The Phase Transition of the Number-Theoretical Spin Chain

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Abstract

The number-theoretical spin chain has exactly one phase transition, which is located at inverse temperature $\beta_{\mathrm{cr}} = 2$. There the magnetization jumps from one to zero. The energy density, being zero in the low temperature phase, grows at least linearly in $\beta_{\mathrm{cr}} - \beta$.

1 Introduction

In [10] one of us showed that the quotient

$$Z(\beta) := \frac{\zeta(\beta - 1)}{\zeta(\beta)}$$

of Riemann zeta functions could be interpreted for $\beta > 2$ as the canonical partition function of an infinite ferromagnetic spin chain.

This partition function was shown to be the thermodynamic limit

$$Z(\beta) = \lim_{k \to \infty} Z_k(\beta)$$

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of k-spin partition functions $Z_k(\beta) := \sum_{\sigma\in\mathbf{G}_k} \exp(-\beta\mathbf{H}_k^C(\sigma))$, $\mathbf{G}_k := \{0,1\}^k$, where the energy function $\mathbf{H}_k^C : \mathbf{G}_k \to \mathbb{R}$ of the canonical ensemble is given by $\mathbf{H}_k^C = \ln(\mathbf{h}_k^C)$ with

$$\mathbf{h}_0^C := 1, \quad \mathbf{h}_{k+1}^C(\sigma,0) := \mathbf{h}_k^C(\sigma) \quad \text{and } \mathbf{h}_{k+1}^C(\sigma,1) := \mathbf{h}_k^C(\sigma) + \mathbf{h}_k^C(1-\sigma), \quad (1)$$

$1-\sigma \equiv (1-\sigma_1,\ldots,1-\sigma_k)$ being the inverted configuration of $\sigma \equiv (\sigma_1,\ldots,\sigma_k)$.

It was shown in [10] that the interaction coefficients $j_k^C : \mathbf{G}_k \to \mathbb{R}$ with

$$\mathbf{H}_k^C(\sigma) = -\sum_{t\in\mathbf{G}_k} j_k^C(t)\cdot(-1)^{\sigma\cdot t}$$

are asymptotically translation invariant and saturate in the length k of the chain. Moreover, the effective interaction between spins at positions r and l was shown to decay like $1/(r-l)^2$.

It turned out to be useful to introduce the grand canonical energy functions $\mathbf{H}_k^G : Gb_k \to \mathbb{R}$, $\mathbf{H}_k^G(\sigma) := \mathbf{H}_{k+1}^C(\sigma,1)$, partly because of their symmetries

$$\mathbf{H}_k^G(1-\sigma_1,\ldots,1-\sigma_k) = \mathbf{H}_k^G(\sigma_1,\ldots,\sigma_k) = \mathbf{H}_k^G(\sigma_k,\ldots,\sigma_1).$$

In [12] the existence of the thermodynamic limit $F(\beta) := \lim_{k\to\infty} F_k(\beta)$ of the free energy $F_k(\beta) := -(\beta\cdot k)^{-1}\ln(Z_k(\beta))$ was shown (due to the lack of strict translation invariance of the interaction standard estimates cannot be applied here).

In [11] thermodynamic expectations

$$\langle O\rangle_k(\beta) := \frac{\sum_{\sigma\in\mathbf{G}_k} O(\sigma)\exp(-\beta\mathbf{H}_k^C(\sigma))}{Z_k(\beta)}$$

of quantities like the internal energy $U_k := \left\langle \frac{1}{k}\mathbf{H}_k^C\right\rangle_k$ and magnetization $M_k := \left\langle \frac{1}{k}\sum_{l=1}^k(-1)^{\sigma_l}\right\rangle_k$ were analyzed. Due to the absolute convergence of the Dirichlet series $Z(\beta) = \sum_{n=1}^\infty \varphi(n)n^{-\beta}$ for $\mathrm{Re}(\beta) > 2$ the limits $U(\beta) := \lim_{k\to\infty} U_k(\beta)$ and $M(\beta) := \lim_{k\to\infty} M_k(\beta)$ can be easily shown to have the values $U(\beta) = 0$, $M(\beta) = 1$ in the frozen low temperature phase $\beta > 2$.

In the high temperature regime $\beta < 2$ the estimates

$$\frac{\ln 2 - \beta\ln(3/2)}{2-\beta} \le U(\beta) \le \ln(3/2) \quad (2)$$

were derived.

In [13] it was shown that the values $\mathbf{H}_k^C(\sigma)$ of the canonical energy function can be naturally interpreted in terms of geodesics coming from and going to the cusp in the modular domain.

These geodesics are naturally organized in families of 2^k members and labelled by $\sigma \in \mathbf{G}_k$. Then $\mathbf{H}_k^C(\sigma)$ is the length difference between the geodesic with index σ and the shortest such geodesic (which carries index 0).

This related the spin chain to the quantum scattering theory in the modular domain, since these length differences arise naturally in the WKB expansion of the scattering matrix.

Moreover, numerical evidence was presented that the Riemann zeta function can be well approximated *within its critical strip* by statistical-mechanical expectations. The reasons for this observation will be discussed in a forthcoming paper [14] by one of us.

The study of the number-theoretical spin chain is mainly motivated by the idea that probabilistic properties of statistical mechanics, and in particular ferromagnetism, could be helpful in deriving new results in number theory.

We have a somewhat opposite motivation for this paper. Namely, we want to use the above model for studying the phase transition of Thouless type.

It is known since a long time that spin chains with an effective $(r-l)^{-\alpha}$ interaction do not have a phase transition if $\alpha > 2$ and have one if $\alpha < 2$ (see, e.g., Dyson [6, 7]).

In [16] Thouless argued that for the borderline case $\alpha = 2$, magnetization should be discontinuous at the critical point. More recently, Aizenman, J. Chayes, L. Chayes and Newman studied the $\alpha = 2$ case with pair interaction, proving discontinuity of the magnetization and giving bounds for the critical temperature [1, 2].

Functions related to Z_k were treated earlier in the literature (but without the interpretation as coming from a spin chain).

In [17] Williams and Browne related the values of the function $\mathbf{h}_k^C$ to the radii of osculating circles and noticed the recursion relation $Z_{k+1}(-1) = 3Z_k(-1)$.

In [8] and [9] Feigenbaum, Procaccia and Tél analyzed functionals on multifractals defined by iterated functions, Using eigenvalue methods, they predicted an infinite order phase transition for a related system (the 'Farey model') describing intermittency.

