Helv Phys Acta
Vol. 69 (1996)

0018-0238/96/060908-41$1.50+0.20/0

Statistical mechanical methods and continued fractions

By O. E. Lanford III and L. Ruedin

Mathematics Department, ETH-Zürich
ETH-Zentrum, 8092 Zürich, Switzerland

(6.V.1996)

Abstract. For a_1, ..., a_n a finite sequence of strictly positive integers, we denote by $q_n(a_1, \ldots, a_n)$ the denominator of the finite continued fraction $[a_1, \ldots, a_n]$ written as a quotient of two relatively prime integers. We show that the sequence of functions $\log q_n(a_1, \ldots, a_n)$, $n = 1, 2, \ldots$, have the formal properties of a Hamiltonian for a one-dimensional lattice system, to which the methods of statistical mechanics can be applied, and we investigate the properties of the system so defined.

1 Introduction

We are going to discuss here a one-dimensional statistical-mechanical system constructed out of continued fractions. We will write continued fractions with the notation $[a_1, \ldots, a_n]$ instead of the typographically inconvenient

$$\cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{\ddots \, \cfrac{}{a_{n-1} + \cfrac{1}{a_n}}}}}$$

Formally, we can define this notation recursively:

$$[a_1] := \frac{1}{a_1}, \quad [a_1, a_2, \ldots, a_n] := \cfrac{1}{a_1 + \cfrac{1}{[a_2, \ldots, a_n]}}.$$

From this definition, it follows easily by induction that

$$[a_1, \ldots, a_k, \ldots a_n] = [a_1, \ldots, (a_k + [a_{k+1}, \ldots, a_n])] \quad \text{for any } k < n.$$

In general, the entries a_j can be elements of an arbitrary field (but it is then necessary to pay attention to the possibility of encountering a zero denominator.) In our application, the a_j will almost always be strictly positive integers; the only exception will be that it is occasionally convenient to let the last entry a_n be a real number ≥ 1. In these cases, there are no problems with zero denominators. Infinite continued fractions are defined as limits of finite ones: It is well known that, if all a_1, a_2, ... is a sequence of numbers all ≥ 1, then the sequence of finite ("truncated") partial fractions $[a_1, \ldots, a_n]$ converges as $n \to \infty$; we denote the limit by $[a_1, \ldots]$.

A finite continued fraction $[a_1, \ldots, a_n]$ with positive integer entries is a rational number between 0 and 1; we define $p_n(a_1, \ldots, a_n)$ and $q_n(a_1, \ldots, a_n)$ as the numerator and denominator of the reduced-form representation of this number:

$$[a_1, \ldots, a_n] =: \frac{p_n(a_1, \ldots, a_n)}{q_n(a_1, \ldots, a_n)},$$

with p_n, q_n relatively prime positive integers.

The starting point for the work reported here is the observation that *the sequence of functions*

$$H_n(a_1, \ldots, a_n) := \log q_n(a_1, \ldots, a_n)$$

can be taken to be the energy functions for a one-dimensional classical lattice system, with single-site state space $\mathbb{N}_+ := \{1, 2, \ldots\}$. In essence what this means is that this sequence of functions is *extensive* in the sense that

$$H_{n+m}(a_1, \ldots, a_{n+m}) \approx H_n(a_1, \ldots, a_n) + H_m(a_{n+1}, \ldots, a_{n+m}).$$

In the case at hand, the "$\approx$" sign in the above equation can be taken to mean that the difference in the two sides is bounded uniformly in n, m, and $a_1, \ldots, a_{n+m}$ (although a bit less would suffice for the construction of a statistical mechanical system.) In many respects, this Hamiltonian defines an extremely well-behaved statistical-mechanical system; notably, the interaction is exponentially decreasing. On the other hand, since the single-site state space is infinite, this system isn't quite covered by the standard theory, and does indeed turn out to display a few – inessential – pathologies.

The investigation of this system is the subject of the second author's Ph.D. dissertation (Ruedin, 1994). This dissertation contains results of two different kinds: On the one hand, extensions of many standard results to a a general framework adequate to cover the Hamiltonian $H_n = \log q_n$ as well as many others, and, on the other hand, proofs of a specific results for this Hamiltonian. We will concentrate here on results specific to this system, referring to Ruedin (1994) for the general theory.

This article is organized as follows: Section 2 reviews a few facts about continued fractions used in the remainder of the article, and the most basic properties of the specific Hamiltonian are established in Section 3. In Sections 4 and 5 respectively, we summarize the properties of the canonical

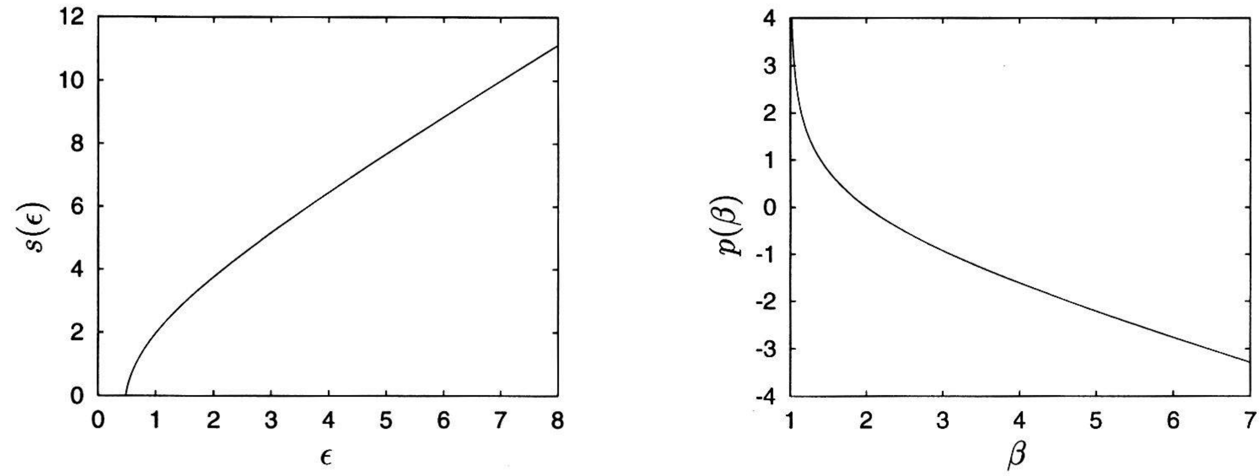

Figure 1: The thermodynamic functions

and microcanonical partition functions, and we introduce some ideas about "letting the size of the system fluctuate," which are natural for applications to continued fractions. The effect of letting the size of the system fluctuate is to fix the temperature at the particular value at which the pressure vanishes; in the present case this turns out to correspond to inverse temperature $\beta = 2$. By applying ideas about equivalence of ensembles, we show that, among rational numbers between 0 and 1 with reduced-form denominators not larger than some given large integer q, an overwhelming majority have continued fraction expansions $[a_1, \ldots, a_n]$ whose length n is approximately equal to $(\epsilon^*)^{-1} \log q$, for a constant ϵ^* (which we later show is equal to $\frac{\pi^2}{12 \log 2}$.)[1] In Section 6, we investigate the question of how thick the energy surface has to be made in order to get the microcanonical ensemble to function for our model, and in Section 7 we show that our system has no zero-point entropy, i.e., satisfies the third law of thermodynamics.

In Section 8, we introduce a second observable (in addition to H_n), the sequence

$$F_n(a_1, \ldots, a_n) = a_1 + \cdots + a_n,$$

and we investigate the joint distribution of H_n and F_n for large n. The quantity F_n has an interesting interpretation: it is the depth in the *Farey tree* enumeration of the rational numbers at which $[a_1, \ldots, a_n]$ occurs (see e.g. Kim and Ostlund (1989), §3). Ideas about equivalence of ensembles in statistical mechanics suggest that there should be a constant k_F such that most rational numbers $[a_1, \ldots, a_n]$ (n variable) with reduced form denominator $q_n \approx q$ have $F_n \approx k_F \log q$. One of the stimuli for this investigation was a considerable body of numerical evidence that this is *not* the case; in Section 8, we show that, in fact, typical values of $F_n / \log q_n$ go to ∞ as q_n does (i.e., loosely, that $k_F = \infty$.) In Section 9, we introduce an alternative representation for our system which is convenient for some kinds of computation, and we evaluate the constant ϵ^* referred to above. In Section 10, we state – without proof – the solution to the problem of maximizing the $q_n(a_1, \ldots, a_n)$ for fixed n and $a_1 + \cdots + a_n$, and we use this result to determine explicitly the "set of compatible values of H_n/n and F_n/n for large n," i.e., the set of points in the plane representable as limits of values of $(H_n/n, F_n/n)$ as $n \to \infty$.

For completeness, we show in Fig. 1 the microcanonical and canonical thermodynamic func-

[1] As we learned after this work was nearly completed, sharper results in this direction were proved more than twenty-five years ago by J. D. Dixon. See the discussion at the end of Section 5.

tions for our system. Aside from a few qualitative features – e.g., $p(\beta) \to \infty$ as $\beta \to 1$ – which will be explained in the course of the development, these graphs seem entirely unremarkable.

The work reported here certainly has some connection with classical ideas about "ergodic properties of the Gauss map," as presented, for example, in Cornfeld *et al.* (1982), §7.4. Exactly what the connection is remains something of a mystery for us; we do not see any strict mathematical implications in either direction. There is a more transparent connection with the work of D. Mayer (Mayer, 1990), who investigates an operator which turns out to be exactly the Ruelle transfer operator for our system and proves a number of striking results about its spectrum. Mayer, however, approaches the subject from a different point of view, and his results and ours seem to be more complementary than overlapping.

The first author thanks D. Ruelle for a number of helpful remarks in the course of this work and H. Epstein for many fruitful discussion.

2 Continued fractions

It is a standard fact from the classical theory of continued fractions[2] that, if we write p_n/q_n as before for the reduced-form representation of the rational number $[a_1, \ldots, a_n]$, then the p_n and q_n both satisfy the same recursion relation, namely

$$p_n = a_n p_{n-1} + p_{n-2}; \quad q_n = a_n q_{n-1} + q_{n-2}.$$

Hence, given the a_n's, and given p_n (or q_n) for two successive values of n, we can determine all other p_n's (respectively q_n's) from the recursion relations. It is immediate that $p_1(a_1) = 1$ and $q_1(a_1) = a_1$. Although p_0 and q_0 are not defined by the above, it is easy to check that, if we set $p_0 = 0$ and $q_0 = 1$, the recursion relations give the correct p_2 and q_2 and hence all later ones as well. Thus, we can alternatively define the p_n's and q_n's by:

$$\begin{aligned} p_n &= a_n p_{n-1} + p_{n-2}; \quad p_0 = 0, \quad p_1 = 1, \\ q_n &= a_n q_{n-1} + q_{n-2}; \quad q_0 = 1, \quad q_1 = a_1. \end{aligned}$$

From these formulas it is clear that $q_n(a_1, \ldots, a_n)$ is a strictly increasing function of each of its arguments, and that $p_n(a_1, \ldots, a_n)$ is independent of a_1 but strictly increasing in all its other arguments.

The smallest value of $q_n(a_1, \ldots, a_n)$ is thus $q_n(1, \ldots 1)$, and these numbers are the *Fibonacci sequence.* To fix the normalization, we define the Fibonacci sequence F_n by:

$$F_n = F_{n-1} + F_{n-2} \quad \text{with } F_0 = F_1 = 1;$$

it then follows from the recurrences for p_n and q_n that

$$\begin{aligned} q_n(1, \ldots, 1) &= F_n, \quad \text{and also} \\ p_n(1, \ldots, 1) &= F_{n-1}. \end{aligned}$$

[2]Results quoted in this section without proof or explicit citation can be found in any of the standard classical texts, e.g., Hardy and Wright (1960), Chapter X

The Fibonacci numbers can be written explicitly via the *Binet formula*

$$F_n = \frac{\gamma^{n+1} + (-1)^n (1/\gamma)^{n+1}}{\sqrt{5}}, \qquad \text{where } \gamma := \frac{\sqrt{5}+1}{2}, \text{ the \textit{golden number.}}$$

Since $\gamma > 1$, we get $F_n \approx \gamma^{n+1}/\sqrt{5}$ for large n and, in particular,

$$F_n > \frac{1}{2}\gamma^n \quad \text{for large enough } n.$$

We prove here a simple result which we will need later concerning exponential falloff of dependence of $[a_1, \ldots, a_n]$ on arguments "far to the right."

Proposition 2.1 *Let*

$$a_1, \ldots, a_n, a_{n+1}, \ldots a_m \quad \textit{and} \quad a_1, \ldots a_n, a'_{n+1}, \ldots a'_{m'}$$

be two sequences of strictly positive integers, both of length at least n*, which agree through the* n*th place. Then*

$$\left| \frac{[a_1, \ldots, a_m]}{[a_1, \ldots a'_{m'}]} - 1 \right| \leq \frac{1}{q_n p_n}.$$

The right-hand side of this inequality is majorized by $1/(F_n F_{n-1})$ *and hence by* $4\gamma^{-2n-1}$ *for large enough* n.

Proof. Let

$$x := \begin{cases} [a_{n+1}, \ldots a_m] & \text{for } m > n \\ 0 & \text{for } m = n \end{cases}$$

Then

$$[a_1, \ldots, a_n, \ldots a_m] = [a_1, \ldots, a_n + x],$$

and we can write $[a_1, \ldots, a'_{m'}]$ similarly. The proof of the recurrences for p_n and q_n shows that

$$[a_1, \ldots a_m] = \frac{p_n + x p_{n-1}}{q_n + x q_{n-1}},$$

where p_n and q_n denote $p_n(a_1, \ldots, a_n)$ and $q_n(a_1, \ldots, a_n)$ respectively. Hence

$$\begin{aligned} & \frac{[a_1, \ldots, a_m]}{[a_1, \ldots, a'_{m'}]} - 1 \\ = \; & \frac{(p_n + x p_{n-1})(q_n + x' q_{n-1}) - (p_n + x' p_{n-1})(q_n + x q_{n-1})}{(q_n + x q_{n-1})(p_n + x' p_{n-1})} \\ = \; & \frac{x p_{n-1} q_n + x' p_n q_{n-1} - x p_n q_{n-1} - x' p_{n-1} q_n}{(q_n + x q_{n-1})(p_n + x' p_{n-1})} \\ = \; & \frac{(x' - x)(p_n q_{n-1} - p_{n-1} q_n)}{(q_n + x q_{n-1})(p_n + x' p_{n-1})} \end{aligned}$$

Now $|p_n q_{n-1} - p_{n-1} q_n| = 1$ and, since $0 \le x, x' \le 1$, $|x' - x| \le 1$, and $(q_n + x q_{n-1})(p_n + x' p_{n-1}) \ge q_n p_n$, so the desired estimate follows. $\square$

It is a classical fact, and not difficult to prove, that $q_n(a_1, \ldots, a_n)$ is symmetric under reversal of its arguments, i.e., that

Proposition 2.2 $q_n(a_1, \ldots, a_n) = q_n(a_n, \ldots, a_1)$.

