2 + \log\,\cosh(\nu\eta+\beta h).$$

The free energy per lattice site is

$$\begin{aligned} f_\Lambda(\beta,h) = -\frac{1}{\beta V}\log Z_\Lambda(\beta,h) &= \frac{\nu}{2\beta V} - \frac{1}{\beta}\log 2 - \frac{1}{2\beta V}\log\left(\frac{\nu V}{2\pi}\right) \\ &- \frac{1}{\beta V}\log\int_{-\infty}^{\infty} \mathrm{e}^{VG(h,\eta)}\mathrm{d}\eta. \end{aligned}$$

Therefore by Laplace's Theorem (see for example [Ell85] or [Dor99]), the free energy per lattice site in the thermodynamic limit is

$$\begin{aligned} f(\beta,h) &= -\frac{1}{\beta}\log 2 - \lim_{V\to\infty}\frac{1}{\beta V}\log\int_{-\infty}^{\infty} \mathrm{e}^{VG(h,\eta)}\mathrm{d}\eta \\ &= -\frac{1}{\beta}\log 2 - \frac{1}{\beta}\sup_{\eta\in\mathbb{R}} G(h,\eta). \end{aligned}$$

Suppose that the supremum of $G(h,\eta)$ is attained at $\eta(h)$. Then

$$f(\beta,h) = -\frac{1}{\beta}\log 2 - \frac{1}{\beta}G(h,\eta(h))$$

and

$$\frac{\partial G}{\partial\eta}(h,\eta(h)) = -\nu\eta(h) + \nu\tanh(\nu(h,\eta(h)) + \beta h) = 0,$$

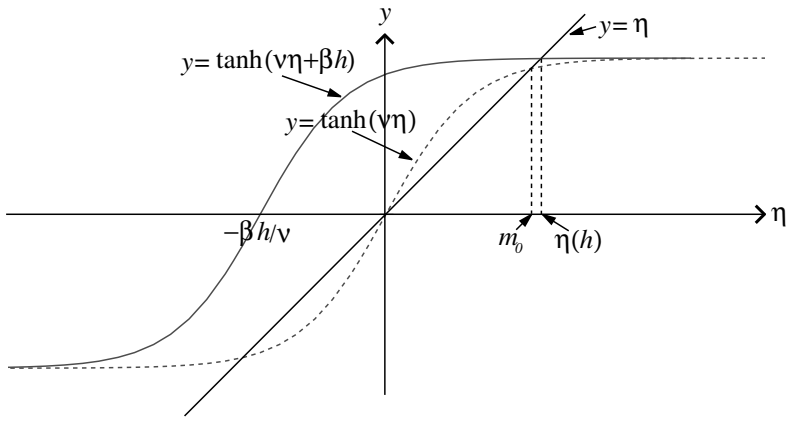

Figure 5: $h > 0$, $\nu > 1$

or

$$\eta(h) = \tanh(\nu\eta(h) + \beta h).$$

The mean magnetisation per site in thermodynamic limit is

$$\begin{aligned} m(\beta, h) &= -\frac{\partial}{\partial h} f(\beta, h) = \frac{1}{\beta}\frac{\partial}{\partial h} G(h, \eta(h)) \\ &= \tanh(\nu\eta(h) + \beta h) + \frac{\partial G}{\partial \eta}(h, \eta(h))\frac{\partial \eta}{\partial h}(h) \\ &= \eta(h), \end{aligned}$$

since $\frac{\partial G}{\partial \eta}(h, \eta(h)) = 0$.

Since

$$f(\beta, -h) = f(\beta, h) \qquad \text{and} \qquad m(\beta, -h) = -m(\beta, h),$$

it is sufficient to consider the case $h \geq 0$ (see Figure 7 and 8). The expression $m_0 = \lim_{h\downarrow 0} m(h)$ is called the **spontaneous magnetisation**, this is the mean magnetisation as the magnetic field is decreased to zero,

$$m_0 = \lim_{h\downarrow 0} m(h) = \lim_{h\downarrow 0} \eta(h).$$

We have from above

$$m_0 \begin{cases} = 0\ , & \text{if } \nu \leq 1 \\ > 0\ , & \text{if } \nu > 1 \end{cases} .$$