In [4] and [5] Artuso, Cvitanović and Kenny stated that (in our notation) the values $Z_k^G(\beta)$ for $-\beta \in \mathbb{N}_0$ of the grand canonical partition function $Z_k^G(\beta) := \sum_{\sigma\in\mathbf{G}_k} \exp(-\mathbf{H}_k^G(\sigma))$ could be written as largest roots of certain polynomials of degree $\leq |\beta|+1$. The coefficients of these polynomials were given by the coefficients of a linear recursion relation between $Z_k^G(\beta)$ and $Z_l^G(\beta)$, $k+\beta-1 \leq l < k$.

Here we shall shortly present a different approach in which the above polynomials are obtained as characteristic polynomials of square matrices $\tilde{C}(\beta)$ of size $|\beta|+1$. This approach will allow us to analyze arbitrary real positive inverse temperatures β afterwards, a question which was posed in [5].

For $-\beta, k \in \mathbb{N}_0$ let

$$Y_k^\beta(m) := \sum_{\sigma\in\mathbf{G}_k} (\mathbf{h}_{k+1}^C(\sigma,1))^{-\beta-m}(\mathbf{h}_{k+1}^C(\sigma,0))^m, \qquad m \in \{0,\ldots,|\beta|\},$$

so that $Y_k^\beta(0) = Z_k^G(\beta)$. Then using the recursion relations $\mathbf{h}_{k+1}^C(\sigma,0) = \mathbf{h}_k^C(\sigma)$ and $\mathbf{h}_{k+1}^C(\sigma,1) = \mathbf{h}_k^C(\sigma) + \mathbf{h}_k^C(1-\sigma)$ for $\mathbf{h}_k^C$, we obtain

$$\begin{aligned}
Y_{k+1}^\beta(m) &= \sum_{\sigma\in\mathbf{G}_{k+1}} (\mathbf{h}_{k+1}^C(\sigma) + \mathbf{h}_{k+1}^C(1-\sigma))^{-\beta-m}(\mathbf{h}_{k+1}^C(\sigma))^m \\
&= \sum_{\mu\in\mathbf{G}_k} (\mathbf{h}_{k+1}^C(\mu,1) + \mathbf{h}_{k+1}^C(1-\mu,0))^{-\beta-m} \cdot \\
&\qquad \left[(\mathbf{h}_{k+1}^C(\mu,1))^m + (\mathbf{h}_{k+1}^C(1-\mu,0))^m\right] \\
&= \sum_{\rho\in\mathbf{G}_k} (\mathbf{h}_{k+1}^C(\rho,1) + \mathbf{h}_{k+1}^C(\rho,0))^{-\beta-m} \cdot \\
&\qquad \left[(\mathbf{h}_{k+1}^C(\rho,1))^m + (\mathbf{h}_{k+1}^C(\rho,0))^m\right],
\end{aligned}$$

since $\mathbf{h}_{k+1}^C(\mu,1) = \mathbf{h}_{k+1}^C(1-\mu,1)$. Thus

$$\begin{aligned}
Y_{k+1}^\beta(m) &= \sum_{r=0}^{|\beta|-m} \binom{|\beta|-m}{r} \sum_{\rho\in\mathbf{G}_k} (\mathbf{h}_{k+1}^C(\rho,1))^{-\beta-r}(\mathbf{h}_{k+1}^C(\rho,0))^r \\
&\quad + \sum_{r=m}^{|\beta|} \binom{|\beta|-m}{r-m} \sum_{\rho\in\mathbf{G}_k} (\mathbf{h}_{k+1}^C(\rho,1))^{-\beta-r}(\mathbf{h}_{k+1}^C(\rho,0))^r \\
&= \sum_{r=0}^{|\beta|-m} \binom{|\beta|-m}{r} Y_k^\beta(r) + \sum_{r=m}^{|\beta|} \binom{|\beta|-m}{r-m} Y_k^\beta(r).
\end{aligned}$$

So the vectors $Y_k^\beta \in \mathbb{R}^{|\beta|+1}$ meet the recursion relation

$$Y_{k+1}^\beta = \tilde{C}(\beta) Y_k^\beta \qquad \text{with } \tilde{C}(\beta)_{m,r} := \binom{|\beta|-m}{r} + \binom{|\beta|-m}{r-m}.$$

Being composed of two Pascal triangles, $\tilde{C}(\beta)$ is a matrix of Perron-Frobenius type, all the entries of $(\tilde{C}(\beta))^s$ being strictly positive for $s \geq 2$. The initial vector Y_0^β has the form $Y_0^\beta(m) = (\mathbf{h}_1^C(1))^{-\beta-m}(\mathbf{h}_1^C(0))^m = 2^{-\beta-m} > 0$. Therefore $\lim_{k\to\infty} Y_k^\beta/\|Y_k^\beta\|$ converges to the normalized right eigenvector of $\tilde{C}(\beta)$ with the eigenvalue $\lambda(\beta)$ of largest modulus, and

$$\lim_{k\to\infty} \frac{Z_{k+1}^G(\beta)}{Z_k^G(\beta)} = \lambda(\beta).$$

Example. For $\beta = -2$,

$$\tilde{C}(\beta) = \begin{pmatrix} 2 & 4 & 2 \\ 1 & 2 & 1 \\ 1 & 0 & 1 \end{pmatrix} \qquad \text{and } \lambda(\beta) = \frac{5+\sqrt{17}}{2}.$$

It is remarkable that the asymptotic of the partition function leads to finite expressions for negative integer arguments.

It is known that the values of zeta functions for integer arguments are related to questions in analysis, topology and number theory. Here the free energy is derived from finite approximants of the zeta function Z, so that the finiteness of the expressions for negative integer arguments should not come as a surprise. But it would be interesting to find a statistical mechanics interpretation for the corresponding property of the analytically continued Riemann zeta function.

2 The Perron-Frobenius operator

We will now make a similar construction in the case of arbitrary non-negative inverse temperatures $\beta \in \mathbb{R}_0^+$. Thus we set for $k \in \mathbb{N}_0$

$$Y_k^\beta(m) := \sum_{\sigma\in\mathbf{G}_k} (\mathbf{h}_{k+1}^C(\sigma,1))^{-\beta-m}(\mathbf{h}_{k+1}^C(\sigma,0))^m, \qquad m \in \mathbb{N}_0. \tag{3}$$

So $Y_k^\beta(m) = \sum_{\sigma\in\mathbf{G}_k} \exp(-(\beta+m)\mathbf{H}_k^G(\sigma)+m\mathbf{H}_k^C(\sigma))$ and in particular $Y_k^\beta(0) = Z_k^G(\beta)$.