This equation follows easily from the *Euler bracket function* representation for q_n, also known as the *Euler-Minding formula.* See Roberts (1977), Ch. XIII, or Perron (1954), §3. None of our proofs actually depend on this fact; we mention it only to avoid having to justify some otherwise odd-looking choices for orders of arguments.

3 The statistical mechanical system

We consider the sequence of functions

$$H_n(a_1, \ldots, a_n) = \log q_n(a_n, \ldots a_1) \quad \text{on } \mathbb{N}_+^n.$$

for $n = 1, 2, 3, \ldots$ (The reversal of the order of arguments on the right is inconsequential in view of Prop. 2.2.) The first thing to be seen is that this system of functions is "extensive," in the sense explained in the introduction. Once this has been established, we can interpret H_n as the "energy" of a lattice system with n sites occupied by identical molecules with countably infinite state space. We start by defining

$$\begin{aligned} h_n(a_1, \ldots, a_n) &= H_n(a_1, \ldots, a_n) - H_{n-1}(a_2, \ldots a_n) \\ &= \log \frac{q_n(a_n, \ldots, a_1)}{q_{n-1}(a_n, \ldots, a_2)} \end{aligned}$$

for $n > 1$ and

$$h_1(a_1) = \log(a_1)$$

Then

$$H_n(a_1, \ldots, a_n) = h_n(a_1, \ldots a_n) + h_{n-1}(a_2, \ldots, a_n) + \cdots + h_1(a_n).$$

We now have

Proposition 3.1

$$\frac{q_n(a_n, \ldots, a_1)}{q_{n-1}(a_n, \ldots, a_2)} = \frac{1}{[a_1, \ldots, a_n]},$$

(with $q_0 := 1$) and hence

$$h_n(a_1, \ldots, a_n) = -\log[a_1, \ldots, a_n].$$

Proof. By induction on n. The asserted formula is true for $n = 1$. The recursion for the q_j gives

$$q_n(a_n, \ldots, a_1) = a_1 q_{n-1}(a_n, \ldots a_2) + q_{n-2}(a_n, \ldots, a_3).$$

Dividing by q_{n-1} gives

$$\begin{aligned} \frac{q_n}{q_{n-1}} &= a_1 + \frac{q_{n-2}}{q_{n-1}} \\ &= a_1 + \frac{1}{[a_2, \ldots a_n]} \quad \text{by the induction hypothesis.} \\ &= \frac{1}{[a_1, \ldots a_n]} \quad \text{by the definition of continued fraction.} \end{aligned}$$

This proves the induction step and hence the formula. □

We now split the energy into an self-interaction part $H^{(0)}$ and a remainder $H^{(I)}$ by:

$$\begin{aligned} H_n^{(0)}(a_1, \ldots, a_n) &:= h_1(a_1) + h_1(a_2) + \cdots + h_1(a_n) \\ H_n^{(I)}(a_1, \ldots, a_n) &:= H_n(a_1, \ldots, a_n) - H_n^{(0)}(a_1, \ldots a_n) \\ &= h_n^{(\mathrm{I})}(a_1, \ldots a_n) + \cdots + h_2^{(\mathrm{I})}(a_{n-1}, a_n), \end{aligned}$$

where

$$\begin{aligned} h_j^{(\mathrm{I})}(a_1, \ldots a_j) &:= h_j(a_1, \ldots a_j) - h_1(a_1) \\ &= -\log(a_1 \cdot [a_1, \ldots, a_j]) \\ &= -\log(\frac{a_1}{a_1 + [a_2, \ldots, a_j]} \\ &= \log(1 + \frac{[a_2, \ldots, a_j]}{a_1}) \end{aligned}$$

for $j > 1$ and $h_1^{(\mathrm{I})}(a_1) = 0$.

Proposition 3.2 *We have*

$$0 \le h_n^{(\mathrm{I})}(a_1, \ldots, a_n) \le \log 2,$$

and there is a constant c such that, for all $n \ge 1$, *and all pairs of sequences*

$$a_1, \ldots, a_n, a_{n+1}, \ldots a_m \quad \textit{and} \quad a_1, \ldots a_n, a'_{n+1}, \ldots a'_{m'} \in \mathbb{N}_+,$$

both with length $\ge n$, *and agreeing in the first* n *places, we have*

$$|h_m^{(\mathrm{I})}(a_1, \ldots, a_m) - h_{m'}^{(\mathrm{I})}(a_1, \ldots, a'_{m'})| \le c \frac{1}{\gamma^{2n}}$$

Proof. The first estimate follows at once from the formula

$$h_m^{(\mathrm{I})}(a_1, \ldots, a_m) = \log(1 + \frac{[a_2, \ldots, a_m]}{a_1}).$$

The second assertion follows from Proposition 2.1 and the preceding formula, together with the observation that the derivative of the logarithm is ≤ 1 on the interval $[1, 2]$. □

Note that it follows that

$$H_n^{(0)} \leq H_n \leq H_n^{(0)} + n \log 2$$

for all n.

The proof that the sequence of functions H_n is extensive is now nearly immediate.

Proposition 3.3 *The difference*

$$H_{n+m}(a_1, \ldots, a_{n+m}) - H_n(a_1, \ldots, a_n) - H_m(a_{n+1}, \ldots, a_{n+m})$$

is bounded uniformly in n, m, a_1, ..., a_{n+m}.

Proof. Since $H_{n+m}^{(0)} = H_n^{(0)} + H_m^{(0)}$ – with the obvious arguments – we get

$$\begin{aligned}
&H_{n+m}(a_1, \ldots, a_{n+m}) - H_n(a_1, \ldots, a_n) - H_m(a_{n+1}, \ldots a_{n+m}) \\
&\quad = H_{n+m}^{(I)}(a_1, \ldots, a_{n+m}) - H_n^{(I)}(a_1, \ldots, a_n) - H_m^{(I)}(a_{n+1}, \ldots, a_{n+m}) \\
&\quad = (h_{n+m}^{(\mathrm{I})}(a_1, \ldots a_{m+n}) - h_n^{(\mathrm{I})}(a_1, \ldots, a_n)) \\
&\qquad + \cdots + (h_{m+2}^{(\mathrm{I})}(a_{n-1}, \ldots a_{n+m}) - h_2^{(\mathrm{I})}(a_{n-1}, a_n)) \\
&\qquad + h_{m+1}^{(\mathrm{I})}(a_n, \ldots a_{n+m}).
\end{aligned}$$

The modulus of the right-hand side is majorized by

$$\log 2 + \sum_{j=2}^{\infty} \frac{c}{\gamma^{2j}},$$

which is finite and independent of n, m, and the a_i. □

It is now also easy to give a potential from which the sequence of H_n's can be reconstructed: We put

$$\begin{aligned}
\Phi_{\{j\}}(a_j) &= \log a_j, \\
\Phi_{\{j,\ldots,k\}}(a_j, \ldots, a_k) &= h_{k-j+1}^{(\mathrm{I})}(a_j, \ldots, a_k) - h_{k-j}^{(\mathrm{I})}(a_j, \ldots, a_{k-1}) \quad \text{for } j < k,
\end{aligned}$$

and $\Phi_J \equiv 0$ for finite subsets J of $\mathbb{Z}$ other than intervals. It is then easy to check that

$$H_n(a_1, \ldots, a_n) = \sum_{J \subset \{1,\ldots,n\}} \Phi_J(a|_J),$$

and it follows from Proposition 3.2 that

$$\|\Phi_J\|_\infty = \mathcal{O}(\gamma^{-2\,\mathrm{diam}(J)}),$$

and hence, in particular, that the interaction is exponentially decreasing.

4 The canonical ensemble

The first observation we need to make is that the canonical ensemble only makes sense for inverse temperature $\beta > 1$. This is already true for the finite system. The canonical partition function for a finite system with n (adjacent) lattice sites is

$$Z_n(\beta) = \sum_{a_1,\ldots a_n=1}^{\infty} \exp(-\beta H_n(a_1,\ldots,a_n)).$$

We denote – temporarily – the corresponding sum for $H_n^{(0)}$ by $Z_n^{(0)}$. From the inequalities

$$H_n^{(0)} \leq H_n \leq H_n^{(0)} + n \cdot \log 2,$$

it follows that

$$Z_n^{(0)}(\beta) \geq Z_n(\beta) \geq 2^{-n\beta} Z_n^{(0)}(\beta).$$

But

$$Z_n^{(0)}(\beta) = (\sum_{a=1}^{\infty} e^{-\beta \log a})^n = (\sum_{a=1}^{\infty} \frac{1}{a^\beta})^n = (\zeta(\beta))^n,$$

and $\zeta(\beta)$, the Riemann zeta function, goes to infinity as β decreases to 1. Hence, the same is true for the finite-system partition function for any n.

On the other hand, for $\beta > 1$, the finite-system partition function is finite for all n. Using the bound on $H_n - H_n^{(0)}$, it is easy to adapt the standard proof of the existence of the thermodynamic limit of the canonical partition function for lattice systems – which assumes that the system at each lattice site has only finitely many states, rather than countably many as in the case at hand – to show that

$$p(\beta) = \lim_{n\to\infty} \frac{1}{n} \log Z_n(\beta)$$

exists for any $\beta > 1$. The limiting function is convex on $(1,\infty)$, since this is true before passing to the limit. From the estimates proved above we get the bounds

$$\log \zeta(\beta) \geq p(\beta) \geq \log \zeta(\beta) - \beta \log 2.$$

It is a standard and simple fact that the zeta function has a simple pole with unit residue at 1; from this it follows that

$$p(\beta) = \log(\beta - 1) + \mathcal{O}(1) \quad \text{as } \beta \to 1.$$

Remark. The above lower bound can be improved – for β near its minimum value 1 – as follows: Since

$$h_j(a_j,\ldots,a_n) = \log(a_j + [a_{j+1},\ldots,a_{jn}]) \leq \log(a_j + 1),$$

we get

$$Z_n(\beta) \geq (\sum_{a=2}^{\infty} \frac{1}{a^\beta})^n = (\zeta(\beta) - 1)^n,$$

and hence

$$p(\beta) \geq \log(\zeta(\beta) - 1) \approx \log \zeta(\beta) - \frac{1}{\zeta(\beta)}.$$

These estimates do not however tell us much about the behavior for $\beta \to \infty$; the upper bound goes to 0 and the lower bound is asymptotic to $-\beta \log 2$. We will get better information about this limiting regime later.

We will need here generalizations of a certain number of results which are standard for one-dimensional lattice systems with finite single-site state spaces to our model (which has $\mathbb{N}_+$ as single-site state space.) We referred above to one such result, the existence of the thermodynamic limit for the canonical partition function. The generalization for that particular result is easy, but we will require here generalizations of two other circles of ideas – Gibbs states and the transfer-operator formalism – which are not quite so straightforward. These extensions have been carried out in all detail in Ruedin (1994); we summarize the results here:

Proposition 4.1 *1. For each $\beta > 1$ there is a unique Gibbs state σ_β, (which is then necessarily translation-invariant,) and*

$$p(\beta) = s(\sigma_\beta) - \beta \bar{\epsilon}_\beta,$$

where $s(\sigma_\beta)$ is the Kolmogorov-Sinai entropy of σ_β and $\bar{\epsilon}_\beta$ the mean energy per lattice site of σ_β.

2. $p(\beta)$ is a real-analytic function of β on $(1, \infty)$ and is strictly convex in the strong sense that its second derivative is everywhere strictly positive.

5 The microcanonical entropy

Once again we need an extension of some standard results to our slightly-nonstandard technical situation. The standard results can be found in Lanford (1973); an extension adequate to the present situation is given in Ruedin (1994). To formulate the result we need, we use the following notation: Let $-\infty \leq \epsilon_1 < \epsilon_2 \leq \infty$; then $\mathcal{V}_n(\epsilon_1, \epsilon_2)$ will denote the number of sequences $a_1, \ldots, a_n$ of length n with

$$\epsilon_1 < \frac{1}{n} H_n(a_1, \ldots, a_n) < \epsilon_2$$

Proposition 5.1 *There is a non-negative concave function $s(\epsilon)$, defined on an open interval $(\epsilon_{\min}, \epsilon_{\max})$, (where $\epsilon_{\min}$ may be $-\infty$ and $\epsilon_{\max}$ may be $+\infty$) such that*

1. *$\lim_{n\to\infty} \frac{1}{n} \log \mathcal{V}_n(\epsilon_1, \epsilon_2) = \sup_{\epsilon_1 < \epsilon < \epsilon_2} s(\epsilon)$ for all intervals (ϵ_1, ϵ_2) intersecting $(\epsilon_{\min}, \epsilon_{\max})$*
2. *$\mathcal{V}_n(\epsilon_1, \epsilon_2) = 0$ for all sufficiently large n for intervals (ϵ_1, ϵ_2) whose closures do not intersect the closure of $(\epsilon_{\min}, \epsilon_{\max})$.*

The formulation of the preceding proposition is a little dense, and it may be helpful to elaborate on it a bit. For purposes of this explanation, let us say that ϵ is an *asymptotically excluded value for* H_n/n if there exists a neighborhood of ϵ which is disjoint from the image of H_n/n for all sufficiently large n and an *asymptotically allowed value* otherwise. The set of asymptotically excluded values is manifestly open. The first non-trivial assertion of the proposition is that the complementary set of asymptotically allowed values is an interval; its interior is the interval $(\epsilon_{\min}, \epsilon_{\max})$ of the proposition. We will accordingly – if not quite precisely – refer to $(\epsilon_{\min}, \epsilon_{\max})$ as the *allowed interval.* The idea is then that, for any "sampling interval" (ϵ_1, ϵ_2), the number $\mathcal{V}_n(\epsilon_1, \epsilon_2)$ of configurations with $H_n/n \in (\epsilon_1, \epsilon_2)$ should be asymptotically – for large n – about $\exp(ns_{\epsilon_1,\epsilon_2})$, with a particular form for the dependence of the exponent $s_{\epsilon_1,\epsilon_2}$ on the sampling interval. Part 1. of the proposition says that this behavior does hold for sampling intervals which overlap the allowed interval, and part 2. says that a natural – and rather strong – variant holds for sampling intervals which stay away from the allowed interval. It turns out, however, that the asserted exponential behavior can fail – or at least is much more delicate to prove – if the sampling interval touches but does not overlap the allowed interval, i.e., if $\epsilon_2 = \epsilon_{\min}$ or $\epsilon_1 = \epsilon_{\max}$; the proposition says nothing in these cases. We remark that the proof of this statement depends not just on the "extensivity" of the sequence of functions H_n in the sense described above; it is also necessary that they "grow at infinity" in an appropriate way so as to guarantee, in particular, that $\mathcal{V}_n(\epsilon_1, \epsilon_2)$ is finite for all finite n, ϵ_1, and ϵ_2. An appropriate general formulation of the growth at infinity condition is given in Ruedin (1994); we note here only that, in the case at hand, adequate growth at infinity is guaranteed by the fact that $H_n \geq H_n^{(0)}$ and that $h_1(a)$ grows adequately fast as $a \to \infty$.