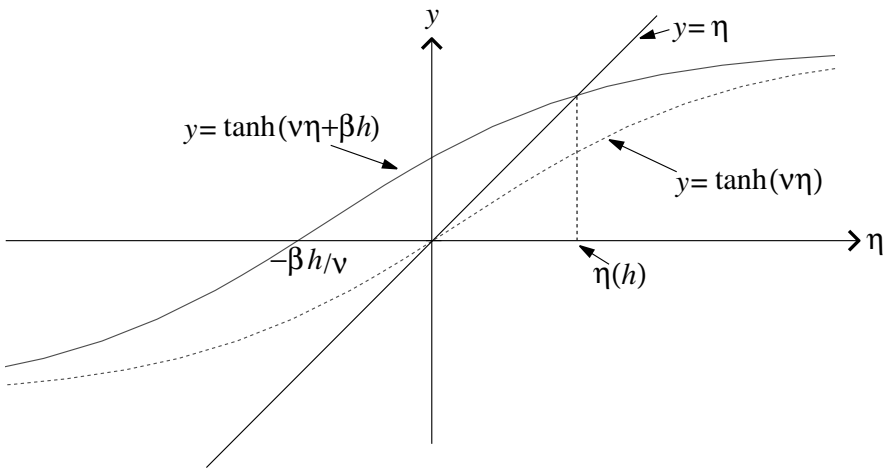

Figure 6: $h > 0$, $\nu \leq 1$

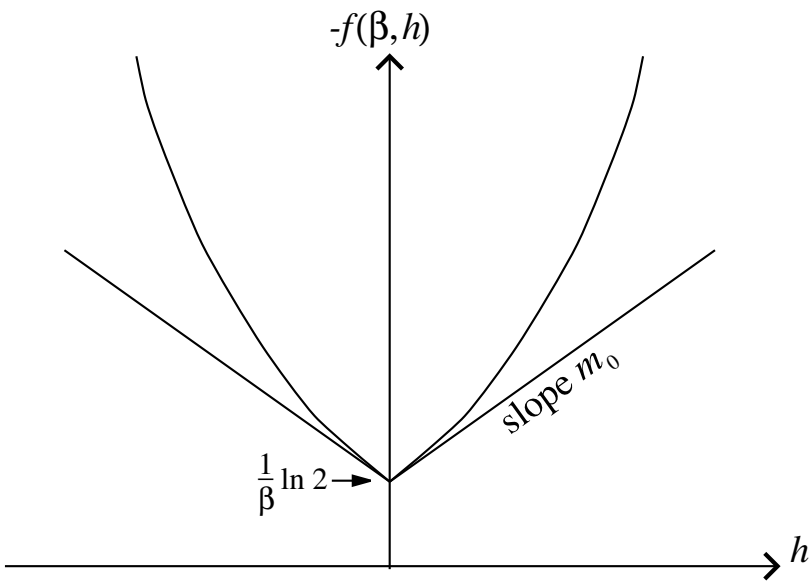

Figure 7: $\nu > 1$

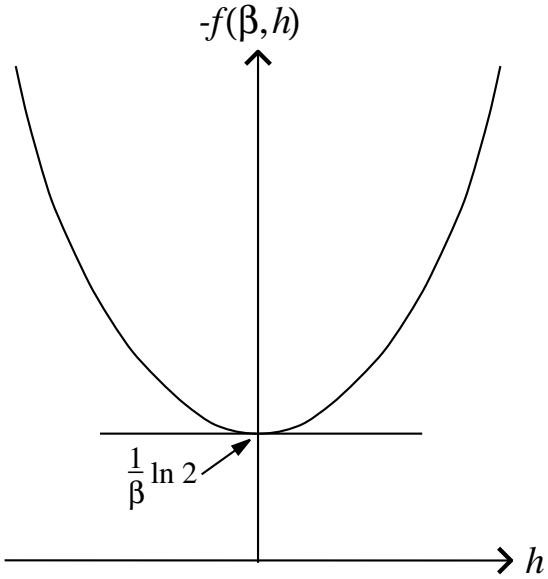

Figure 8: $\nu \leq 1$

Let $T_c = \frac{\alpha}{k}$; T_c is called the **Curie Point**. $T \geq T_c$ corresponds to $\nu \leq 1$ (see figure 8) and $T < T_c$ to $\nu > 1$ (see Figure 7).

$$m_0 \begin{cases} > 0 \ , & \text{when } T < T_c \\ = 0 \ , & \text{when } T \geq T_c \end{cases} .$$

We have a phase transition at the Curie Point corresponding to the onset of spontaneous magnetisation.

We can consider this model from the point of view of a lattice gas. Consider a lattice gas with potential energy

$$H_\Lambda(\omega) = -\frac{\gamma}{V} \sum_{i \leq i < j \leq V} \omega_i \omega_j = -\frac{\gamma}{2V} \left(\sum_{i=1}^{V} t_i \right)^2 + \frac{\gamma}{2V} \sum_{i=1}^{V} \omega_i$$

Let $t_i = \frac{(\sigma_i + 1)}{2}$. Then

$$\sum_{i=1}^{V} \omega_i = \frac{1}{2} (\sum_{i=1}^{V} \sigma_i + V).$$

Therefore

$$H_\Lambda(\omega) = -\frac{\gamma}{8V}\left(\sum_{i=1}^{V}\sigma_i\right)^2 - \frac{\gamma}{4}\sum_{i=1}^{V}\sigma_i - \frac{\gamma V}{8} + \frac{\gamma}{4V}\sum_{i=1}^{V}\sigma_i + \frac{\gamma}{4}.$$