Lemma 1 *For $\beta \geq 0$ the vector $Y_{k+1}^{\beta} = \tilde{C}(\beta) Y_k^{\beta}$ with*

$$\tilde{C}(\beta)_{m,r} := \frac{2^{-\beta-m}}{r!} \frac{d^r}{dx^r} \left. \frac{1+(1-x)^m}{(1-x/2)^{m+\beta}} \right|_{x=0}, \quad (m, r \in \mathbb{N}_0). \tag{4}$$

Proof. We derive the recursion by decomposing $Y_{k+1}^{\beta} = A + B$ with

$$A(m) := \sum_{\mu \in \mathbf{G}_k} (\mathbf{h}_{k+1}^C(\mu, 1) + \mathbf{h}_{k+1}^C(1-\mu, 0))^{-\beta-m} (\mathbf{h}_{k+1}^C(\mu, 1))^m$$

and

$$B(m) := \sum_{\mu \in \mathbf{G}_k} (\mathbf{h}_{k+1}^C(\mu, 1) + \mathbf{h}_{k+1}^C(1-\mu, 0))^{-\beta-m} (\mathbf{h}_{k+1}^C(1-\mu, 0))^m.$$

Now $\mathbf{h}_{k+1}^C(1-\mu, 0) = \mathbf{h}_{k+1}^C(\mu, 1) - \mathbf{h}_{k+1}^C(\mu, 0)$ so that

$$\begin{aligned}
A(m) &= \sum_{\mu \in \mathbf{G}_k} (2\mathbf{h}_{k+1}^C(\mu, 1) - \mathbf{h}_{k+1}^C(\mu, 0))^{-\beta-m} (\mathbf{h}_{k+1}^C(\mu, 1))^m \\
&= \sum_{r=0}^{\infty} 2^{-\beta-m-r} \binom{-\beta-m}{r} (-1)^r \sum_{\mu \in \mathbf{G}_k} (\mathbf{h}_{k+1}^C(\mu, 1))^{-\beta-r} (\mathbf{h}_{k+1}^C(\mu, 0))^r \\
&= \sum_{r=0}^{\infty} 2^{-\beta-m-r} \binom{-\beta-m}{r} (-1)^r Y_k^{\beta}(r)
\end{aligned}$$

with generalized binomial coefficients $\binom{a}{b} = (\prod_{i=0}^{b-1}(a-i))/b!$, $a \in \mathbb{R}$, $b \in \mathbb{N}_0$.

The above series expansion converges since $\mathbf{h}_{k+1}^C(\mu, 0) < \mathbf{h}_{k+1}^C(\mu, 1)$. Furthermore $(-1)^r \binom{-\beta-m}{r} \geq 0$ since $\beta + m \geq 0$.

The treatment of the vector B is slightly different.

$$\begin{aligned}
B(m) &= \sum_{\mu \in \mathbf{G}_k} (2\mathbf{h}_{k+1}^C(\mu, 1) - \mathbf{h}_{k+1}^C(\mu, 0))^{-\beta-m} (\mathbf{h}_{k+1}^C(\mu, 1) - \mathbf{h}_{k+1}^C(\mu, 0))^m \\
&= \sum_{r=0}^{\infty} 2^{-\beta-m-r} \binom{-\beta-m}{r} (-1)^r \sum_{\mu \in \mathbf{G}_k} (\mathbf{h}_{k+1}^C(\mu, 1))^{-\beta-m-r} (\mathbf{h}_{k+1}^C(\mu, 0))^r \cdot \\
&\quad \sum_{s=0}^{m} (-1)^s \binom{m}{s} (\mathbf{h}_{k+1}^C(\mu, 1))^{m-s} (\mathbf{h}_{k+1}^C(\mu, 0))^s \\
&= \sum_{r=0}^{\infty} \sum_{s=0}^{m} 2^{-\beta-m-r} (-1)^{r+s} \binom{-\beta-m}{r} \binom{m}{s} Y_k^{\beta}(r+s) \\
&= \sum_{r=0}^{\infty} (-1)^r \sum_{s=0}^{m} 2^{-\beta-m-r+s} \binom{-\beta-m}{r-s} \binom{m}{s} Y_k^{\beta}(r).
\end{aligned}$$

Now

$$\frac{1}{r!}\frac{d^r}{dx^r}\left.\frac{1}{(1-x/2)^{m+\beta}}\right|_{x=0} = (-1)^r 2^{-r}\binom{-\beta-m}{r}$$

and

$$\begin{aligned}
&\frac{1}{r!}\frac{d^r}{dx^r}\left.\frac{(1-x)^m}{(1-x/2)^{m+\beta}}\right|_{x=0} \\
&= \frac{(-1)^r}{r!}\sum_{s=0}^{m}\binom{r}{s}2^{s-r}\prod_{i=0}^{r-s-1}(-\beta-m-i)\prod_{j=0}^{s-1}(m-j) \\
&= (-1)^r\sum_{s=0}^{m}2^{s-r}\binom{-\beta-m}{r-s}\binom{m}{s}
\end{aligned}$$

so that the formula for $\tilde{C}(\beta)$ is proven. □

Lemma 2 *For $\beta > 0$ and $m, r \in \mathbb{N}_0$ the entry $\tilde{C}(\beta)_{m,r} > 0$.*

Proof. We first consider the case $\beta = 0$. For $|x| < 2$ the Taylor series of $(1-x/2)^{-m}$ converges, and

$$\frac{1+(1-x)^m}{(1-x/2)^m} = \left(1+\sum_{k=1}^{\infty}(x/2)^k\right)^m + \left(1-\sum_{k=1}^{\infty}(x/2)^k\right)^m$$

is a convergent power series with non-negative coefficients, the zeroth coefficient being 2.

Moreover for $\beta > 0$ the Taylor expansion of the multiplicative factor $(1-x/2)^{-\beta}$ in (4) has strictly positive coefficients. Thus the product $(1+(1-x)^m)/(1-x/2)^{m+\beta}$, too has strictly positive Taylor coefficients, proving the lemma. □

We want to estimate the k-dependence of Y_k^β, using the recursion $Y_{k+1}^\beta = \tilde{C}(\beta)Y_k^\beta$ and starting with

$$Y_0^\beta(m) = 2^{-\beta-m}, \qquad (m \in \mathbb{N}_0). \tag{5}$$

Since $Y_0^\beta \in l^2(\mathbb{N}_0)$ for all $\beta > 0$, it is natural to consider $\tilde{C}(\beta)$ as an operator on $l^2(\mathbb{N}_0)$.