The above proposition is a general result, using only qualitative properties of H_n. In the case at hand, we can be more specific.

Proposition 5.2 *For $H_n(a_1, \ldots, a_n) = \log q_n(a_1, \ldots, a_n)$, we have:*

- $\epsilon_{\min} = \log \gamma$ *(with, as above,* $\gamma = \dfrac{\sqrt{5}+1}{2}$*),*
- $\epsilon_{\max} = \infty$,
- $s(\epsilon)$ *is strictly increasing on* $(\log \gamma, \infty)$*, and* $s(\epsilon) \to \infty$ *as* $\epsilon \to \infty$.

Proof. We have already noted that

$$q_n(a_1, \ldots, a_n) \geq q_n(1, \ldots, 1) = F_n \approx \text{const}\, \gamma^n.$$

Hence,

$$\mathcal{V}_n(-\infty, \epsilon_2) = 0 \quad \text{for large } n\text{, if } \epsilon_2 < \log \gamma,$$

and

$$\mathcal{V}_n(-\infty, \epsilon_2) \geq 1 \quad \text{for large } n\text{, if } \epsilon_2 > \log \gamma.$$

From these two assertions it follows that $\epsilon_{\min} = \log \gamma$.

We now claim that

$$\sup_{\epsilon < \epsilon_1} s(\epsilon) \to \infty \quad \text{as } \epsilon_1 \to \infty.$$

From this claim, it follows that $s(\epsilon)$ is not bounded; hence, since it is concave, that it it is strictly increasing on its whole interval of definition and goes to ∞ with ϵ, and these are the remaining assertions of the proposition

To prove the claim, we begin by considering the sequence $q_n(p, \ldots, p)$ for general $p \in \mathbb{N}_+$. By the recursion relation

$$q_n(p, \ldots, p) = p\, q_{n-1}(p, \ldots, p) + q_{n-2}(p, \ldots, p).$$

It follows from simple standard arguments – generalizing the derivation of the Binet formula for the Fibonacci numbers, see also §10 – that

$$q_n(p, \ldots, p) \approx \text{const} \cdot \gamma_p^n,$$

where γ_p is the positive root of the quadratic equation $t^2 - pt - 1 = 0$, i.e.,

$$\gamma_p = \frac{1}{2}(p + \sqrt{p^2 + 4})(\approx p \quad \text{for } p \text{ large.})$$

Thus, if $\epsilon_1 > \log \gamma_p$ and n is large enough,

$$\frac{1}{n} \log q_n(p, \ldots, p) \leq \epsilon_1,$$

and hence the same inequality holds for $q_n(a_1, \ldots, a_n)$ provided that all the a_i are $\leq p$. Thus:

$$\mathcal{V}_n(-\infty, \epsilon_1) \geq p^n \quad \text{for } \epsilon_1 > \log \gamma_p \text{ and } n \text{ sufficiently large.}$$

Taking logarithms, dividing by n, and letting $n \to \infty$ gives

$$\sup_{\epsilon \leq \epsilon_1} s(\epsilon) \geq \log p \quad \text{for } \epsilon_1 > \log \gamma_p;$$

letting ϵ_1 decrease to $\log \gamma_p$ gives

$$\sup_{\epsilon \leq \log \gamma_p} s(\epsilon) \geq \log p.$$

By letting p go to ∞ we see that $s(\epsilon)$ is unbounded, as asserted, and this completes the proof of the proposition. We can now in fact say a little more about the behavior of $s(\epsilon)$ as $\epsilon \to \infty$. Now that we know that $s(\epsilon)$ is increasing, we can simplify the above lower bound to

$$s(\log \gamma_p) \geq \log p,$$

On the other hand, $\gamma_p/p \to 1$ as $p \to \infty$, so $s(\epsilon)$ in fact grows at least as fast as ϵ as $\epsilon \to \infty$. □

The next step is to argue that $p(\beta)$ is the Legendre transform of $s(\epsilon)$ and to deduce analyticity and strict concavity for $s(\epsilon)$ from analyticity and strict convexity for $p(\beta)$.

Proposition 5.3 *$s(\epsilon)$ is real-analytic, strictly increasing, and strictly convex on $(\epsilon_{\min}, \infty)$. The function $\beta(\epsilon) = -s'(\epsilon)$ maps $(\epsilon_{\min}, \infty)$ diffeomorphically onto $(1, \infty)$; its inverse is $\epsilon(\beta) = p'(\beta)$. For every β between 1 and ∞,*

$$p(\beta) = \sup_{\epsilon}(s(\epsilon) - \beta\epsilon);$$

the supremum is taken on at $\epsilon = \epsilon(\beta)$, and nowhere else.

Proof. The argument is standard, but we give it in detail anyway, since there are a few places where special features of the situation at hand have to be invoked to rule out pathologies. We begin from the fact that, since $s(\epsilon)$ is concave, it is differentiable except at most at a countable set of points and its derivative – where defined – is monotone decreasing. We define temporarily

$$\beta_{\min} := \lim_{\epsilon \to \infty} s'(\epsilon) \quad \text{and} \quad \beta_{\max} := \lim_{\epsilon \to \epsilon_{\min}^+} s'(\epsilon),$$

with the understanding that the limits are to be taken along the set where the derivative exists. Nothing said so far rules out the possibility that $\beta_{\min} = \beta_{\max}$. Nevertheless, the microcanonical analysis leads to

Proposition 5.4 *1. If $\beta_{\min} < \beta < \beta_{\max}$, then*

$$p(\beta) = \sup_{\epsilon}(s(\epsilon) - \beta\epsilon),$$

and the supremum is taken on.

2. If $\beta < \beta_{\min}$, then

$$\lim_{n \to \infty} \frac{1}{n} \log Z_n(\beta) = +\infty.$$

3. If $\beta > \beta_{\max}$, then

$$p(\beta) = s_0 - \beta\epsilon_{\min},$$

where s_0 denotes $\lim_{\epsilon \to \epsilon_{\min}^+} s(\epsilon)$.[3]

Again, we refer to Ruedin (1994) for the proof. The argument is essentially the standard one, but a little extra effort is needed to work around the fact that $\mathcal{V}_n(\epsilon, \infty)$ is infinite.

It follows from 1 and 2, together with what we know about $p(\beta)$, that $\beta_{\min} = 1$. If $\beta_{\max}$ were finite, $p(\beta)$ would have to be linear from $\beta_{\max}$ to ∞, and this violates the strict convexity of $P(\beta)$; hence, $\beta_{\max}$ must be infinite. Thus, the Legendre transformation formula

$$p(\beta) = \sup_{\epsilon}(s(\epsilon) - \beta\epsilon)$$

holds for $1 < \beta < \infty$, with the supremum taken on. Furthermore, except for at most a countable set of β's, the supremum is taken on at a single point. We denote this point by $\epsilon(\beta)$; if the supremum is taken on at more than one point – i.e., on an interval of non-zero length – then $\epsilon(\beta)$ is not defined.

For all relevant ϵ and β, we have

$$p(\beta) + \epsilon\beta \leq s(\epsilon),$$

with equality for $\epsilon = \epsilon(\beta)$. Out of this we can read the following: Let β_0 be such that $\epsilon(\beta_0)$ is defined; this excludes at most countably many values. Put $\epsilon_0 = \epsilon(\beta_0)$. Then $\beta \mapsto p(\beta) + \beta\epsilon_0$

[3]We are in fact going to show in §7 that $s_0 = 0$, but we don't need this fact for the moment.

takes on its maximum at $\beta = \beta_0$, which implies $p'(\beta_0) = -\epsilon_0$. In other words: $\epsilon(\beta) = -p'(\beta)$ whenever $\epsilon(\beta)$ is defined. But the only way $\epsilon(\beta)$ can fail to be defined is for the graph of $s(\epsilon)$ to contain a linear segment with slope β, and this implies that $\epsilon(\beta)$ has a jump discontinuity there. This, however, is ruled out by the fact that $p'(\beta)$ is real-analytic. The conclusion is that $\epsilon(\beta)$ is defined for all $\beta \in (1, \infty)$, and that $\epsilon(\beta) = -p'(\beta)$ for all these values of β.

Substituting into an earlier formula, we thus get the parametric representation

$$s(-p'(\beta)) = p(\beta) - \beta p'(\beta),$$

which, together with the analyticity and strict convexity of $p(\beta)$, ensures that $s(\epsilon)$ is real-analytic on the image of the mapping $\beta \mapsto -p'(\beta)$. By continuity, this image is an interval. Since $p(\beta) \to \infty$ as $\beta \to 1^+$, the same must be true of $-p'(\beta)$, i.e., the image interval must extend to ∞. On the other hand, the fact that $\beta_{\max} = \infty$ means that $s'(\epsilon)$ goes to ∞ as ϵ approaches $\epsilon_{\min}$ and hence implies that there exists a sequence ϵ_n converging to $\epsilon_{\min}$ such that $s'(\epsilon_n)$ exists for all n. Denoting $s'(\epsilon_n)$ by β_n, we get that $s(\epsilon) - \beta_n\epsilon$ takes on its supremum at ϵ_n, i.e., that $\epsilon_n = \epsilon(\beta_n) = -p'(\beta_n)$. Hence, the image interval also extends to $\epsilon_{\min}$, so the above formula represents $s(\epsilon)$ over its full range of definition. Thus, $s(\epsilon)$ is real-analytic where defined, and differentiation of the formula gives $s''(\epsilon) < 0$ everywhere.

We have just argued that $\beta \mapsto \epsilon(\beta) = -p'(\beta)$ sends $(1, \infty)$ diffeomorphically onto $(\log\gamma, \infty)$. We denote the inverse mapping by $\beta(\epsilon)$; a standard calculation shows that $\beta(\epsilon) = s'(\epsilon)$. We then have:

$$p(\beta) = s(\epsilon(\beta)) + \beta \cdot \epsilon(\beta) \qquad \text{for all } \beta \in (1, \infty).$$

This completes the proof of Prop. 5.3 □

Everything said so far has used only qualitative properties of $H_n = \log q_n$. We will now make a first contact with "number theory." The argument is the reverse of what we ultimately want to do – we will use some classical facts from number theory to prove something about $s(\epsilon)$. The argument is also illuminating as a simple example of how to compute more concrete quantities in terms of $s(\epsilon)$. The question we want to address is:

Question. *How does the total number $N(q)$ of sequences $a_1, \ldots, a_n$ with*

$$q_n(a_1, \ldots, a_n) < q$$

(n variable) behave as $q \to \infty$?

Determining $N(q)$ is almost the same as counting rational numbers between 0 and 1 with reduced-form denominator $< q$. There is in fact exactly a factor of 2 difference between the two question: A rational number has *exactly two* continued fraction representations:

- the "standard" one – given by the Euclidean algorithm – which has the form $[a_1, \ldots, a_n]$ with $a_n \geq 2$, and
- a second one $[a_1, \ldots, a_n - 1, 1]$

(e.g., $1/2 = [2] = [1,1]$.)Furthermore, the number of rational numbers between 0 and 1 with reduced-form denominator q is exactly $\varphi(q)$, the Euler φ-function. Thus, we have the exact formula

$$N(q) = 2\sum_{j=2}^{q-1} \varphi(j).$$

By classical number theory (e.g. Hardy and Wright, 1960, Theorem 330) this sum is asymptotically a constant multiple of q^2. We now proceed to compute the asymptotic behavior of $N(q)$ in terms of the function $s(\epsilon)$; comparing that answer with the one just obtained will tell us something about $s(\epsilon)$.

We start from the fact that the number of sequences *of length* n with $\log q_n < n\epsilon$ is, by definition, $\mathcal{V}_n(-\infty, \epsilon)$. Unraveling the notation: The number of sequences of length n with $q_n < q$ is $\mathcal{V}_n(-\infty, (\log q)/n)$. Thus, the total number of sequences – of arbitrary n – is

$$N(q) = \sum_{n=1}^{\infty} \mathcal{V}_n(-\infty, \frac{\log q}{n}).$$

Although we have written the sum as running to ∞, there are in fact only finitely many non-zero terms for given q: $q_n(a_1, \ldots, a_n) \geq F_n$, so

$$\mathcal{V}_n(-\infty, \frac{\log q}{n}) = 0 \quad \text{for } F_n > q,$$

i.e., for

$$\frac{1}{n} \log F_n > \frac{1}{n} \log q,$$

i.e., for

$$n \geq \log q \frac{n}{\log F_n} \approx \frac{\log q}{\log \gamma}.$$

In particular: The number of terms in the above sum is $\mathcal{O}(\log q)$ for large q. From this, we want to argue that *for our purposes, it is adequate to approximate the above sum by its largest term.* The justification for this assertion runs as follows: For given q, let $n(q)$ be such as to make

$$\mathcal{V}_{n(q)}(-\infty, \frac{\log q}{n(q)})$$

as large as possible, and put

$$y(q) := \frac{n(q)}{\log q}.$$

Then $y(q)$ is certainly not much larger than $1/\log \gamma$ for large q. We will argue later that $y(q)$ converges to a finite non-zero limit as $q \to \infty$; for the moment, we accept this without proof to see how the rest of the argument goes. The largest term in the sum is then

$$\mathcal{V}_{n(q)}(-\infty, \frac{1}{y(q)}) \sim \exp(n(q)s(1/y(q))) = \exp(t(q)\log q)$$

where $t(q)$ denotes $y(q)s(1/y(q))$. Taking logarithms and dividing by $\log q$ gives a sequence which has a chance of remaining of order unity as $q \to \infty$. We can now justify the claim that the largest term is an adequate approximation to the sum: We have

$$\begin{aligned}\frac{1}{\log q}\log \mathcal{V}_{n(q)}(-\infty,\frac{1}{y(q)}) &\leq \frac{1}{\log q}\log\Big(\sum_{n=1}^{\infty}\mathcal{V}_n(-\infty,\frac{\log q}{n})\Big)\\ &\leq \frac{1}{\log q}\log \mathcal{V}_{n(q)}(-\infty,\frac{1}{y(q)}) + \mathcal{O}(\frac{\log\log q}{\log q}),\end{aligned}$$

so the sequence built from the sum and the one built from its largest term do have the same limiting behavior in the sense that their difference goes to zero.