We can neglect the last two terms, because γ is small and the expectation of a single spin is zero, and we take

$$H_\Lambda(\omega) = -\frac{\gamma}{8V}\left(\sum_{i=1}^{V}\sigma_i\right)^2 - \frac{\gamma}{4}\sum_{i=1}^{V}\sigma_i - \frac{\gamma V}{8}.$$

Then

$$\begin{aligned} H_\Lambda(\omega) - \mu\sum_{i=1}^{V}\omega_i &= -\frac{\gamma}{8V}\left(\sum_{i=1}^{V}\sigma_i\right)^2 - (\frac{\gamma}{4}+\frac{\mu}{2})\sum_{i=1}^{V}\sigma_i - (\frac{\gamma}{8}+\frac{\mu}{2})V \\ &= -\mathcal{E}(\sigma) - (\frac{\gamma}{4}+\frac{\mu}{2})\sum_{i=1}^{V}\sigma_i - (\frac{\gamma}{8}+\frac{\mu}{2})V. \end{aligned}$$

with $\alpha = \frac{\gamma}{4}$ and

$$\pi(\beta,\mu) = (\frac{\gamma}{8}+\frac{1}{2}\mu) - f(\beta, \frac{\gamma}{4}+\frac{1}{2}\mu)$$

and

$$\rho(\beta,\mu) = \frac{1}{2}(1 + m(\beta, \frac{\gamma}{4}+\frac{1}{2}\mu)).$$

Let $\mu_0 = -\frac{\gamma}{2}$, then

$$\pi(\beta,\mu) = (\frac{\gamma}{8}+\frac{1}{2}\mu) - f(\beta, \frac{1}{2}(\mu-\mu_0))$$

and

$$\rho(\beta,\mu) = \frac{1}{2}(1 + m(\beta, \frac{1}{2}(\mu-\mu_0))).$$

If $\beta > \frac{4}{\gamma}$, then $\pi(\beta,\mu)$ has a discontinuity in its derivative at μ_0 and $\rho(\beta,\mu)$ has a discontinuity at μ_0 (see Figure 9).