We will show that $\tilde{C}(\beta)$ is conjugate to a positive operator $C(\beta)$ by using the following representation

Lemma 3 *For $\beta > 0$ and $m, r \in \mathbb{N}_0$*

$$\tilde{C}(\beta)_{m,r} = 2^{-\beta-m-r} \sum_{l=0}^{\min(m,r)} (1+(-1)^l) \binom{m}{l} \binom{r+\beta-1}{r-l}$$

Proof. For $|x| < 2$

$$\begin{aligned} \frac{1+(1-x)^m}{(1-x/2)^m} &= \left(1+\frac{x/2}{1-x/2}\right)^m + \left(1-\frac{x/2}{1-x/2}\right)^m \\ &= \sum_{l=0}^{m} (1+(-1)^l) \left(\frac{x/2}{1-x/2}\right)^l \binom{m}{l}. \end{aligned} \tag{6}$$

Using

$$\left.\frac{d^a}{dx^a}(1-x/2)^{-\beta}\right|_{x=0} = 2^{-a} a! \binom{\beta+a-1}{a}$$

and

$$\left.\frac{d^b}{dx^b}\left(\frac{x/2}{1-x/2}\right)^l\right|_{x=0} = 2^{-b} b! \binom{b-1}{l-1}$$

for $a \in \mathbb{N}_0$, $b, l \in \mathbb{N}$, we have for $r \geq l$

$$\begin{aligned} &\left.\frac{d^r}{dx^r}(1-x/2)^{-\beta}\left(\frac{x/2}{1-x/2}\right)^l\right|_{x=0} \\ &= 2^{-r} r! \sum_{s=l}^{r} \binom{s-1}{l-1} \binom{\beta+r-s-1}{r-s} \\ &= 2^{-r} r! \binom{\beta+r-1}{r-l}. \end{aligned} \tag{7}$$

This formula holds true for $l = 0$, too. Thus inserting (7) in the representation of $\tilde{C}(\beta)$ of Lemma 1, we obtain with (6)

$$\tilde{C}(\beta)_{m,r} = 2^{-\beta-m-r} \sum_{l=0}^{m} (1+(-1)^l) \binom{m}{l} \binom{r+\beta-1}{r-l}.$$

Clearly we need only sum up to $l = \min(m, r)$ since for $l > r$ eq. (7) $= 0$. □

In order to develop some understanding of $\tilde{C}(\beta)$, consider the special case $\beta = 1$. Then $\tilde{C}(\beta)$ is symmetric:

$$\begin{aligned}\tilde{C}(1)_{m,r} &= 2^{-1-m-r}\sum_{l=0}^{\min(m,r)}(1+(-1)^l)\binom{m}{l}\binom{r}{l}\\ &= 2^{-1-m-r}\left[\binom{m+r}{r}+\sum_{l=0}^{\min(m,r)}(-1)^l\binom{m}{l}\binom{r}{l}\right]\end{aligned}$$

and large only near the diagonal.

For general $\beta > 0$ define the diagonal operator $g(\beta)$ by

$$g(\beta)_{i,k} := \delta_{i,k}\Big/\sqrt{\binom{\beta+k-1}{k}}, \qquad (i,k\in\mathbb{N}_0)\ .$$

Lemma 4 *For* $\beta > 0$

$$\tilde{C}(\beta) = g(\beta)C(\beta)g(\beta)^{-1} \qquad \textit{with } C(\beta) := D(\beta)^T D(\beta)$$

where for $k, r \in \mathbb{N}_0$

$$D(\beta)_{k,r} := 2^{-\frac{1}{2}(\beta+1)-r}\cdot\sqrt{\frac{\binom{\beta+r-1}{r}}{\binom{\beta+k-1}{k}}}(1+(-1)^k)\binom{r}{k}.$$

Proof.

$$\begin{aligned}C_{m,r} = (D^T D)_{m,r} &= 2^{-\beta-m-r}\sqrt{\binom{\beta+r-1}{r}\binom{\beta+m-1}{m}}\cdot\\ &\quad\sum_{l=0}^{\min(m,r)}(1+(-1)^l)\frac{\binom{m}{l}\binom{r}{l}}{\binom{\beta+l-1}{l}}.\end{aligned} \tag{8}$$

On the other hand

$$\begin{aligned}(g^{-1}\tilde{C}g)_{m,r} &= \tilde{C}_{m,r}\sqrt{\frac{\binom{\beta+m-1}{m}}{\binom{\beta+r-1}{r}}}\\ &= 2^{-\beta-m-r}\sqrt{\binom{\beta+r-1}{r}\binom{\beta+m-1}{m}}\sum_{l=0}^{\min(m,r)}(1+(-1)^l)\frac{\binom{m}{l}\binom{\beta+r-1}{r-l}}{\binom{\beta+r-1}{r}}\end{aligned}$$

which equals (8) since

$$\frac{\binom{\beta+r-1}{r-l}}{\binom{\beta+r-1}{r}} = \frac{\binom{r}{l}}{\binom{\beta+l-1}{l}}. \tag{9}$$

□

Lemma 5 *For $\beta > 0$ $C(\beta)$ is a bounded positive operator on $l_2(\mathbb{N}_0)$, and the part $\sigma(C(\beta)) \cap (1, \infty)$ of the spectrum is purely discrete.*

Proof. First we show that the operator norms $\|\tilde{C}(\beta)\|_1 < \infty$ and $\|\tilde{C}(\beta)^T\|_1 < \infty$, if one considers $\tilde{C}(\beta)$ as an operator on the Banach space $l_1(\mathbb{N}_0)$. Since the entries of $\tilde{C}(\beta)$ are positive (Lemma 2), we can do this by estimating the column sums of $\tilde{C}(\beta)$ resp. of $\tilde{C}(\beta)^T$.

For $r \in \mathbb{N}_0$ by Taylor's formula and analyticity of $x \mapsto (1+(1-x)^m)/(1-x/2)^{m+\beta}$ for $|x| < 2$

$$\begin{aligned}\sum_{m=0}^{\infty} \tilde{C}(\beta)_{m,r} &= \frac{1}{r!}\frac{d^r}{dx^r}(2-x)^{-\beta}\sum_{m=0}^{\infty}\left[\left(\frac{1}{2-x}\right)^m + \left(\frac{1-x}{2-x}\right)^m\right]\Bigg|_{x=0} \\ &= \frac{1}{r!}\frac{d^r}{dx^r}\left.\frac{(2-x)^{2-\beta}}{1-x}\right|_{x=0} \\ &= \sum_{l=0}^{r}(-1)^l\binom{2-\beta}{l}2^{2-\beta-l}. \end{aligned} \tag{10}$$

As

$$\begin{aligned} 2^{2-\beta}\sum_{l=0}^{\infty}(-1)^l\binom{2-\beta}{l}2^{-l} &= 2^{2-\beta}\sum_{l=0}^{\infty}\frac{1}{l!}\frac{d^l}{dx^l}\left.(1-x/2)^{2-\beta}\right|_{x=0} \\ &= 2^{2-\beta}\left.(1-x/2)^{2-\beta}\right|_{x=1} = 1, \end{aligned}$$

the sum of the rth column converges to one as $r \to \infty$, so that $\|\tilde{C}(\beta)\|_1 < \infty$. More precisely, one sees from (10) that

$$\|\tilde{C}(\beta)\|_1 = \sup_{r \in \mathbb{N}_0}\sum_{m=0}^{\infty}\tilde{C}(\beta)_{m,r} = \max(2^{2-\beta}, 1).$$

Similarly for $m \in \mathbb{N}_0$

$$\sum_{r=0}^{\infty} \tilde{C}(\beta)_{m,r} = 2^{-\beta-m} \sum_{r=0}^{\infty} \frac{1}{r!} \frac{d^r}{dx^r} \left. \frac{1+(1-x)^m}{(1-x/2)^{m+\beta}} \right|_{x=0}$$
$$= 2^{-\beta-m} \left. \frac{1+(1-x)^m}{(1-x/2)^{m+\beta}} \right|_{x=1} = 1 + \delta_{m,0}, \qquad (11)$$

So $\|\tilde{C}(\beta)^T\|_1 = 2$.