We now make a heuristic argument, intended as motivation for a subsequent precise result: Assuming that $y(q)$ converges to a limit y^*, and assuming also the validity of an obvious exchange of limits, we would expect that

$$\lim_{q\to\infty}\frac{1}{\log q}\log N(q) = \lim_{q\to\infty}\frac{1}{\log q}\log \mathcal{V}_{n(q)}(-\infty,\frac{1}{y(q)}) = y^* s(1/y^*).$$

Furthermore, $n(q)$ was chosen to make the corresponding term in the sum as large as possible, and y^* is the limit of the $n(q)/\log q$'s, so it should be at least plausible that

$$y^* s(1/y^*) = \sup_y y\, s(1/y) = \sup_\epsilon s(\epsilon)/\epsilon.$$

On the other hand, we showed above that

$$N(q) \approx \text{const}\cdot q^2 \quad \text{so} \quad \lim_{q\to\infty}\frac{1}{\log q}\log N(q) = 2,$$

so, finally, we expect that

$$y^* s(1/y^*) = 2, \quad \text{i.e.,} \quad \sup_\epsilon \frac{s(\epsilon)}{\epsilon} = 2.$$

With this as introduction and motivation, we formulate the following result:

Proposition 5.5 *The function $p(\beta)$ has a unique zero, which we denote by β^*. The function $s(\epsilon)/\epsilon$ takes on its supremum at $\epsilon = \epsilon^* := \epsilon(\beta^*)$. This is the only place where the supremum is taken on, and the function is strictly increasing to the left of ϵ^* and strictly decreasing to the right. We have, furthermore,*

$$2 = \beta^* = \sup_\epsilon \frac{s(\epsilon)}{\epsilon} = \lim_{q\to\infty}\frac{1}{\log q}\log N(q),$$

where $N(q)$ denotes as above the number of sequences $a_1,\ldots,a_n$ (n variable) with

$$q_n(a_1,\ldots,a_n) < q.$$

Proof. The logic is:

- We investigate first the problem of maximizing $s(\epsilon)/\epsilon$. We show that on the one hand the supremum is taken on exactly at $\epsilon(\beta^*)$ and on the other hand the supremum is also *equal to* β^*.
- We then fill in the gaps in the earlier heuristic analysis to show that
$$\lim_{q\to\infty} \frac{1}{\log q} \log N(q) = \sup_{\epsilon} \frac{s(\epsilon)}{\epsilon}.$$
- Comparing with the formula for $N(q)$ in terms of the Euler φ-function, we find
$$\lim_{q\to\infty} \frac{1}{\log q} \log N(q) = 2,$$
which completes the proof.

We will prove later – by quite different methods – the explicit formula
$$\epsilon^* = \frac{\pi^2}{12 \log 2}.$$

That $s(\epsilon)/\epsilon$ takes on its supremum at ϵ^*, and that the value of the supremum is β^*, can be motivated by putting the derivative of $s(\epsilon)/\epsilon$ equal to zero. For a proof, it is more convenient to proceed less directly.[4] From the fact that $p'(\beta) = -\epsilon(\beta) < -\log\gamma < 0$, it follows that $p(\beta) \to -\infty$ for $\beta \to \infty$. We know, on the other hand, that $p(\beta) \to +\infty$ for $\beta \to 1$. Hence, there is a β^* such that
$$p(\beta^*) = 0,$$
and since $p'(\beta) < 0$ everywhere, this β^* is unique. From the Legendre transform
$$0 = p(\beta^*) = \sup_{\epsilon}(s(\epsilon) - \beta^*\epsilon),$$
and the supremum is taken on exactly for $\epsilon = \epsilon^*$. In other words:
$$s(\epsilon) \le \beta^*\epsilon, \quad \text{with equality if and only if } \epsilon = \epsilon^*.$$
Since all relevant ϵ's are $> \epsilon_{\min} = \log\gamma > 0$, we can divide by ϵ to get
$$\frac{s(\epsilon)}{\epsilon} \le \beta^*, \quad \text{with equality if and only if } \epsilon = \epsilon^*,$$
which is the desired assertion about where the supremum is taken on and what its value is. To show that $s(\epsilon)/\epsilon$ is strictly decreasing with increasing separation from ϵ^*, we use the general fact that (strict) concavity of $s(\epsilon)$ on $(\epsilon_{\min}, \infty)$ implies (strict) concavity of
$$g(y) := ys(\frac{1}{y}) \quad \text{on } (0, 1/\epsilon_{\min}).$$

[4] The argument we are about to give is standard in the application of statistical mechanics to dynamical systems.

This is true without smoothness assumptions, but can be proved particularly easily in the smooth case by verifying that

$$g''(y) = \frac{s''(1/y)}{y^3}.$$

Since $s(\epsilon)/\epsilon$ takes on its supremum at an interior point of its interval of definition, the same is true for $g(y)$; since $g(y)$ is concave, it is strictly monotone decreasing with increasing distance from the place where it takes on its supremum, so the same is true for $s(\epsilon)/\epsilon$.

This completes our analysis of the behavior of $s(\epsilon)/\epsilon$; we turn now to the behavior of $N(q)$ for large q. We have already given an outline of the argument; what remains to be shown is

$$\frac{1}{\log q} \log \mathcal{V}_{n(q)}(-\infty, \frac{\log q}{n(q)}) \longrightarrow \frac{s(\epsilon^*)}{\epsilon^*},$$

(where, as before, $n(q)$ denotes a value of n maximizing $\mathcal{V}_n(-\infty, \log q/n)$.) The first step in proving this is:

Lemma 5.6 *Let $m(q)$ be a sequence of integers such that*

$$\frac{\log q}{m(q)} \longrightarrow \tilde{\epsilon} \in (\epsilon_{\min}, \infty)$$

Then

$$\frac{1}{\log q} \log \mathcal{V}_{m(q)}(-\infty, \frac{\log q}{m(q)}) \longrightarrow \frac{s(\tilde{\epsilon})}{\tilde{\epsilon}}.$$

Proof. Let $\epsilon_1 < \tilde{\epsilon}$. Then, for sufficiently large q, $\log q/m(q) > \epsilon_1$, so

$$\mathcal{V}_{m(q)}(-\infty, \frac{\log q}{m(q)}) \geq \mathcal{V}_{m(q)}(-\infty, \epsilon_1),$$

again for sufficiently large q. Taking logarithms and dividing by $\log q$ gives

$$\frac{1}{\log q} \log \mathcal{V}_{m(q)}(-\infty, \frac{\log q}{m(q)}) \geq \frac{m(q)}{\log q} \frac{1}{m(q)} \log \mathcal{V}_{m(q)}(-\infty, \epsilon_1) \longrightarrow \frac{s(\epsilon_1)}{\tilde{\epsilon}}.$$

Hence,

$$\liminf_{q\to\infty} \frac{1}{\log q} \log \mathcal{V}_{m(q)}(-\infty, \frac{\log q}{m(q)}) \geq \frac{s(\epsilon_1)}{\tilde{\epsilon}}.$$

This holds for all $\epsilon_1 < \tilde{\epsilon}$, and $s(\epsilon)$ is continuous, so we can replace ϵ_1 on the right by $\tilde{\epsilon}$. In exactly the same way – starting with $\epsilon_1 > \tilde{\epsilon}$ – we show that

$$\limsup_{q\to\infty} \frac{1}{\log q} \log \mathcal{V}_{m(q)}(-\infty, \frac{\log q}{m(q)}) \leq \frac{s(\tilde{\epsilon})}{\tilde{\epsilon}},$$

and the lemma follows. It is clear that this argument also works, with the obvious modification in the formulation, if $m(q)$ is only defined for a subsequence of q's going to ∞. □

As a consequence of the lemma, we note that the sequence $(\log q)/n(q)$ – with $n(q)$ defined as above – cannot have any accumulation point in $(\epsilon_{\min}, \infty)$ other than ϵ^*. Otherwise, letting $\hat{n}(q)$ be a sequence such that $(\log q)/\hat{n}(q) \to \epsilon^*$, we would eventually encounter a q for which

$$\mathcal{V}_{\hat{n}(q)}(-\infty, \frac{\log q}{\hat{n}(q)}) > \mathcal{V}_{n(q)}(-\infty, \frac{\log q}{n(q)}),$$

contradicting the assumed maximizing property of $n(q)$.

By the same sort of argument as used in the proof of the preceding lemma, we see that if

$$\limsup_{q\to\infty} \frac{\log q}{m(q)} \leq \epsilon_{\min},$$

then

$$\limsup_{q\to\infty} \frac{1}{\log q} \log \mathcal{V}_{m(q)}(-\infty, \frac{\log q}{m(q)}) \leq \lim_{\epsilon\to\epsilon_{\min}^+} \frac{s(\epsilon)}{\epsilon} < \sup_{\epsilon} \frac{s(\epsilon)}{\epsilon},$$

Thus, it is also impossible that $(\log q)/n(q)$ have an accumulation point in $[0, \epsilon_{\min}]$, so the only remaining possible accumulation points for the sequence $\log q/n(q)$ are ϵ^* and $+\infty$. If we eliminate the second possibility, it will follow that $\log q/n(q) \to \epsilon^*$ and hence, applying again the lemma, that

$$\frac{1}{\log q} \log \mathcal{V}_{n(q)}(-\infty, \frac{\log q}{n(q)}) \longrightarrow \frac{s(\epsilon^*)}{\epsilon^*},$$

as asserted.

Lemma 5.7 *Let $m(q)$ be a sequence such that*

$$\frac{m(q)}{\log q} \longrightarrow 0.$$

Then

$$\limsup \frac{1}{\log q} \log \mathcal{V}_{m(q)}(-\infty, \frac{\log q}{m(q)}) \leq 1$$

Proof. Fix $\beta > 1$, and let B denote an upper bound for the $Z_m(\beta)^{1/m}$. For any m and any real number r, we get

$$\begin{aligned} B^m &\geq Z_m(\beta) = \sum_{a_1,\ldots,a_m} \exp(-\beta H_m(a_1,\ldots,a_m)) \\ &\geq \sum \{\exp(-\beta H_m(a_1,\ldots,a_n)) : H_m(a_1,\ldots,a_m) < rm\} \\ &\geq \exp(-\beta rm)\mathcal{V}_m(-\infty, r), \end{aligned}$$

i.e.,

$$\mathcal{V}_m(-\infty, r) \leq \exp(\beta rm)B^m.$$

Thus,

$$\frac{1}{\log q} \log \mathcal{V}_{m(q)}(-\infty, \frac{\log q}{m(q)}) \leq \frac{m(q)}{\log q} \log B + \beta.$$

The first term on the right drops out as $q \to \infty$, so we get

$$\limsup_{q\to\infty} \frac{1}{\log q} \log \mathcal{V}_{m(q)}(-\infty, \frac{\log q}{m(q)}) \leq \beta.$$

Since this holds for all $\beta > 1$, the lemma – and hence also the proposition – is proved.

We can expand on the above argument to establish a statistical relation between n and q. Let $\epsilon_{\min} < \epsilon_1 < \epsilon^*$ and let $N^{(<)}(q, \epsilon_1)$ denote the number of n-tuples $a_1, \ldots, a_n$ (n variable) with

$$q_n(a_1, \ldots, a_n) \leq q \quad \text{and} \quad \frac{\log q_n(a_1, \ldots, a_n)}{n} < \epsilon_1,$$

i.e., with

$$q_n(a_1, \ldots, a_n) \leq q \quad \text{and} \quad n > (\epsilon_1)^{-1} \log q_n(a_1, \ldots, a_n).$$

The proof of Proposition 5.5 can easily be generalized to show that

$$\lim_{q\to\infty} \frac{1}{\log q} \log N^{(<)}(q, \epsilon_1) = \sup_{\epsilon<\epsilon_1} \frac{s(\epsilon)}{\epsilon} < \frac{s(\epsilon^*)}{\epsilon^*}.$$

Hence, in particular,

$$\lim_{q\to\infty} \frac{N^{(<)}(q, \epsilon_1)}{N(q)} = 0.$$

The ratio $N^{(<)}(q, \epsilon_1)/N(q)$ is the fraction of sequences $a_1, \ldots, a_n$ with $q_n < q$ which satisfy the further condition that $n > (\epsilon_1)^{-1} \log q_n$. Thus, we can say that, for q large, the overwhelming majority of sequences with $q_n < q$ have $n \leq (\epsilon_1)^{-1} \log q_n$, and this holds *for all* $\epsilon_1 < \epsilon^*$.

In exactly the same way, we argue that, for all $\epsilon_2 > \epsilon^*$, the fraction of these sequences with $n < (\epsilon_2)^{-1} \log q_n$ also goes to zero as $q \to \infty$. Hence:

Proposition 5.8 *Let $\epsilon_1 < \epsilon^* < \epsilon_2$. Then for q sufficiently large, an overwhelming majority of configurations with $q_n < q$ satisfy*

$$(\epsilon_2)^{-1} \log q_n \leq n \leq (\epsilon_1)^{-1} \log q_n.$$

Loosely formulated: For q large, nearly all configurations with $q_n < q$ satisfy $n \approx (\epsilon^*)^{-1} \log q$. We have already observed that the number of configurations with $q_n < q$ is twice the number of rational numbers between 0 and 1 with reduced-form denominator $< q$; each rational number has exactly two continued-fraction representations. The two representations of such a number have lengths differing by one, which is unimportant at the resolution at which we are working. Thus, we can reformulate what we have shown to say: *For q large, nearly all rational numbers with reduced-form denominator $< q$ have continued fraction expansions of length $\approx (\epsilon^*)^{-1} \log q$.*

After we had obtained the result formulated in the preceding paragraph, we learned that a sharper assertion had been proved in Dixon (1970). (See also Knuth (1981), §4.5.3, for a readable survey of work in this direction.) Part of what Dixon proves can be formulated as follows: For any $\epsilon > 0$, and for q large, the overwhelming majority of rational numbers r between 0 and 1 with reduced-form denominator $q(r) \leq q$, have continued fraction expansion with length $n(r)$ satisfying

$$|n(r) - \lambda \log q(r)| \leq (\log q(r))^{1/2+\epsilon},$$

where λ denotes $\dfrac{12\log 2}{\pi^2}$. Loosely: For typical rational numbers r, with large $q(r)$, $n(r)$ differs from $\lambda \log q(r)$ by something not much larger that $(\log q(r))^{1/2}$, whereas our results show only that the difference is typically $o(\log q(r))$. Dixon also gives an estimate for the number of configurations which do *not* satisfy the asserted inequality. Although Dixon's proof is based on detailed estimates in the spirit of analytic number theory, rather than the general statistical mechanical ideas we have used, there are many points of resemblance between his argument and ours.

6 Full entropy

We are now going to explore the possibility of improving, e.g., Proposition 5.8 by replacing the phrase "the overwhelming majority of configurations with $q_n < q$" by "the overwhelming majority of configurations with $q_n \approx q$." This is a version of a standard problem in statistical mechanics: How thick must the energy shell be to get the microcanonical ensemble to work properly? We can formulate the question somewhat more precisely as follows: Suppose we choose, for each q, a quantity $\delta(q)$ between zero and one, and we let $\widetilde{N}(q)$ denote the number of configurations with $q - \delta(q) \cdot q < q_n < q$. If we can show that

$$\lim_{q\to\infty} \frac{1}{\log q} \log \widetilde{N}(q) = \lim_{q\to\infty} \frac{1}{\log q} \log N(q),$$

i.e., if we can show that the set of configurations with $q-\delta(q)\cdot q < q_n < q$ has "the same entropy" as the larger set of all configurations with $q_n < q$, then the argument of the preceding section applies to show that the overwhelming majority of configurations with $q-\delta(q)\cdot q < q_n < q$ have $n \approx \epsilon^* \log q$. The question thus becomes: How small can $\delta(q)$ be without excluding too many configurations? In particular: Is $\delta(q)$ small and constant allowed?