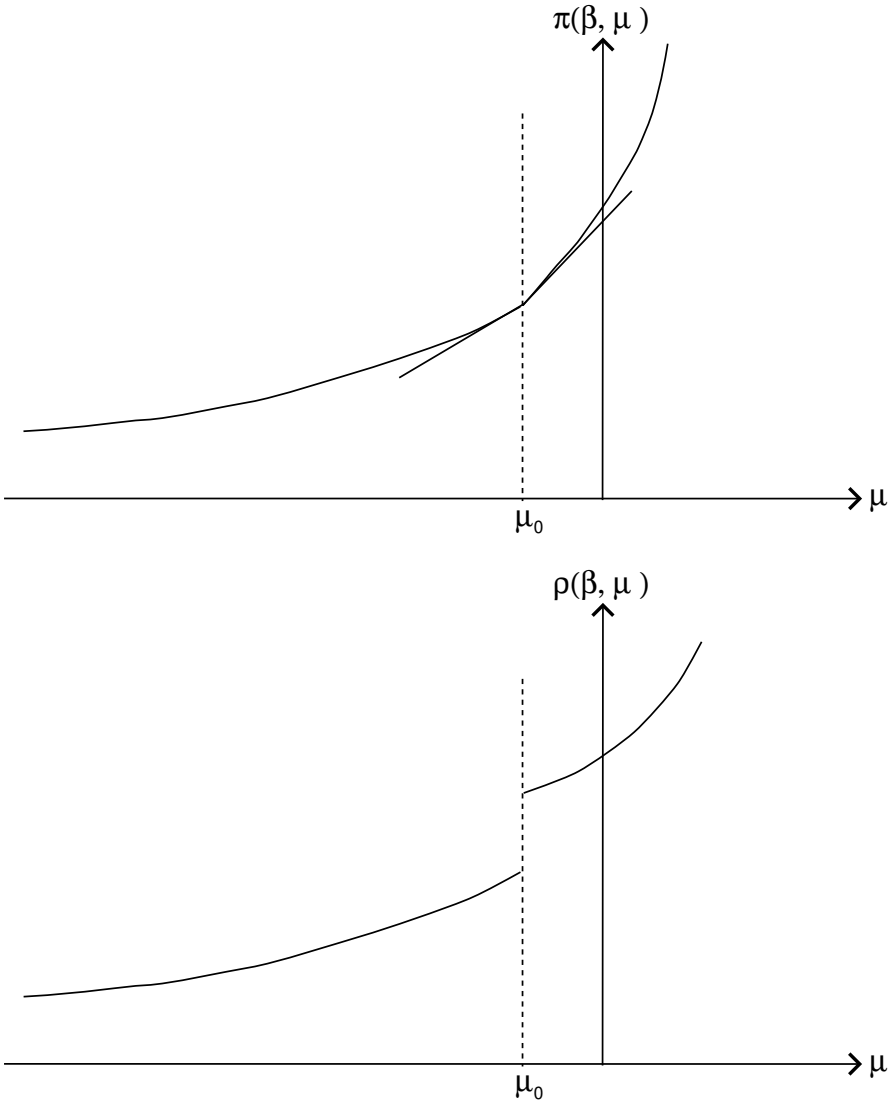

Figure 9: $\beta > \frac{4}{\gamma}$

9.4 Continuous Ising model

In the continuous Ising model the state space $E = \{-1, +1\}$ is replaced by the real numbers $\mathbb{R}$. Let $\Omega = \mathbb{R}^{\mathbb{Z}^d}$ denote the space of configurations. Due to the non-compactness of the state space severe mathematical difficulties arise. We note that the continuous Ising model can be seen as an effective model describing the height of an interface, here the functions $\phi \in \Omega$ give the height of an interface for some reference height; and any collection $(\sigma_x)_{x\in\mathbb{Z}^d}$ or probability measure $P \in \mathcal{P}(\Omega, \mathcal{F})$ is called **random field of heights**. Details about this model can be found in [Gia00] and [Fun05]. One first considers the so-called **massive** model, where there is a mass $m > 0$ implying a self-interaction. Let $\Lambda \in \mathcal{S}, \psi \in \Omega$ and $m > 0$. We write synonymously $\phi_x = \phi(x)$ for $\phi \in \Omega$. Nearest neighbour heights do interact with an *elastic interaction potential* $V\colon \mathbb{R} \to \mathbb{R}$, which we assume to be strictly convex with quadratic growth, and which depends only on the difference in the heights of the nearest neighbours. In the simplest case $V(r) = \frac{r^2}{2}$ one gets the Hamiltonian

$$H_\Lambda^\psi(\phi) = \sum_{x\in\Lambda} \frac{m^2}{2}\phi_x^2 + \frac{1}{4d} \sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} (\phi_x - \phi_y)^2,$$

with $\phi_x = \psi_x$ for $x \in \Lambda^c$. The interface here is said to be anchored at ψ outside of Λ. A random interface anchored at ψ outside of Λ is given by the Gibbs distribution

$$\gamma_\Lambda^\psi(\mathrm{d}\phi) = \frac{1}{Z_\Lambda(\psi)} \mathrm{e}^{-\beta H_\Lambda^\psi(\phi)} \lambda_\Lambda^\psi(\mathrm{d}\phi),$$

where

$$\lambda_\Lambda^\psi(\mathrm{d}\phi) = \prod_{x\in} \mathrm{d}\phi_x \prod_{x\notin\Lambda} \delta_{\psi_x}(\mathrm{d}\phi_x)$$

is the product of the Lebesgue measure at each single site in Λ and the Dirac measure at ψ_x for $x \in \Lambda^c$. The term λ_Λ^ψ is called reference measure in Λ with boundary ψ. The thermodynamic limit exists for the model with $m > 0$ in any dimension. However, for the most interesting case $m = 0$ this exists only for $d \geq 3$. These models are called **massless models** or **harmonic crystals**. The interesting feature of these models is that there are infinitely many Gibbs measures due to the continuous symmetry. Hence we are in a regime of phase transitions (see [BD93] for some rigorous results for this regime). The massless models have been studied intensively during the last fifteen years (see [Gia00] for an overview). The main technique applied is the random walk representation. This can be achieved when one employs summation by parts to obtain a discrete elliptic problem.

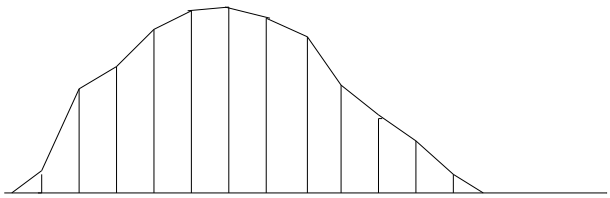

Figure 10: height-functions $\phi\colon \mathbb{Z}^d \to \mathbb{R}$

This gives also the hint that we need $d \geq 3$ due to this random walk representation and the transience of the random walk. Luckily, if one goes over to the **random field of gradient**, i.e. the field derived with the discrete gradient mapping from the random field of heights, one has the existence of infinite Gibbs measure for any dimension ([Gia00],[Fun05]). However, one looses the product structure of the reference measure and one has to deal with the curl free condition. The fundamental result concerning these gradient Gibbs measures is given in [FS97]. For a recent review see [Fun05].

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