Using these estimates we can bound $C(\beta)$:

$$\tilde{C}_{m,r} = C_{m,r} \cdot x_{m,r} \quad \text{and} \quad (\tilde{C}^T)_{m,r} = C_{m,r}/x_{m,r}$$

with $x_{m,r} := g_{m,m}/g_{r,r}$. So

$$C_{m,r} \cdot (x_{m,r} + 1/x_{m,r}) = \tilde{C}_{m,r} + (\tilde{C}^T)_{m,r}.$$

But $(x + 1/x)/2 \geq 1$ for $x > 0$ so that

$$\|C(\beta)\|_1 \leq \tfrac{1}{2}(\|\tilde{C}(\beta)\|_1 + \|\tilde{C}(\beta)^T\|_1) \qquad (\beta > 0).$$

We can also interpret $\tilde{C}(\beta)$, $\tilde{C}(\beta)^T$ and $C(\beta)$ as operators acting on the dual space $l_\infty(\mathbb{N}_0) = l_1(\mathbb{N}_0)^*$. Then the matrix transpose $\tilde{C}(\beta)^T$ on $l_\infty(\mathbb{N}_0)$ is the Banach space adjoint of $\tilde{C}(\beta)$ on $l_1(\mathbb{N}_0)$, and similarly for $\tilde{C}(\beta)$ and $C(\beta)$. Thus $\|\tilde{C}(\beta)\|_\infty = \|\tilde{C}(\beta)^T\|_1$, $\|\tilde{C}(\beta)^T\|_\infty = \|\tilde{C}(\beta)\|_1$ and $\|C(\beta)\|_\infty = \|C(\beta)\|_1$.

Now for $1 \leq p \leq q \leq \infty$ we have the inclusion $l_p(\mathbb{N}_0) \subset l_q(\mathbb{N}_0)$. Therefore, using the Riesz-Thorin interpolation theorem (Thm. IX.17 of Reed and Simon [15], Vol. II), we conclude that $\tilde{C}(\beta)$, $\tilde{C}(\beta)^T$ and $C(\beta)$ have also finite norms as operators on $l_p(\mathbb{N}_0)$, $1 \leq p \leq \infty$, and in particular on the Hilbert space $l_2(\mathbb{N}_0)$ of sequences.

¿From the definition of $C(\beta)$ in Lemma 4 we see that it is a positive operator.

By the estimates (10) and (11) for $\beta > 0$ and $\varepsilon > 0$ there exist an $m_0 \in \mathbb{N}$ such that for $m \geq m_0$

$$\sum_{r=m_0}^{\infty} \tilde{C}(\beta)_{m,r} < 1 + \varepsilon \quad \text{and} \quad \sum_{r=m_0}^{\infty} \tilde{C}(\beta)_{r,m} < 1 + \varepsilon.$$

Thus defining for $n \in \mathbb{N}_0$ the projector P_n by

$$(P_n v)_r := \begin{cases} v_r & r \geq n \\ 0 & 0 \leq r < n \end{cases} ,$$

we get

$$\|P_{m_0} \tilde{C}(\beta) P_{m_0}\|_1 < 1 + \varepsilon \quad \text{and} \quad \|P_{m_0} \tilde{C}(\beta)^T P_{m_0}\|_1 < 1 + \varepsilon$$

which implies $\|P_{m_0} \tilde{C}(\beta)^T P_{m_0}\|_2 < 1 + \varepsilon$, using Riesz-Thorin interpolation.

The range of P_{m_0} has codimension m_0. But that implies that the spectral projection of $C(\beta)$ on the interval $(1+\varepsilon, \infty)$ is at most m_0-dimensional, because otherwise that subspace would have non-empty intersection with the range of P_{m_0}. So $\sigma(C(\beta)) \cap (1, \infty)$ is purely discrete. □

Remark. One can show that there is at most one eigenvalue of $C(\beta)$ which is strictly larger than one, using eq. (11). This is of interest when one discusses the convergence speed of the free energy $F_k(\beta)$ in the thermodynamic limit $k \to \infty$.

Lemma 6 *For $0 < \beta < 2$ the operator $C(\beta)$ on $l_2(\mathbb{N}_0)$ has a largest eigenvalue $\lambda(\beta) > 1$, and*

$$\lambda(\beta) \geq 1 + c \frac{2 - \beta}{Z(4 - \beta)} \qquad \text{for } 1 \leq \beta < 2,$$

with $c := (1 - \ln(2)) \cdot \exp(-\pi^2/48) \approx 0.2498$.

Proof. For arbitrary $\beta > 0$ let $\hat{v}(\beta) : \mathbb{N}_0 \to \mathbb{R}^+$ be given by

$$\hat{v}(\beta)_r := \frac{\sqrt{\binom{\beta+r-1}{r}}}{r+1}.$$

For $\beta = 2$ we have $\hat{v}(\beta)_r = 1/\sqrt{r+1}$, whereas for $0 < \beta < 2$ the vector $\hat{v}(\beta) \in l_2(\mathbb{N}_0)$. This follows from

$$\binom{\beta + r - 1}{r} = \prod_{i=0}^{r-1} \left(1 + \frac{\beta - 1}{r - i}\right) = \exp\left(\sum_{l=1}^{r} \ln(1 + \frac{\beta - 1}{l})\right). \qquad (12)$$

In particular $\binom{\beta+r-1}{r}$ is monotone increasing in $\beta > 0$. We estimate (12) from below and above.