We will cast this question in slightly more general terms: We consider two sequences $\epsilon_n^{(1)}$ and $\epsilon_n^{(2)}$ with

- $\epsilon_n^{(1)} < \epsilon_n^{(2)}$ for all n, and
- $\epsilon_n^{(2)} \to \epsilon$, with $\epsilon_{\min} < \epsilon < \infty$,

and we ask for condition sufficing to guarantee

$$\lim_{n\to\infty} \frac{1}{n} \log \mathcal{V}_n(\epsilon_n^{(1)}, \epsilon_n^{(2)}) = s(\epsilon).$$

The following proposition gives such a condition:

Proposition 6.1 *Let the general setup be as described in the preceding paragraph, and assume that $\epsilon_n^{(2)} - \epsilon_n^{(1)}$ goes to zero, if at all, more slowly than exponentially in n, in the sense that*

$$\limsup_{n\to\infty} \frac{-\log(\epsilon_n^{(2)} - \epsilon_n^{(1)})}{n} \leq 0.$$

Then

$$\lim_{n\to\infty} \frac{1}{n} \log \mathcal{V}_n(\epsilon_n^{(1)}, \epsilon_n^{(2)}) = s(\epsilon).$$

Proof. We note first that it is always true that

$$\limsup_{n\to\infty} \frac{1}{n} \log \mathcal{V}_n(\epsilon_n^{(1)}, \epsilon_n^{(2)}) \leq \lim_{n\to\infty} \frac{1}{n} \log \mathcal{V}_n(-\infty, \epsilon_n^{(2)}) = s(\epsilon),$$

so we have only to prove

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathcal{V}_n(\epsilon_n^{(1)}, \epsilon_n^{(2)}) \geq s(\epsilon).$$

We can thus assume without loss of generality that $\epsilon_n^{(2)} - \epsilon_n^{(1)} \to 0$. Fix $\bar{\epsilon} < \epsilon$; we are going to argue that, for n sufficiently large, any configuration $a_1, \ldots, a_{n-1}$ of length $n-1$ with

$$\log q_{n-1}(a_1, \ldots, a_{n-1}) < (n-1)\bar{\epsilon}$$

can be extended, by proper choice of a_n, to a configuration of length n with

$$n\epsilon_n^{(1)} < \log q_n(a_1, \ldots, a_n) < n\epsilon_n^{(2)}.$$

This will imply

$$\mathcal{V}_n(\epsilon_n^{(1)}, \epsilon_n^{(2)}) \geq \mathcal{V}_{n-1}(-\infty, \bar{\epsilon}),$$

and hence

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathcal{V}_n(\epsilon_n^{(1)}, \epsilon_n^{(2)}) \geq \lim_{n\to\infty} \frac{1}{n} \log \mathcal{V}_{n-1}(-\infty, \bar{\epsilon}) = s(\bar{\epsilon}).$$

This holds for all $\bar{\epsilon} < \epsilon$, so

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathcal{V}_n(\epsilon_n^{(1)}, \epsilon_n^{(2)}) \geq s(\epsilon),$$

which is what we want to prove.

It remains only to prove the assertion about extension of configurations $a_1, \ldots, a_{n-1}$ with

$$\log q_{n-1}(a_1, \ldots, a_{n-1}) < n\,\bar{\epsilon}.$$

For any a_n we have

$$q_n(a_1, \ldots, a_n) = a_n q_{n-1}(a_1, \ldots, a_{n-1}) + q_{n-2}(a_1, \ldots, a_{n-2}).$$

Clearly, by taking a_n large enough, we can make $q_n > \exp(n\epsilon_n^{(1)})$. We choose the smallest a_n which accomplishes this and show that then $q_n < \exp(n\epsilon_n^{(2)})$, provided that n is large enough. Note first that

$$a_n = \frac{q_n}{q_{n-1}} - \frac{q_{n-2}}{q_{n-1}} \geq \exp(n(\epsilon_n^{(1)} - \bar{\epsilon})) - 1,$$

which is $\geq \exp(\alpha n)$ for all sufficiently large n, for an appropriately chosen $\alpha > 0$. Next,

$$\begin{aligned}\frac{q_n(a_1,\ldots,a_{n-1},a_n)}{q_n(a_1,\ldots,a_{n-1},a_n-1)} &= 1+\frac{1}{a_n-1+\frac{q_{n-2}}{q_{n-1}}}\\ &\leq 1+\mathcal{O}(\exp(-\alpha n)).\end{aligned}$$

Hence,

$$\log q_n(a_1,\ldots,a_n)-\log q_n(a_1,\ldots,a_n-1)=\mathcal{O}(\exp(-\alpha n));$$

since – by the choice of a_n –

$$\log q_n(a_1,\ldots,a_n-1)\leq n\epsilon_n^{(1)},$$

and since, by assumption,

$$\epsilon_n^{(2)}-\epsilon_n^{(1)}\gg\exp(-n\alpha)\quad\text{for large } n,$$

it follows that

$$\log q_n(a_1,\ldots,a_n)<n\epsilon_n^{(2)}\quad\text{for } n \text{ large enough.}$$

This completes the proof of the proposition. □

It is easy to translate this result to apply to the statistical relation between q and n:

Proposition 6.2 *Let $\delta(q)$ be a sequence in $(0,1]$ such that*

$$\limsup_{q\to\infty}\frac{\log(1/\delta(q))}{\log q}=0,$$

(i.e., $\delta(q)$ goes to zero, if at all, less rapidly than any inverse power of q), and let $\widetilde{N}(q)$ denote the number of configurations $a_1,\ldots,a_n$ with

$$(1-\delta(q))q<q_n(a_1,\ldots,a_n)<q. \tag{$*$}$$

Then

$$\lim_{q\to\infty}\frac{1}{\log q}\log\widetilde{N}(q)=\sup_{\epsilon}\frac{s(\epsilon)}{\epsilon}. \tag{$\dagger$}$$

Hence: For any $\eta>0$, and for large q, the overwhelming majority of configurations satisfying $(*)$ have continued-fraction expansion of length between $(1-\eta)(\epsilon^*)^{-1}\log q$ and $(1+\eta)(\epsilon^*)^{-1}\log q$.

We omit the proof; it is a straightforward adaptation of the proofs of Propositions 5.5 and 5.8, using Proposition 6.1. We remark that the condition that $\delta(q)$ decrease less rapidly than any inverse power of q is also *necessary* for $(\dagger)$; this follows from the elementary upper bound

$$\widetilde{N}(q)\leq 2\sum_{j=(1-\delta(q))q}^{q} j=\mathcal{O}(q^2\delta(q)).$$

7 The third law of thermodynamics

We are going to show here that

Proposition 7.1

$$\lim_{\epsilon\to\epsilon_{\min}^+} s(\epsilon) = 0.$$

In other words: Our statistical mechanical system has no zero-point entropy, i.e., it satisfies the third law of thermodynamics. There are available general methods for proving the third law; see, for example Simon (1993) §III.9 or Schrader (1970). Although these methods could certainly be used here, we will instead give a simple "bare-hands" argument. In general terms, the argument goes as follows:

- We show that our system has, in a particularly clean sense, a unique ground state and a "mass gap."
- From this, we argue that the unique Gibbs state σ_β converges to the point mass at the ground state as $\beta \to \infty$. Intuitively, this means that the entropy of σ_β should go to zero, and we show that convergence takes place in a sufficiently strong sense that this expectation is realized.
- To finish the argument, we invoke a version of the "variational principle," saying that the entropy of σ_β is equal to the microcanonical entropy for $\epsilon = \bar{\epsilon}_\beta$, where $\bar{\epsilon}_\beta$ means the mean energy per lattice site in σ_β. (For this conclusion, we need only the "easy" half of the variational principle, i.e., the fact that Gibbs states maximize the free energy, and not the converse assertion that states maximizing the free energy are Gibbs states.)

The heart of the matter is the "mass gap." Recall that the Hamiltonian of an n-site finite system is $\log q_n(a_1,\ldots,a_n)$, and that q_n is strictly increasing in each a_i separately. Hence, the unique ground state of the n-site system is the configuration $(1,\ldots,1)$. Something much stronger is true in our case: If we start from a non-ground state $(a_1,\ldots,a_n)$, pick any i for which $a_i \neq 1$, and replace the corresponding a_i by 1, keeping all the other a_j's fixed, then the energy decreases by at least a fixed nonzero amount independent of n, i, and the configuration.

Lemma 7.2 *There is a strictly positive number ϵ_{g} such that,*

$$\log q_n(a_1,\ldots,a_{i-1},a_i,a_{i+1},\ldots a_n) \geq \log q_n(a_1,\ldots,a_{i-1},1,a_{i+1},\ldots a_n) + \epsilon_{\mathrm{g}}$$

for all n, all i between 1 and n, and all configurations $(a_1,\ldots,a_n)$ with $a_i \neq 1$.

Proof. Since $q_n(a_1,\ldots,a_i,\ldots,a_n)$ is nondecreasing in a_i, it suffices to consider $a_i = 2$. We will write q_j for $q_j(a_1,\ldots,a_{i-1},1,a_{i+1},\ldots a_j)$ (with the obvious simplifications for $j \leq i+1$), and we put

$$\begin{aligned} d_j &:= q_j(a_1,\ldots,a_{i-1},2,a_{i+1},\ldots,a_j) - q_j \quad \text{for } j \geq i \text{ and} \\ d_j &:= 0 \quad \text{for } j < i. \end{aligned}$$

Since

$$\begin{aligned} q_i(a_1,\ldots,a_{i-1},2) &= 2q_{i-1}+q_{i-2} \quad \text{and} \\ q_i(a_1,\ldots,a_{i-1},1) &= q_{i-1}+q_{i-2}, \end{aligned}$$

we get

$$d_i = q_{i-1}.$$

The d_{i+k} satisfy the recurrence

$$d_{i+k} = a_{i+k}d_{i+k-1} + d_{i+k-2},$$

i.e., the same recurrence as the $q_k(a_{i+1},\ldots,a_{i+k})$. In view of the initial condition

$$d_{i-1} = 0 \quad \text{and} \quad d_i = q_{i-1},$$

(which differs only by a factor of q_{i-1} for that for $q_k(a_{i+1},\ldots,a_{i+k})$), we see

$$d_{i+k} = q_{i-1}q_k(a_{i+1},\ldots,a_{i+k}).$$

Hence, setting $i+k=n$,

$$q_n(a_1,\ldots,2,\ldots,a_n) - q_n = q_{i-1}(a_1,\ldots,a_{i-1})q_{n-i}(a_{i+1},\ldots,a_n),$$

so we have only to show that

$$\frac{q_{i-1}(a_1,\ldots,a_{i-1})q_{n-i}(a_{i+1},\ldots,a_n)}{q_n(a_1,\ldots,a_{i-1},1,a_{i+1},\ldots a_n)} \tag{$*$}$$

is bounded away from zero.

Now let $\tilde{q}_k$ and $\tilde{p}_k$ denote $q_k(a_{i+1},\ldots,a_{i+k})$ and $p_k(a_{i+1},\ldots,a_{i+k})$ respectively. The $\tilde{q}_k$ and $\tilde{p}_k$ satisfy the same recurrence as the q_{i+k}, but with initial conditions

$$\begin{aligned} \tilde{q}_0 &= 1 \qquad \tilde{q}_{-1} = 0 \\ \tilde{p}_0 &= 0 \qquad \tilde{p}_{-1} = 1. \end{aligned}$$

It follows that

$$q_{i+k} = q_i\tilde{q}_k + q_{i-1}\tilde{p}_k.$$

Setting $k = n-i$, we see that we can rewrite $(*)$ as

$$\begin{aligned} \frac{q_{i-1}\tilde{q}_{n-i}}{q_i\tilde{q}_{n-i}+q_{i-1}\tilde{p}_{n-i}} &= \frac{1}{q_i/q_{i-1}+\tilde{p}_{n-i}/\tilde{q}_{n-i}} \\ &= \frac{1}{1+q_{i-2}/q_{i-1}+\tilde{p}_{n-i}/\tilde{q}_{n-i}} \quad \text{since } q_i = q_{i-1}+q_{i-2} \\ &= \frac{1}{1+[a_{i-1},\ldots,a_1]+[a_{i+1},\ldots,a_n]} \\ &> \frac{1}{3}, \end{aligned}$$

so the assertion is proved □

The next step will be to show, using this lemma, that as $\beta \to \infty$ the Gibbs state converges to the point mass on the unique ground state configuration in a strong enough way to ensure that the entropy of the Gibbs state goes to 0. We first need to recall the definition of entropy in the present context. Let μ denote a translation-invariant probability measure on $\{1, 2, \dots\}^{\mathbb{Z}}$, and let $\mu(a_0, \dots, a_{n-1})$ denote the μ-probability of the configuration $(a_0, \dots, a_{n-1})$ in the finite subset $\{0, \dots, n-1\}$ of the index set ("lattice") $\mathbb{Z}$. We then define

$$S_n(\mu) = \sum_{a_0,\dots,a_{n-1}} -\mu(a_0, \dots, a_{n-1}) \log \mu(a_0, \dots, a_{n-1}),$$

with, as usual, the convention $0 \log 0 = 0$. Then S_n is a subadditive function of n, so $\lim_{n\to\infty} \frac{1}{n} S_n(\mu)$ exists and is equal to $\inf_n \frac{1}{n} S_n(\mu)$; the common value is the entropy $s(\mu)$ of μ. We can now formulate:

Proposition 7.3 *Let σ_β denote the unique Gibbs state with inverse temperature β. Then $s(\sigma_\beta) \to 0$ when $\beta \to \infty$.*

Proof. We are going to show that, in the notation of the preceding paragraph, $S_1(\sigma_\beta)$ converges to 0 as $\beta \to \infty$; since

$$0 \le s(\sigma_\beta) \le \cdots \le S_n(\sigma_\beta) \le \cdots \le S_1(\sigma_\beta),$$

the assertion follows. We will need some notation related to Gibbs states. For Λ any subset of $\mathbb{Z}$, we denote by X_Λ the set of configurations in Λ, i.e., of mappings $\Lambda \to \{1, 2, \dots\}$. For Λ a *finite* subset of $\mathbb{Z}$, the interaction gives rise to a function Ψ_Λ, defined on $X_\Lambda \times X_{\Lambda^c}$ with the interpretation that $\Psi_\Lambda(a_\Lambda, a_{\Lambda^c})$ is the sum of the self-energy of the finite configuration a_Λ and its energy of interaction with the outside configuration a_{Λ^c}.[5] A Gibbs state with inverse temperature β is a probability measure on $X_{\mathbb{Z}}$ with the property that, for any finite Λ, the conditional probability of finding a_Λ inside Λ given that the configuration outside Λ is a_{Λ^c} is

$$\frac{\exp(-\beta \Psi_\Lambda(a_\Lambda, a_{\Lambda^c}))}{Z_\Lambda(\beta, a_{\Lambda^c})},$$

with

$$Z_\Lambda(\beta, a_{\Lambda^c}) = \sum_{a'_\Lambda \in X_\Lambda} \exp(-\beta \Psi_\Lambda(a'_\Lambda, a_{\Lambda^c})).$$

It follows from the considerations of §3 that

$$\Psi_\Lambda(a_\Lambda, a_{\Lambda^c}) - \sum_{i\in\Lambda} \log(a_i)$$

is bounded (for fixed Λ.)