So for $0 < \beta < 2$ and $r \in \mathbb{N}$, using the inequality $\ln(1+x) \leq x$, $x > -1$,

$$\sum_{l=1}^{r} \ln(1 + \frac{\beta - 1}{l}) \leq (\beta - 1)\ln(r+1) + C_E$$

with Euler's constant $C_E \approx 0.5772$. This implies

$$\binom{\beta + r - 1}{r} \leq e^{C_E} \cdot (r+1)^{\beta-1}, \qquad (r \in \mathbb{N}_0), \tag{13}$$

so that for $0 < \beta < 2$ the vectors $\hat{v}(\beta) \in l_2(\mathbb{N}_0)$.

For more precise estimates we specialize to the interval $1 \leq \beta < 2$.

The function $f_r(\beta) := \sum_{l=1}^{r} \ln(1 + (\beta-1)/l)$ is concave so that

$$f_r(\beta) \geq (\beta - 1)f_r(2) + (2 - \beta)f_r(1) = (\beta - 1)\ln(r+1).$$

On the other hand

$$0 \leq -f_r''(\beta) = \sum_{l=1}^{r}(l + \beta - 1)^{-2} \leq \sum_{l=1}^{r} l^{-2} < \sum_{l=1}^{\infty} l^{-2} = \pi^2/6.$$

This estimate can be used to improve the upper bound (13). Namely, we have for $1 \leq \beta < 2$

$$f_r(\beta) \leq p_r(\beta) := (\beta - 1)f_r(2) + (2 - \beta)f_r(1) + \frac{\pi^2}{12}(\beta - 1)\cdot(2 - \beta),$$

since $f_r(1) = p_r(1)$, $f_r(2) = p_r(2)$, and $f_r''(\beta) \geq p_r''(\beta) = -\pi^2/6$. Thus $f_r(\beta) \leq (\beta-1)\ln(r+1) + \pi^2/48$, since $(\beta - 1)\cdot(2-\beta) \leq 1/4$, and including the case $r = 0$

$$(r+1)^{\beta-1} \leq \binom{\beta + r - 1}{r} \leq \exp(\pi^2/48)\cdot(r+1)^{\beta-1}, \qquad (r \in \mathbb{N}_0). \tag{14}$$

The choice of the vectors $\hat{v}(\beta)$ is motivated by the fact that $\hat{v}(2)$ is an l_∞-eigenvector of $C(2)$.

We will derive the inequality

$$\hat{\lambda}(\beta) := \frac{(\hat{v}(\beta), C(\beta)\hat{v}(\beta))}{(\hat{v}(\beta), \hat{v}(\beta))} > 1, \qquad (\beta < 2) \tag{15}$$

for the expectation which then, together with Lemma 5, implies the existence of a largest eigenvalue $\lambda(\beta) \geq \hat{\lambda}(\beta) > 1$ of $C(\beta)$.

By Lemma 4 $C(\beta)\hat{v}(\beta) = D(\beta)^T D(\beta)\hat{v}(\beta)$.

$$\begin{aligned}
\sum_{r=0}^{\infty} D_{k,r}\hat{v}_r &= \frac{2^{-\frac{1}{2}(\beta+1)}}{\sqrt{\binom{\beta+k-1}{k}}}(1+(-1)^k)\sum_{r=0}^{\infty}\frac{2^{-r}}{r+1}\binom{r}{k}\binom{\beta+r-1}{r} \\
&= \frac{2^{-\frac{1}{2}(\beta+1)}}{\sqrt{\binom{\beta+k-1}{k}}}(1+(-1)^k)\binom{\beta+k-1}{k}\sum_{r=k}^{\infty}\frac{2^{-r}}{r+1}\binom{\beta+r-1}{r-k}
\end{aligned}$$

since the (9) holds.

On the other hand for $|x| < 1$

$$\sum_{r=k}^{\infty} x^r \binom{\beta+r-1}{r-k} = \frac{x^k}{(1-x)^{k+\beta}}$$

and $2^{-r}/(r+1) = 2\int_0^{1/2} x^r dr$ so that

$$\sum_{r=0}^{\infty} D_{k,r}\hat{v}_r = 2^{-\frac{1}{2}(\beta-1)}(1+(-1)^k)\sqrt{\binom{\beta+k-1}{k}}\int_0^{1/2}\frac{x^k}{(1-x)^{k+\beta}}dx.$$

$$\begin{aligned}
(C\hat{v})_l &= \sum_{k,r=0}^{\infty} D_{k,l}D_{k,r}\hat{v}_r \\
&= 2^{-\frac{1}{2}(\beta+1)-l}\sqrt{\binom{\beta+l-1}{l}}\,2^{-\frac{1}{2}(\beta-1)} \\
&\qquad \cdot\sum_{k=0}^{l} 2(1+(-1)^k)\binom{l}{k}\int_0^{1/2}\frac{x^k}{(1-x)^{k+\beta}}dx \\
&= 2^{-\beta-l+1}\sqrt{\binom{\beta+l-1}{l}}\int_0^{1/2}(1-x)^{-\beta}\left[\left(\frac{1}{1-x}\right)^l + \left(2-\frac{1}{1-x}\right)^l\right]dx \\
&= \sqrt{\binom{\beta+l-1}{l}}\int_{1/2}^{1} z^{\beta-2}\left[z^l + (1-z)^l\right]dz \qquad (16)
\end{aligned}$$

with $z := 1/(2(1-x))$.

Thus for $\beta = 2$

$$(C\hat{v})_l = \sqrt{\binom{l+1}{l}} \int_{1/2}^{1} \left[z^l + (1-z)^l \right] dz = \frac{1}{\sqrt{l+1}} = \hat{v}_l.$$

For $0 < \beta < 2$ we write $(C(\beta)\hat{v}(\beta))_l = \hat{v}(\beta)_l(1 + I(\beta, l))$ with

$$I(\beta, l) := (l+1) \int_{1/2}^{1} \left(z^{\beta-2} - 1 \right) \left[z^l + (1-z)^l \right] dz.$$

But for these values of β and z we can estimate $z^{\beta-2} - 1 = \exp((\beta-2)\ln(z)) - 1 \geq (\beta - 2)\ln(z)$ so that

$$I(\beta, l) \geq (\beta - 2) \cdot (l+1) \int_{1/2}^{1} \ln(z) \left[z^l + (1-z)^l \right] dz. \tag{17}$$

So $I(\beta, 0) \geq (2 - \beta) \cdot (1 - \ln(2))$ and for $l \geq 1$

$$\begin{aligned} I(\beta, l) &\geq (\beta - 2) \cdot (l+1) \int_{1/2}^{1} \ln(z) z^l dz \\ &= (2 - \beta) \left(\frac{1 - 2^{-(l+1)}}{l+1} - 2^{-(l+1)} \ln(2) \right) \geq \frac{2 - \beta}{l+1} \cdot (1 - \ln(2)). \end{aligned}$$

Using (14) we get for $1 \leq \beta < 2$ the estimates $(\hat{v}, \hat{v}) \leq \exp(\pi^2/48) \cdot \zeta(3 - \beta)$ and

$$(\hat{v}, C\hat{v}) \geq (\hat{v}, \hat{v}) + (1 - \ln(2)) \cdot (2 - \beta)\zeta(4 - \beta).$$

So

$$\frac{(\hat{v}(\beta), C(\beta)\hat{v}(\beta))}{(\hat{v}(\beta), \hat{v}(\beta))} \geq 1 + c\frac{2 - \beta}{Z(4 - \beta)},$$

with $c := (1 - \ln(2)) \exp(-\pi^2/48)$.

So $\lambda(\beta) \geq \hat{\lambda}(\beta) \geq 1 + c(2 - \beta)/Z(4 - \beta)$ for $1 \leq \beta < 2$. Moreover, the strict positivity of (17) implies that $\hat{\lambda}(\beta) > 1$ for $0 < \beta < 2$. □

Now we can apply the Perron-Frobenius and Kato-Rellich theorems.

Lemma 7 *For $0 < \beta < 2$ the largest eigenvalue λ and the corresponding positive eigenvector v, $\|v\|_2 = 1$, of C are analytic functions of β.*

Proof. For $\beta > 0$ the operator $C(\beta)$ on $l_2(\mathbb{N}_0)$ is bounded, positive, and *positivity improving*, that is, for $w \in l_2(\mathbb{N}_0) \setminus \{0\}$ with entries $w_k \geq 0$ one has $(C(\beta)w)_k > 0$ for all $k \in \mathbb{N}_0$. This follows since by Lemma 2 the entries $\tilde{C}(\beta)_{m,r} > 0$ and thus by Lemma 4 the entries $C(\beta)_{m,r} > 0$, too.

Moreover, for $0 < \beta < 2$ its operator norm $\|C(\beta)\|_2$ on $l_2(\mathbb{N}_0)$ is an eigenvalue, since $C(\beta)$ is positive so that $\|C(\beta)\|_2 = \sup \sigma(C(\beta))$, and since by Lemma 6 $\sup \sigma(C(\beta)) = \lambda(\beta)$ is an eigenvalue.

Thus by the Perron-Frobenius Theorem XIII.43 of [15], Vol. IV $\lambda(\beta)$ is a simple eigenvalue with strictly positive eigenvector $v(\beta)$.

Moreover, the map $\mathbb{R}^+ \to B(l_2(\mathbb{N}_0))$, $\beta \mapsto C(\beta)$ is an analytic family in the sense of Kato. Therefore, by the Kato-Rellich Theorem (Thm. XII.8 of [15], Vol. IV) for $0 < \beta < 2$ the eigenvalue λ is an analytic function of β, and the positive normalized eigenvector v is analytic in β, too. □

Lemma 8 *For $0 < \beta < 2$ the free energy F is given by*

$$\beta F(\beta) = -\ln(\lambda(\beta)).$$

Proof. First we show that for these inverse temperatures the limit

$$\lim_{k\to\infty} Z^G_{k+1}(\beta)/Z^G_k(\beta)$$

of quotients of grand canonical partition functions exists and equals $\lambda(\beta)$.

¿From Definition (3) of the vector Y^β_k we see that its zeroth component

$$Y^\beta_k(0) = \sum_{\sigma\in\mathbf{G}_k} (\mathbf{h}^C_{k+1}(\sigma,1))^{-\beta} = \sum_{\sigma\in\mathbf{G}_k} \exp(-\beta\mathbf{H}^G_k(\sigma)) = Z^G_k(\beta). \tag{18}$$

Now by (5) $Y^\beta_k = \tilde{C}(\beta)^k Y^\beta_0$ with $Y^\beta_0(m) = 2^{-\beta-m}$, $(m \in \mathbb{N}_0)$. Lemma 4 allows us to write $\tilde{C}(\beta) = g(\beta)C(\beta)g(\beta)^{-1}$ so that

$$Y^\beta_k = g(\beta)C(\beta)^k\hat{Y}^\beta_0 \qquad \text{with } \hat{Y}^\beta_0 := g(\beta)^{-1}Y^\beta_0. \tag{19}$$

$\hat{Y}^\beta_0 \in l_2(\mathbb{N}_0)$ since $\hat{Y}^\beta_0(m) = \sqrt{\binom{\beta+m-1}{m}}2^{-\beta-m}$. We have the norm limit

$$\lim_{k\to\infty} \lambda(\beta)^{-k}C(\beta)^k\hat{Y}^\beta_0 = \Pi(\beta)\hat{Y}^\beta_0 \tag{20}$$

with the orthogonal projector $\Pi(\beta)$ on $\mathrm{span}(v(\beta))$.

We prove (20) by decomposing

$$\lambda(\beta)^{-k}C(\beta)^k\hat{Y}_0^\beta = \lambda(\beta)^{-k}C(\beta)^k(\mathbb{1}-\Pi(\beta))\hat{Y}_0^\beta + \Pi(\beta)\hat{Y}_0^\beta.$$

Then $\mathbb{1}-\Pi(\beta)$ is an orthogonal projector commuting with $C(\beta)$. So $C(\beta)\cdot(\mathbb{1}-\Pi(\beta))$ is self-adjoint, and

$$\|C(\beta)^k(\mathbb{1}-\Pi(\beta))\|_{B(l_2(\mathbb{N}_0))} = \|C(\beta)(\mathbb{1}-\Pi(\beta))\|^k_{B(l_2(\mathbb{N}_0))} = \mu(\beta)^k,$$

where $\mu(\beta) < \lambda(\beta)$ is the supremum of $\sigma(C(\beta)) \setminus \{\lambda(\beta)\}$. So

$$\|\lambda(\beta)^{-k}C(\beta)^k(\mathbb{1}-\Pi(\beta))\hat{Y}_0^\beta\|_{l_2(\mathbb{N}_0)} \le \left(\frac{\mu(\beta)}{\lambda(\beta)}\right)^k \|\hat{Y}_0^\beta\|_{l_2(\mathbb{N}_0)}$$

converges to zero as $k \to \infty$. On the other hand, $\Pi(\beta)\hat{Y}_0^\beta > 0$ since $v(\beta)$ and $\hat{Y}_0^\beta$ have strictly positive entries.

By (18) and (19) we have $Z_k^G(\beta) = (C(\beta)^k\hat{Y}_0^\beta)_0$, using that $g(\beta)_{0,k} = \delta_{0,k}$ independent of the temperature. So by (20) we obtain

$$\lim_{k\to\infty} \frac{Z_{k+1}^G(\beta)}{Z_k^G(\beta)} = \lambda(\beta). \tag{21}$$

The free energy $F(\beta) = \lim_{k\to\infty} F_k(\beta)$ is defined in terms of the canonical partition function $Z_k(\beta)$: $\beta F_k(\beta) = -\frac{1}{k}\ln(Z_k(\beta))$.