We apply these considerations in the very simple case $\Lambda = \{0\}$. We define

$$V(a_0, \hat{a}) := \Psi_{\{0\}}(a_0, \hat{a}) - \Psi_{\{0\}}(1, \hat{a}),$$

where $\hat{a}$ denotes a general configuration of $\mathbb{Z} \setminus \{0\}$. Then

[5] Although these individual energies are not unambiguously defined, the sum is unambiguous, at least up to an additive constant.

- $V(1, \hat{a}) = 0$
- $V(a_0, \hat{a}) \geq \epsilon_g$ for $a_0 > 1$, by Lemma 7.2
- $V(a_0, \hat{a}) - \log a_0$ is bounded.

We put

$$Z_0(\beta, \hat{a}) := \sum_{a_0 \geq 1} \exp(-\beta V(a_0, \hat{a})) = 1 + \sum_{a_0 > 1} \exp(-\beta V(a_0, \hat{a})).$$

By the preceding remarks, $\exp(-\beta V(a_0, \hat{a}))$ converges to zero for any fixed $a_0 > 1$ and is furthermore $< a_0^{-\beta/2}$ (for example) for any sufficiently large a_0, all uniformly in $\hat{a}$. Hence, in particular, $Z_0(\beta, \hat{a}) \to 1$ as $\beta \to \infty$. From the definition of Gibbs state, the conditional probability of finding a_0 at the origin given the configuration $\hat{a}$ away from the origin is

$$\frac{\exp(-\beta V(a_0, \hat{a}))}{Z_0(\beta, \hat{a})},$$

which converges to 1 for $a_0 = 1$ and to 0 for $a_0 > 1$, and is bounded by $a_0^{-\beta/2}$ for all sufficiently large a_0, again uniformly in $\hat{a}$.

Now let $\sigma_\beta(a_0)$ denote the probability, with respect to the unique Gibbs state σ_β of having a_0 at the origin. Since this probability is a convex combination of the above conditional probabilities, it follows that

$$\sigma_\beta(1) \to 1, \quad \sigma_\beta(a_0) \to 0 \quad \text{for} \quad a_0 > 1, \quad \text{as} \quad \beta \to \infty,$$

and

$$\sigma_\beta(a_0) < a_0^{-\beta/2} \quad \text{for all sufficiently large } a_0.$$

Hence,

$$-\sigma_\beta(a_0) \log \sigma_\beta(a_0)$$

converges to zero with $\beta \to \infty$, for all a_0, and furthermore is $\leq a_0^{-\beta/4}$ for all sufficiently large a_0 (since $-t \log t \leq t^{1/2}$ for t positive and sufficiently small.) From this it follows that

$$S_1(\sigma_\beta) = \sum_{a_0=1}^{\infty} -\sigma_\beta(a_0) \log \sigma_\beta(a_0) \longrightarrow 0 \quad \text{with} \quad \beta \longrightarrow \infty.$$

□

It remains to relate $s(\sigma_\beta)$ to the microcanonical entropy. To avoid confusion, we will, for this section, denote the microcanonical entropy by $s_{\mathrm{mc}}(\epsilon)$; s without subscript means the entropy of a translation-invariant measure, as defined above.

- from Proposition 4.1,

  $$p(\beta) = s(\sigma_\beta) - \beta\, \bar{\epsilon}(\beta),$$

  where $\bar{\epsilon}(\beta)$ denotes the mean energy per lattice site in the Gibbs state σ_β.

- from the theory of thermodynamic limits for partition functions and the Legendre transform, we have
$$p(\beta) = s_{\mathrm{mc}}(\epsilon(\beta)) - \beta\,\epsilon(\beta),$$
where $\epsilon(\beta)$ is defined as the unique ϵ for which $s_{\mathrm{mc}}(\epsilon) - \beta\epsilon$ takes on its supremum,

- and finally, from a standard argument using Propositions 4.1 and 5.3
$$\bar{\epsilon}(\beta) = \epsilon(\beta),$$

Putting all this together, we see that

$$s(\sigma_\beta) = s_{\mathrm{mc}}(\epsilon(\beta)).$$

As $\beta \to \infty$, one the one hand $s(\sigma_\beta) \to 0$ – by what was shown above – and on the other hand, $\epsilon(\beta)$ is continuous and strictly decreasing, and converges to ϵ_{min}. This completes the proof of Proposition 7.1

8 Joint distribution of $\log q$ and the Farey depth

We consider here, in addition to $H_n = \log q_n(a_1, \ldots, a_n)$, the function

$$F_n(a_1, \ldots, a_n) := a_1 + \cdots + a_n$$

on $\mathbb{N}_+^n$. As noted in the introduction, F_n has a number-theoretic significance: It is the level in the Farey-tree representation of rational numbers at which $[a_1, \ldots, a_n]$ appears. We will accordingly refer to F_n as the *Farey depth.* The sequence of functions F_n is trivially extensive; if interpreted as an energy, it corresponds to a non-interacting system. We put the two quantities $\log q_n$ and F_n together and regard them as components of a single $\mathbb{R}^2$-valued extensive quantity

$$g_n(a_1, \ldots, a_n) := (\log q_n(a_1, \ldots, a_n), F_n(a_1, \ldots, a_n)).$$

The theory of the microcanonical entropy of such vector-valued extensive quantities is developed under technically favorable assumptions in Lanford (1973) and has been generalized to apply to the present situation in Ruedin (1994). To formulate the results, we will use the following notation: For J a subset of $\mathbb{R}^2$ and $n = 1, 2, \ldots$, $\mathcal{V}_{q,F}(n, J)$ will denote the number of configurations $(a_1, \ldots, a_n)$, of length n, with

$$\frac{g(a_1, \ldots, a_n)}{n} \in J.$$

The main results are as follows:

Proposition 8.1 *There exist:*

- *a (non-empty) convex open set $\mathcal{D}_{q,F}$ in $\mathbb{R}^2$ and*

– *a non-negative concave function* $s_{q,F}$ *on* $\mathcal{D}_{q,F}$

such that:

– *If* J *is an open convex subset of* $\mathbb{R}^2$ *with* $J \cap \mathcal{D}_{q,F} \neq \emptyset$, *then*

$$\lim_{n\to\infty} \frac{1}{n} \log \mathcal{V}_{q,F}(n, J) = \sup_{x \in J\cap\mathcal{D}_{q,F}} s_{q,F}(x).$$

– *if* J *is an open convex set whose distance from* $\mathcal{D}_{q,F}$ *is strictly positive, then* $\mathcal{V}_{q,F}(n, J)$ *vanishes for all sufficiently large* n.

The intuitive meaning is: If $(\epsilon, f) \in \mathcal{D}_{q,F} \subset \mathbb{R}^2$, then there exist, for arbitrarily large n, configurations with – simultaneously – $\log q_n \approx n\,\epsilon$ and $F_n \approx n\, f$; the number of such configurations is furthermore $\approx \exp(n s_{q,F}(\epsilon, f))$. If, on the other hand, (ϵ, f) is outside the closure of $\mathcal{D}_{q,F}$, then $(n\,\epsilon, n\, f)$ is *excluded* as a value for $(\log q_n, F_n)$ for large n. As in the single-observable case, this proposition evades the potentially delicate question of the behavior of $\mathcal{V}_{q,F}(n, J)$ when J has distance zero from $\mathcal{D}_{q,F}$ but does not actually intersect it. Comparing the defining properties of $s_{q,F}$ with those of the single-observable s, we see that

$$s(\epsilon) = \sup_f s_{q,F}(\epsilon, f).$$

Furthermore, $s_{q,F}$ has the following interpretation: If I is any interval for which

$$\sup_{f\in I} s_{q,F}(\epsilon, f) < s(\epsilon),$$

then, for large n, among configurations of length n with $q_n \approx \exp(n\epsilon)$, only a vanishingly small fraction have $F_n/n \in I$. Somewhat less precisely: For large n, among configurations with $q_n \approx \exp(n\epsilon)$, the values of F_n/n are strongly concentrated around values of f where $s_{q,F}(\epsilon, f)$ is maximal.

The preceding proposition is a version of a result which holds with great generality. A first special feature of the particular situation we are considering is

Proposition 8.2 *Let* $(\epsilon_0, f_0) \in \mathcal{D}_{q,F}$, *and let* $f_1 > f_0$. *Then* $(\epsilon_0, f_1) \in \mathcal{D}_{q,F}$, *and* $s_{q,F}(\epsilon_0, f_1) \geq s_{q,F}(\epsilon_0, f_0)$.

Roughly: $s_{q,F}(\epsilon, f)$ is non-decreasing in f for fixed ϵ.

Proof. For purposes of this argument, we denote by $R_\delta(\epsilon, f)$ the open square of side-length 2δ centered at $(\epsilon, f) \in \mathbb{R}^2$. We are going to argue:

Claim. *For sufficiently large* n,

$$\mathcal{V}_{q,F}(n+1, R_{2\delta}(\epsilon_0, f_1)) \geq \mathcal{V}_{q,F}(n, R_\delta(\epsilon_0, f_0)).$$

Before proving the claim, we show how it implies the proposition. In the first place, it follows at once that (ϵ_0, f_1) must be in the *closure* of $\mathcal{D}_{q,F}$; otherwise, for small enough δ, $\mathcal{V}_{q,F}(n+1, R_{2\delta}(\epsilon_0, f_1))$ would have to vanish for large n whereas $\mathcal{V}_{q,F}(n, R_\delta(\epsilon_0, f_0))$ is non-zero. By applying the same argument, with ϵ_0 moved a little, we see that *a neighborhood of* (ϵ_0, f_1) *lies inside the closure of* $\mathcal{D}_{q,F}$. But $\mathcal{D}_{q,F}$ is a convex open set, so this implies that (ϵ_0, f_1) itself is in $\mathcal{D}_{q,F}$. It then follows that $s_{q,F}$ is continuous at (ϵ_0, f_1) (as it is at (ϵ_0, f_0)). Thus,

$$s_{q,F}(\epsilon_0, f_1) = \inf_{\delta>0} \lim_{n\to\infty} \frac{1}{n+1} \log \mathcal{V}_{q,F}(n+1, R_{2\delta}(\epsilon_0, f_1)),$$

but, on the other hand, applying the claim again,

$$\begin{aligned}
\lim_{n\to\infty} \frac{1}{n+1} &\log \mathcal{V}_{q,F}(n+1, R_{2\delta}(\epsilon_0, f_1)) \\
&\geq \lim_{n\to\infty} \frac{1}{n+1} \log \mathcal{V}_{q,F}(n, R_\delta(\epsilon_0, f_0)) \\
&= \sup\{s_{q,F}(\epsilon, f) : (\epsilon, f) \in R_\delta(\epsilon_0, f_0)\} \\
&\geq s_{q,F}(\epsilon_0, f_0),
\end{aligned}$$

so the proposition follows from the claim.

Proof of Claim: Let $(a_1, \ldots, a_n)$ be a configuration with

$$\frac{1}{n}(\log q_n(a_1, \ldots, a_n), F_n(a_1, \ldots, a_n)) \in R_\delta(\epsilon_0, f_0).$$

We are going to make a configuration of length $n+1$ by adjoining a single large a_n and show that, for sufficiently large n, the augmented configuration always has

$$\frac{1}{n+1}(\log q_{n+1}(a_1, \ldots, a_{n+1}), F_n(a_1, \ldots a_{n+1})) \in R_{2\delta}(\epsilon_0, f_1);$$

this will establish the claim. We choose a_{n+1} to be the smallest integer with $a_1 + \ldots + a_n + a_{n+1} \geq (n+1)f_1$. Since $a_1 + \ldots + a_n \approx n f_0$, it is easy to find upper and lower bounds for a_{n+1} both of which go to infinity linearly with n (We need to assume here, as we may without loss of generality, that δ is chosen small enough so that $f_0 + \delta < f_1$.) Since

$$q_{n+1}(a_1, \ldots, a_{n+1}) = a_{n+1} q_n + q_{n-1},$$

we get

$$a_{n+1} q_n < q_{n+1} < (a_{n+1} + 1) q_n,$$

and hence – in view of the growth rate of the a_n's –

$$\log q_{n+1} = \log q_n + \mathcal{O}(\log n).$$

Since

$$\frac{1}{n} \log q_n \in (\epsilon_0 - \delta, \epsilon_0 + \delta),$$

it follows that, for n sufficiently large,

$$\frac{1}{n+1}\log q_{n+1} \in (\epsilon_0 - 2\delta, \epsilon_0 + 2\delta),$$

which completes the argument. $\square$

This gives us at least a rough picture of $\mathcal{D}_{q,F}$: We know from the outset that it lies to the right of the vertical line $\{\epsilon = \epsilon_{\min}\}$, since smaller values of ϵ are asymptotically excluded without any condition on F. It also extends arbitrarily far to the right, since $s(\epsilon)$ is defined for arbitrary large ϵ. In view of the preceding proposition, it is a union over ϵ of semi-infinite vertical lines:

$$\mathcal{D}_{q,F} = \{(\epsilon, f) : \epsilon > \epsilon_{\min}, f > f_{\min}(\epsilon)\}.$$

The function $f_{\min}(\epsilon)$ defined in the preceding formula is convex – since its epigraph $\mathcal{D}_{q,F}$ is – and hence continuous. It is not difficult to see that $f_{\min}(\epsilon)$ is monotone non-decreasing and not constant; hence, by convexity, that it goes to ∞ with ϵ. We will in fact determine $f_{\min}(\epsilon)$ explicitly in §10; somewhat surprisingly, it turns out to be piecewise linear.

We turn next to the canonical ensemble. We set

$$Z_n(\beta,\gamma) := \sum_{a_1,\ldots,a_n} \exp(-\beta H_n(a_1,\ldots,a_n) - \gamma F_n(a_1,\ldots a_n)).$$

In view of

$$\begin{aligned} H_n &= \log a_1 + \cdots + \log a_n + \text{bounded}, \\ F_n &= a_1 + \cdots + a_n, \end{aligned}$$

it is easy to see that the sum converges for *all* β, positive and negative, for $\gamma > 0$; for $\beta > 1$ for $\gamma = 0$ – the case already studied – and not at all for $\gamma < 0$. We refer to Ruedin (1994) for the proof of the following result, which involves only straightforward generalizations of standard results:

Proposition 8.3 *1. For $\gamma > 0$,*

$$\lim_{n\to\infty} \frac{1}{n} \log Z_n(\beta,\gamma) =: p_{q,F}(\beta,\gamma)$$

exists, and is given by the Legendre transform of $s_{q,F}$:

$$p_{q,F}(\beta,\gamma) = \sup\{s_{q,F}(\epsilon,f) - \beta\epsilon - \gamma f : (\epsilon,f) \in \mathcal{D}_{q,F}.\}$$

2. $p_{q,F}(\beta,\gamma)$ is a real-analytic and strictly convex function of (β,γ) in $\{\gamma > 0\}$.

By "Legendre duality," $s_{q,F}$ is the inverse Legendre transform of $p_{q,F}$. To be precise:

For $(\epsilon, f) \in \mathcal{D}_{q,F}$,

$$s_{q,F}(\epsilon,f) = \inf_{\beta,\gamma} p_{q,F}(\beta,\gamma) + \beta\epsilon + \gamma f;$$

the infimum on the right-hand side is $-\infty$ for (ϵ, f) outside the closure of $\mathcal{D}_{q,F}$.

(There are a number of versions of "Legendre duality." The preceding assertions follow from Theorem I.6.4 of Simon (1993) and the following observation: We have taken the definition domain of $s_{q,F}$ to be open. If we extend $s_{q,F}$ to the closure of the domain by defining it at boundary points to be the lim sup of values at nearby interior points, then the subgraph of the extended function is convex and closed. Hence, except for a sign, the extended function and the closure of the original domain form a *Fenchel pair* in the sense of Simon (1993).)

In particular, if we define

$$\epsilon_{q,F}(\beta,\gamma) := -\frac{\partial p_{q,F}}{\partial \beta}(\beta,\gamma), \quad f_{q,F}(\beta,\gamma) := -\frac{\partial p_{q,F}}{\partial \gamma}(\beta,\gamma),$$

for $\gamma > 0$ and β arbitrary, then $p(\beta,\gamma) + \beta\epsilon_{q,F}(\beta_0,\gamma_0) + \gamma f_{q,F}(\beta_0,\gamma_0)$ has vanishing gradient – and therefore a minimum – at $\beta = \beta_0$, $\gamma = \gamma_0$. Hence, by Legendre duality, $(\epsilon_{q,F}(\beta_0,\gamma_0), f_{q,F}(\beta_0,\gamma_0))$ is in the closure of $\mathcal{D}_{q,F}$, and this holds for all (β_0,γ_0) with $\gamma_0 > 0$. By strict convexity of $p_{q,F}$, the mapping

$$(\beta,\gamma) \mapsto (\epsilon_{q,F}(\beta,\gamma), f_{q,F}(\beta,\gamma))$$

is open and injective. Its image must therefore lie in $\mathcal{D}_{q,F}$, not just in its closure, and we have

$$s_{q,F}(\epsilon_{q,F}(\beta,\gamma), f_{q,F}(\beta,\gamma)) = p(\beta,\gamma) + \beta\epsilon_{q,F}(\beta,\gamma) + \gamma f_{q,F}(\beta,\gamma).$$

The right-hand side is a real-analytic function of (β,γ), and the inverse of

$$(\beta,\gamma) \mapsto (\epsilon_{q,F}(\beta,\gamma), f_{q,F}(\beta,\gamma))$$

is real-analytic by the inverse function theorem, so $s_{q,F}$ is real-analytic and, by a straightforward computation, strictly concave *on the image $\mathcal{D}^{(0)}_{q,F}$ of the upper half plane $\{\gamma > 0\}$ under*

$$(\beta,\gamma) \mapsto (\epsilon_{q,F}(\beta,\gamma), f_{q,F}(\beta,\gamma)).$$

Our next task is to determine the image domain $\mathcal{D}^{(0)}_{q,F}$ of the "analytic" Legendre transform. We do this in a way which produces some extra information which we will need later.

Lemma 8.4 *For any $\gamma > 0$ and any $\epsilon > \epsilon_{\min}$, there is a unique β with*

$$\epsilon_{q,F}(\beta,\gamma) = \epsilon.$$

We will denote this β by $\hat{\beta}(\epsilon,\gamma)$.

- *$\hat{\beta}$ is a real-analytic function of ϵ, γ.*
- *$f_{q,F}(\hat{\beta}(\epsilon,\gamma),\gamma)$ is strictly decreasing in γ.*
- *$\frac{\partial s_{q,F}}{\partial f}(\epsilon, f_{q,F}(\hat{\beta},\gamma)) = \gamma$.*

- *For $\epsilon > \epsilon_{\min}$, $\hat{\beta}(\epsilon, \gamma) \to \beta(\epsilon)$ as $\gamma \to 0^+$; convergence is uniform on compact sets in $(\epsilon_{\min}, \infty)$.*

- $$f_{q,F}(\hat{\beta}(\epsilon,\gamma),\gamma) \longrightarrow \begin{cases} f_{\min}(\epsilon) & \gamma \to \infty \\ \bar{f}(\beta(\epsilon)) & \gamma \to 0^+, \beta(\epsilon) > 2 \\ \infty, & \gamma \to 0^+, \beta(\epsilon) \leq 2. \end{cases}$$
  Here, $\bar{f}(\beta)$ means the means value of F_n/n in the Gibbs state with inverse temperature β (and $\gamma = 0.$).

Proof. For fixed γ, $\epsilon_{q,F}(\beta, \gamma)$ is a strictly decreasing real-analytic function of β. We are going to argue that it converges to $\epsilon_{\min}$ as $\beta \to \infty$ and ∞ as $\beta \to -\infty$; continuity then implies that it takes on every intermediate value exactly once, i.e., that $\hat{\beta}(\epsilon, \gamma)$ is defined. For this argument, we use the fact that $\epsilon_{q,F}(\beta, \gamma)$ is equal to the mean value, in the unique Gibbs state for (β, γ), of the function $-\log([a_0, a_1, \ldots])$.

- An easy extension of the arguments of §7 shows that, as $\beta \to \infty$ with fixed γ, the corresponding Gibbs state converges to the point mass at $(\ldots, 1, 1, \ldots)$, in a strong enough sense to allow us to conclude that $\epsilon_{q,F}(\beta, \gamma) \to -\log([1, 1, \ldots]) = \epsilon_{\min}$.

- The difference between $-\log([a_0, \ldots])$ and $\log a_0$ is bounded, so it is enough to show that the mean value of $\log a_0$ goes to ∞ as $\beta \to -\infty$. By the arguments of §7, the Gibbs state assigns a probability to a_0 which can be written as
  $$c_1(\beta)\exp(-\gamma a_0 - \beta(\log a_0 + c_2(\beta, a_0))$$
  with $c_2(\beta, a_0)$ uniformly bounded in a_0, β. From this form, it is clear that, as $\beta \to -\infty$, the probability distribution becomes concentrated on large values of a_0 and hence that the mean value of $\log a_0$ goes to ∞.

Thus, the existence of $\hat{\beta}(\epsilon, \gamma)$ is established; real analyticity follows from the inverse function theorem (using the strict convexity of $p_{q,F}(\,.\,)$.) Strict positivity of the derivative of $f_{q,F}(\hat{\beta}(\epsilon, \gamma), \gamma)$ with respect to γ follows from the strict convexity of $p_{q,F}(\,.\,)$ by a straightforward computation. The formula
$$\frac{\partial s_{q,F}}{\partial f}(\epsilon_{q,F}(\beta,\gamma), f_{q,F}(\beta,\gamma)) = \gamma$$
holds for all (β, γ) by the elementary properties of the Legendre transform; inserting $\hat{\beta}$ for β and remembering how $\hat{\beta}$ was defined gives
$$\frac{\partial s_{q,F}}{\partial f}(\epsilon, f_{q,F}(\hat{\beta},\gamma) = \gamma.$$

As $\gamma \to 0$ with β fixed > 1, $\epsilon_{q,F}(\beta, \gamma) \to \epsilon(\beta)$ and the convergence is uniform for β is any compact set in $(1, \infty)$. Hence, for fixed $\epsilon > \epsilon_{\min}$ and any $\beta_1 < \beta(\epsilon) < \beta_2$,
$$\epsilon_{q,F}(\beta_1,\gamma) > \epsilon(\beta) > \epsilon_{q,F}(\beta_2,\gamma) \quad \text{for all sufficiently small } \gamma.$$

For γ small enough so that these inequalities hold, $\beta_1 < \hat{\beta}(\epsilon,\gamma) < \beta_2$; this shows that $\hat{\beta}(\epsilon,\gamma)$ converges for $\gamma \to 0^+$ to $\beta(\epsilon)$, and it is easy to see that the convergence is in fact uniform on compact subintervals of $(\epsilon_{\min},\infty)$. It is also easy to see that, for $\gamma \to 0$, $f(\beta,\gamma)$ converges to $\bar{f}(\beta)$ for $\beta > 2$ and to ∞ for $1 < \beta < 2$; the convergence is uniform on compact subsets of $(1,\infty)$. Hence, also for $\gamma \to 0$, $f_{q,F}(\hat{\beta}(\epsilon,\gamma),\gamma)$ converges to $\bar{f}(\beta(\epsilon))$ for $\epsilon < \epsilon^*$ and to ∞ for $\epsilon \geq \epsilon^*$, as asserted. □

Proposition 8.5 *$\mathcal{D}^{(0)}_{q,F} = \{(\epsilon,f) \in \mathcal{D}_{q,F} : \epsilon \geq \epsilon^*$ or $f < \bar{f}(\beta(\epsilon))\}$. For $\epsilon \geq \epsilon^*$, $f \mapsto s_{q,F}(\epsilon,f)$ is strictly increasing and real-analytic on $(f_{\min}(\epsilon),\infty)$; for $\epsilon_{\min} < \epsilon < \epsilon^*$, $f \mapsto s_{q,F}(\epsilon,f)$ is real-analytic and strictly increasing on $(f_{\min}(\epsilon),\bar{f}(\beta(\epsilon)))$, but constant – equal to $s(\epsilon)$ – for $f \geq \bar{f}(\beta(\epsilon))$.*

Proof. The image under the inverse Legendre transformation of the parametrized curve

$$\gamma \mapsto (\hat{\beta}(\epsilon_0,\gamma),\gamma)$$

is a vertical segment above ϵ_0 in the (ϵ,f) plane which evidently lies $\mathcal{D}^{(0)}_{q,F}$. As γ runs from 0 to ∞, the segment is traversed downward. The f-coordinate of the upper end of the segment is $\lim_{\gamma\to 0^+} f_{q,F}(\hat{\beta}(\epsilon_0,\gamma),\gamma)$, which, by the preceding lemma is ∞ for $\epsilon_0 \geq \epsilon^*$ and $\bar{f}(\beta(\epsilon))$ otherwise. We temporarily denote the lower end of the segment by (ϵ_0, f_∞). f_∞ is evidently $\geq f_{\min}(\epsilon_0)$; we want to show that equality actually holds. To see this, we note that $f \mapsto s_{q,F}(\epsilon_0,f)$ is concave and nondecreasing on $(f_{\min}(\epsilon_0),\infty)$. At $f = f_{q,F}(\hat{\beta}(\epsilon_0),\gamma)$, its derivative is equal to γ. Hence, as $f \to f_\infty^+$, the derivative goes to ∞. This is not compatible with concavity unless $f_\infty = f_{\min}$. Furthermore, in the case $\epsilon_0 < \epsilon^*$, the derivative approaches 0 as $f \to \bar{f}(\beta(\epsilon_0))$; concavity and monotonicity then imply that the function must be constant for $f \geq \bar{f}$. As a consequence: If $\epsilon_0 < \epsilon^*$ and $f \geq \bar{f}$, then (ϵ_0,f) cannot lie in the image $\mathcal{D}^{(0)}_{q,F}$ of the analytic Legendre transform, i.e., the set of points above ϵ_0 in $\mathcal{D}^{(0)}_{q,F}$ are exactly those with $f_{\min}(\epsilon_0) < f < \bar{f}(\beta(\epsilon_0))$. Together with the analyticity and strict monotonicity of the analytic Legendre transform onto $\mathcal{D}^{(0)}_{q,F}$, this proves all the assertions of the proposition. □

Our intuition about statistical-mechanical systems suggests that fixing the energy – in the absence of phase transitions – determines all other extensive quantities. In the present context, this suggests that fixing $\log q_n/n$ – within some appropriate thickened energy surface – ought to determine F_n/n statistically. We will argue here, on the basis of the above results, that this is *not* the case, if we allow the size of the system to fluctuate. What happens instead is that the typical values of F_n/n go to infinity as the size of the system goes to infinity.

We consider a q – which will tend to ∞ – and a fixed parameter y and denote by $p(q,y)$ the fraction of set of configurations – of whatever length – with $q_n < q$ which also satisfy $F_n < y\log q$. Since configurations with $q_n < q$ nearly all have $\log q_n \approx \log q$, this means roughly the set of configurations with $F_n/\log q_n < y$. The kinds of arguments used in the proof of Proposition 5.5 show that

$$\lim_{q\to\infty} \frac{1}{\log q} \log p(q,y) = \sup_\epsilon \frac{s_{q,F}(\epsilon,\epsilon y)}{\epsilon} - \sup_\epsilon \frac{s(\epsilon)}{\epsilon},$$

provided that y is large enough so that the line $f = y\epsilon$ intersects $\mathcal{D}_{q,F}$. We are going to argue that the right-hand side is < 0 for all values of y, i.e., the probability that $F_n/\log q_n$ is $< y$ – given that $q_n < q$ – becomes exponentially small at $q \to \infty$ for all y. The argument goes as follows: It is always true that

$$s_{q,F}(\epsilon, f) \leq s(\epsilon),$$

and it follows from Proposition 5.3 that $s'(\epsilon) \to 1$ for $\epsilon \to \infty$ and hence that $s(\epsilon)/\epsilon \to 1$ in the same limit. Hence, if

$$\sup_{\epsilon} \frac{s_{q,F}(\epsilon, y\epsilon)}{\epsilon}$$

is not taken on at a finite ϵ, then it is ≤ 1, whereas $\sup_\epsilon s(\epsilon)/\epsilon$ was shown earlier to be equal to 2. Thus, the assertion is proved if the supremum is not taken on. Suppose now that the supremum is taken on, at, say, ϵ_1. If $\epsilon_1 \neq \epsilon^*$, then

$$\frac{s_{q,F}(\epsilon_1, y\epsilon_1)}{\epsilon_1} \leq \frac{s(\epsilon_1)}{\epsilon_1} < \frac{s(\epsilon^*)}{\epsilon^*};$$

the last inequality is strict since $s(\epsilon)/\epsilon$ takes on its supremum only at ϵ^*. Thus, the assertion is also proved if the supremum is taken on at any ϵ other than ϵ^*. Finally, if the supremum is taken on at ϵ^*, then we have

$$\frac{s_{q,F}(\epsilon^*, y\epsilon^*)}{\epsilon^*} < \frac{s(\epsilon^*)}{\epsilon^*},$$

since $f \mapsto s_{q,F}(\epsilon^*, f)$ is strictly increasing on $(f_{\min}(\epsilon^*), \infty)$ with asymptotic value $s(\epsilon^*)$. Thus, the assertion is proved in this case too, so all cases are covered.

9 The continuum representation

We describe here a neat and convenient representation for the Ruelle transfer operator for our system. We deviate here from Ruedin (1994), where the theory of the transfer operator is extended to a general class of systems including the one we are treating. This extension turns out to be technical and complicated. What we do here is to use the special features of our system to give a simple, if limited, treatment.

We start from the observation that the mapping

$$(a_0, a_1, \ldots) \longmapsto [a_0, a_1, \ldots]$$

sends the space of semi-infinite configurations

$$\Omega_+ := \{1, 2, \ldots\}^{\mathrm{N}}$$

bijectively onto the irrational numbers in $[0, 1]$. We will use this mapping to transport various objects from the configuration space to the unit interval, where they may be easier to work with. We start by looking at

- the Gibbs state of the semi-infinite system (index set $\{0, 1, \ldots\}$)

- the Gibbs state for the two-sided infinite system (index set $\mathbb{Z}$) projected onto the semi-infinite configuration space.

These are both probability measures on Ω_+; the second of them is shift-invariant and the first presumably not. However, as Ruelle observed, the Gibbs state for the semi-infinite system has the advantage of satisfying a relatively simple equation. This comes about as follows: We can construct the semi-infinite Gibbs state by

- Constructing the semi-infinite Gibbs state "with one fewer lattice site," i.e., on configurations labeled by $1, 2, 3, \ldots$ rather than $0, 1, 2, 3, \ldots$. Because of uniqueness, this is the same as the semi-infinite Gibbs state of Ω_+ shifted one place to the right.
- appending a new lattice site at the left-hand end,
- assigning weights proportional to $\exp(-A(a_0, a_1, \ldots))$ to the possible state a_0 at the new lattice site, and
- normalizing.

In other words, the assertion is that

$$e^{-A(a_0,a_1,\ldots)}\, da_0\, \sigma_+(da_1, da_2, \ldots) = \lambda \sigma_+(da_0, da_1, da_2, \ldots). \qquad (*)$$

Here,

- σ_+ denotes the semi-infinite Gibbs state
- $A(a_0, a_1, \ldots)$ denotes $-\beta \log[a_0, a_1, \ldots]$ (or $-\beta \log[a_0, \ldots] + \gamma a_0$, if we are talking about the two-observable situation.)
- the da_i's appearing inside σ_+ are "symbolic," but the da_0 on the left stands for counting measure on $\{1, 2, \ldots\}$.
- λ – or perhaps its reciprocal – is the normalizing factor.

The left-hand side of $(*)$ defines a linear operator $\mathcal{L}^*$ from measures on Ω_+ to measures on Ω_+; $(*)$ says that σ_+ is an eigenvector for $\mathcal{L}^*$ with eigenvalue λ. Iterating $(*)$ n times corresponds to adding n sites to the left. It is easy to see, using standard ideas from the theory of Gibbs states, that the semi-infinite Gibbs state σ_+ is the *unique* probability measure satisfying $(*)$, i.e., the unique probability measure which is an eigenvector of $\mathcal{L}^*$. The same set of considerations shows that the partition function $Z_n(\beta, \gamma)$ admits upper and lower bounds of the form $c\lambda^n$, c a strictly positive constant independent of n; hence, that

$$p(\beta, \gamma) = \log \lambda.$$

We now transport this whole picture to the unit interval. We will generally use the same notation for objects on the sequence space and the corresponding transported objects on the unit interval; for example, σ_+ will also denote the measure on the unit interval obtained by transporting the semi-infinite Gibbs state. We recall that the left shift

$$(a_0, a_1, a_2, \ldots) \longmapsto (a_1, a_2, \ldots)$$

carries over to the Gauss map

$$t \longmapsto \mathrm{fract}(\frac{1}{t}).$$

The construction on the right-hand side of $(*)$ translates into the following: Given a measure μ on $[0, 1]$ (assigning measure zero to the rational numbers), we construct a new measure $\mathcal{L}^*\mu$ by specifying that the $\mathcal{L}^*\mu$-measure of any set contained in one of the intervals $(1/(a_0 + 1), 1/a_0)$ is the integral of $e^{\gamma a_0}/(a_0 + t)^\beta$ over the preimage of the set in question under $t \mapsto 1/(a_0 + t)$. Then σ_+ is characterized as the unique probability measure transformed into a multiple of itself by $\mathcal{L}^*$.

We now have:

Proposition 9.1 *For $\beta = 2$ and $\gamma = 0$,*

- *σ_+ is Lebesgue measure on $[0, 1]$, and*
- *The transported projected two-sided infinite Gibbs state σ is the Gauss measure $\frac{1}{\log 2}\frac{dt}{1+t}$*
- $\epsilon^* = \dfrac{\pi^2}{12 \log 2}$

Proof. σ_+ is uniquely characterized by the fact that it is transformed into a multiple of itself by the operation of the preceding paragraph. To prove the first assertion, it is therefore enough to show that Lebesgue measure is unchanged by this operation. Concretely, it is enough to show that Lebesgue measure itself and the transform of Lebesgue measure assign the same measure to any interval J contained in some one of the intervals $(1/(a_0+1), 1/a_0)$, $a_0 = 1, 2, \ldots$. In other words, we want to show that the length of J is the integral of the function $(a_0 + t)^{-2}$ over the preimage of the interval under $t \mapsto 1/(a_0+t)$, and this follows at once from the fact that the absolute value of the derivative of $t \mapsto 1/(a_0 + t)$ is $(a_0 + t)^{-2}$. Thus, the transform of the one-sided Gibbs state is identified with Lebesgue measure, and the rescaling factor λ is shown to be one.

We now turn to the determination of the image of the projected Gibbs measure for the doubly infinite system under the mapping

$$(a_0, a_1, \ldots) \mapsto [a_0, a_1, \ldots].$$

We denote both the projected Gibbs state and the corresponding measure on $[0, 1]$ by σ. From the general theory of Gibbs states, we know that

- σ_+ and σ are equivalent, i.e., have the same null sets.
- σ is ergodic (with respect to the left shift respectively the Gauss map)

From these facts it follows that σ *is the only invariant probability measure equivalent to* σ_+. For $\beta = 2$, in the unit interval representation, this means that σ is the only probability measure on the unit interval equivalent to Lebesgue measure and invariant under the Gauss map. But it is well known – and in any case follows from an easy computation – that the Gauss measure is invariant under the Gauss map; hence, the Gauss measure must coincide with σ. Since ϵ^* is the mean value of $-\log[a_0, a_1, \ldots]$ with respect to the projected Gibbs state, we conclude that

$$\epsilon^* = -\frac{1}{\log 2}\int_0^1 \frac{\log t\, dt}{1+t} = \frac{\pi^2}{12\log 2}.$$

It is easy to see that the operator $\mathcal{L}^*$ on measures described above is the adjoint of an operator on continuous functions given by

$$(\mathcal{L}f)(t) = \sum_{a_0=1}^{\infty} \frac{e^{-\gamma a_0}}{(a_0+t)^\beta} f\left(\frac{1}{a_0+t}\right).$$

This operator – with $\gamma = 0$ – has been studied extensively in Mayer (1990). It is easy to see from the preceding formula that this operator is compact when restricted to act on a Banach space of functions bounded and analytic on an appropriate domain. A relatively elementary version of the Perron-Frobenius theorem applies and says that the eigenvalue of largest modulus is positive and simple. As might be expected, it can be shown that this eigenvalue is exactly λ. Efficient numerical methods are available for the computation of this principal eigenvalue; this provides an effective method for the numerical computation of the thermodynamic functions of our system.

10 Determining $\mathcal{D}_{q,F}$

We need the solution to the following elementary (finite!) optimization problem:

Given n and F, find the maximum of $q_n(a_1, \ldots, a_n)$ over all configurations with $a_1 + \cdots + a_n = F$.

To formulate the answer, we need to introduce some notation. We write

$$F = mn + r, \quad \text{with } 0 \le r < n;$$

in order that there be any configurations at all, it is necessary that $m \ge 1$, and this will always be assumed in what follows.

Proposition 10.1 *If $r = 0$, there is only one maximizing configuration – the one with $a_i = m$ for $1 \le i \le n$. For $r > 0$, the configurations*

$$a_1 = m+1,\ a_2 = \cdots = a_{n-r+1} = m,\ a_{n-r+2} = \cdots = a_n = m+1$$

is maximizing, as is its reversal, and there are no others. Thus, there is a unique maximizing configuration for $r = 0$ and $r = 2$, and exactly two maximizing configurations for each other value of r.

Although this fact must be known, we have seen no trace of it in the literature. The proof we have found is relatively straightforward but neither short nor particularly enlightening, so we will not give it here. We will nevertheless use the result to get a simple description of the right-hand boundary of the domain $\mathcal{D}_{q,F}$ of asymptotically allowed values for $((\log q_n)/n, F_n/n)$.

Corollary 10.2 *Let $n_j \to \infty$ and $F_j \to \infty$, with*

$$\frac{F_j}{n_j} \to p + \alpha, \quad \textit{with } p = 1, 2, \ldots \textit{ and } 0 \le \alpha < 1,$$

and let $H_{j,\max}$ denote the maximum of $\log(q_{n_j})$ over all configurations of length n_j with $a_1 + \cdots + a_{n_j} = F_j$. Then

$$\frac{H_{j,\max}}{n_j} \to (1-\alpha)\log\gamma_p + \alpha \log \gamma_{p+1},$$

where

$$\gamma_p := \frac{1}{2}\left(p + \sqrt{p^2+4}\right).$$

Proof. Let M_p denote the 2×2 matrix

$$M_p := \begin{pmatrix} p & 1 \\ 1 & 0 \end{pmatrix}.$$

Then, if q_j satisfies the recurrence

$$q_{j+1} = p\, q_j + q_{j-1} \quad \text{for } j = n, \ldots, n+m-1,$$

we get

$$\begin{pmatrix} q_{n+m} \\ q_{n+m-1} \end{pmatrix} = M_p^m \begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix}.$$

A simple computation shows that the eigenvalues of $M(p)$ are γ_p (as defined above) and $-\gamma_p^{-1}$. We let Φ_p and Ψ_p denote eigenvectors of M_p and its transpose respectively with eigenvalue γ_p; we can take these vectors to have strictly positive entries and to be normalized so that their scalar product is unity. (There is no particular difficulty in writing explicit formulas ...) Then

$$M_p^n = \gamma_p^n \Phi_p \otimes \Psi_p + \mathcal{O}(\gamma_p^{-n}) \quad \text{for } n \to \infty.$$

The case $\alpha = 0$ requires a slightly special argument, and we treat first the contrary case $\alpha > 0$. Then, if we define r_j by

$$F_j = pn_j + r_j, \tag{$*$}$$

we get $r_j \to \infty$ and $n_j - r_j \to \infty$. By Proposition 10.1, and denoting by e_0 the 2-vector (1,0),

$$\begin{aligned}
\exp(H_{j,\max}) &= q_n(p+1, \underbrace{p, \ldots p,}_{n_j - r_j} \underbrace{p+1, \ldots, p+1}_{r_j - 1}) \\
&= (e_0, M_{p+1}^{r_j-1} M_p^{n_j-r_j} M_{p+1} e_0) \\
&= \gamma_{p+1}^{r_j-1}\gamma_p^{n_j-r_j-1}(e_0, \Phi_{p+1})(\Psi_{p+1}, \Phi_p)(\Psi_p, M_{p+1}e_0) + o(1)
\end{aligned}$$

Since the coefficient $(e_0, \Phi_{p+1})(\Psi_{p+1}, \Phi_p)(\Psi_p, M_{p+1}e_0)$ is non-zero, it follows that

$$H_{j,\max} = r_j \log \gamma_{p+1} + (n_j - r_j) \log \gamma_p + \mathcal{O}(1),$$

so, since $r_j/n_j \to \alpha$,

$$\frac{1}{n_j} H_{j,\max} \to (1-\alpha) \log \gamma_p + \alpha \log \gamma_{p+1}$$

as asserted.

For $\alpha = 0$ we can still use $(*)$ to define r_j, but this time all we know is that $r_j/n_j \to 0$. By passing to subsequences, we can reduce to the cases

- $r_j \to \infty$, in which case the above argument works as it stands.
- $r_j \to -\infty$, in which case a straightforward modification of the above argument – replacing $p, p+1$ by $p-1, p$ – works.
- $r_j = r$ independent of j, in which case we write

$$\exp(H_{j,\max}) = (e_0, M_{p+1} M_p^{n_j - r} M_{p+1}^{r-1} e_0)$$

 and argue as before.

□

It follows easily from the preceding corollary that the intersection of $\mathcal{D}_{q,F}$ with the horizontal line $f = p + \alpha$ is the interval $(\epsilon_{\min}, (1-\alpha) \log \gamma_p + \alpha \log \gamma_{p+1})$ In other words:

Proposition 10.3 *The right-hand boundary of $\mathcal{D}_{q,F}$ is the polygonal arc consisting of the segments joining* $(\log \gamma_p, p)$ *to* $(\log \gamma_{p+1}, p+1)$*, for* $p = 1, 2, \ldots$.

References

Cornfeld, I. P., Fomin, S. V., and Sinai, Y. G. (1982). *Ergodic Theory.* Springer-Verlag, New York/Heidelberg/Berlin.

Dixon, J. D. (1970). The number of steps in the euclidean algorithm. *J. Number Theory*, **2**, 414–422.

Hardy, G. H. and Wright, E. M. (1960). *An Introduction to the Theory of Numbers.* Clarendon Press, Oxford, UK, fourth edition.

Kim, S. and Ostlund, S. (1989). Universal scaling in circle maps. *Physica D*, **39**, 365–392.

Knuth, D. E. (1981). *Seminumerical Algorithms*, volume 2 of *The Art of Computer Programming.* Addison-Wesley, Reading, MA, USA, second edition.

Lanford, O. E., III (1973). Entropy and equilibrium states in classical statistical mechanics. In A. Lenard, editor, *Statistical Mechanics and Mathematical Problems, Battelle Seattle 1971 Rencontres*, volume 20 of *Springer Lecture Notes in Physics*, pages 1–113, Berlin/Heidelberg/New York. Springer-Verlag.

Mayer, D. (1990). On the thermodynamic formalism for the Gauss map. *Comm. Math. Phys.*, **130**, 311–333.

Perron, O. (1954). *Die Lehre von den Kettenbrücken*, volume 1. B. G. Teubner, Stuttgart, third edition.

Roberts, J. (1977). *Elementary Number Theory: A Problem Oriented Approach.* The MIT Press, Cambridge, MA.

Ruedin, L. (1994). *Statistical Mechanical Methods and Continued Fractions.* Ph.D. thesis, Mathematics Department, ETH-Zürich.

Schrader, R. (1970). Ground states in classical lattice systems with hard core. *Comm. Math. Phys.*, **16**, 247–264.

Simon, B. (1993). *The Statistical Mechanics of Lattice Gases*, volume 1. Princeton University Press, Princeton, NJ, USA.