In turn, $Z_k(\beta)$ is related to the grand canonical partition functions $Z_l^G(\beta)$ via

$$Z_k(\beta) = 1 + \sum_{l=0}^{k-1} Z_l^G(\beta), \tag{22}$$

since

$$\begin{aligned}
Z_k(\beta) &= \sum_{\sigma\in\mathbf{G}_k} \exp(-\beta\mathbf{H}_k^C(\sigma)) \\
&= \exp(-\beta\mathbf{H}_k^C(0)) + \sum_{l=1}^{k}\sum_{\rho\in\mathbf{G}_{l-1}} \exp(-\beta\mathbf{H}_k^C(\rho,1,0_{k-l})) \\
&= 1 + \sum_{l=1}^{k}\sum_{\rho\in\mathbf{G}_{l-1}} \exp(-\beta\mathbf{H}_l^C(\rho,1)) = 1 + \sum_{l=0}^{k-1}\sum_{\rho\in\mathbf{G}_l} \exp(-\beta\mathbf{H}_l^G(\rho)) \\
&= 1 + \sum_{l=0}^{k-1} Z_l^G(\beta)
\end{aligned}$$

with $0_{k-l} = (0, \ldots, 0) \in \mathbf{G}_{k-l}$.

If the quotient (21) were < 1, the statement of the lemma would be wrong. But here we can set $\lambda_\pm(\beta) := \lambda(\beta) \pm \varepsilon$ with $0 < \varepsilon \leq (\lambda(\beta) - 1)/2$ and get constants $c_\pm > 0$ such that

$$c_- \lambda_-^k \leq Z_k^G(\beta) \leq c_+ \lambda_+^k \qquad (k \in \mathbb{N}_0).$$

Thus

$$c_- \frac{\lambda_-^k - 1}{\lambda_- - 1} \leq Z_k(\beta) \leq c_+ \frac{\lambda_+^k - 1}{\lambda_+ - 1} + 1$$

so that $\lambda_- \leq \exp(-\beta F(\beta)) \leq \lambda_+$ and $\lambda(\beta) = \exp(-\beta F(\beta))$. □

Lemma 9 *If the largest eigenvalue $\lambda(\beta) > 1$, then the magnetization $M(\beta) = 0$.*

Proof. We only have to prove that $\limsup_{k \to \infty} M_k(\beta) \leq 0$, since the spin chain of length $k \in \mathbb{N}$ has been shown to be weakly ferromagnetic in [10]. Then the GKS inequalities imply that $M_k(\beta) \geq 0$. Let $\lambda_\pm(\beta) := \lambda(\beta) \pm \varepsilon$ with $0 < \varepsilon \leq (\lambda(\beta) - 1)/2$. Then by (21) there exists a $k_{\min}$ such that for all $k \geq k_{\min}$

$$\lambda_+^{l-k} Z_k^G(\beta) \leq Z_l^G(\beta) \leq \lambda_-^{l-k} Z_k^G(\beta), \qquad (l \in \{0 \ldots, k\}). \tag{23}$$

Thus we have for $k \geq k_{\min} + 1$ by (22)

$$\begin{aligned} Z_k(\beta) &= 1 + \sum_{l=0}^{k-1} Z_l^G(\beta) \geq \left(\sum_{l=0}^{k-1} \lambda_+^{l-k+1} \right) Z_{k-1}^G(\beta) \\ &= \frac{1 - \lambda_+^{-k}}{1 - \lambda_+^{-1}} Z_{k-1}^G(\beta). \end{aligned} \tag{24}$$

The idea of the proof now consists in writing a generic spin configuration $\sigma \in \mathbf{G}_k \setminus \{0\}$ in the form $\sigma = (\tau, 1, 0_{k-m-1})$ with $\tau \in \mathbf{G}_m$, $1 \in \mathbf{G}_1$ and $0_{k-m-1} = (0, \ldots, 0) \in \mathbf{G}_{k-m-1}$. That is, we sort according to the position $m+1$ with $m \in \{0, \ldots, k-1\}$ of the rightmost 1. Then we have $\mathbf{H}_k^C(\sigma) = \mathbf{H}_{m+1}^C(\tau, 1) = \mathbf{H}_m^G(\tau)$, but the grand canonical energy function $\mathbf{H}_m^G$ is invariant w.r.t. spin flip $\tau = (\tau_1, \ldots, \tau_m) \mapsto 1 - \tau = (1 - \tau_1, \ldots, 1 - \tau_m)$: $\mathbf{H}_m^G(\tau) = \mathbf{H}_m^G(1 - \tau)$. That is, the first m spins do not contribute to the magnetization if $\sigma_{m+1} = 1$.

The spin configurations $\sigma = (0, \ldots, 0)$ and $\sigma = (1, 0, \ldots, 0)$ are treated separately.

$$
\begin{aligned}
& Z_k(\beta) \cdot M_k(\beta) \\
&= \sum_{\sigma \in \mathbf{G}_k} \left(\frac{1}{k} \sum_{l=1}^{k} (-1)^{\sigma_l} \right) \exp(-\beta \mathbf{H}_k^C(\sigma)) \\
&= 1 + (1 - \frac{2}{k}) 2^{-\beta} + \sum_{m=1}^{k-1} \sum_{\tau \in \mathbf{G}_m} \frac{1}{k} (k - m - 2 + \sum_{l=1}^{m} (-1)^{\tau_l}) \exp(-\beta \mathbf{H}_m^G(\tau)) \\
&= 1 + (1 - \frac{2}{k}) 2^{-\beta} + \sum_{m=1}^{k-1} \frac{k - m - 2}{k} Z_m^G(\beta).
\end{aligned}
$$

Now we use the upper bound in (23) for the grand canonical partition function Z_l^G.

$$
\begin{aligned}
Z_k(\beta) \cdot M_k(\beta) &= 1 + \sum_{m=0}^{k-1} \frac{k - m - 2}{k} Z_m^G(\beta) \\
&= 1 + \sum_{l=0}^{k-1} \frac{l - 1}{k} Z_{k-1-l}^G(\beta) \\
&\leq 1 + Z_{k-1}^G(\beta) \cdot \sum_{l=0}^{k-1} \frac{l - 1}{k} \lambda_-^{-l} \\
&= 1 + \frac{Z_{k-1}^G(\beta)}{k} \cdot \frac{d}{d\lambda_-} \left(- \sum_{l=0}^{k-1} \lambda_-^{-l+1} \right) \\
&= 1 + \frac{Z_{k-1}^G(\beta)}{k} \cdot \frac{d}{d\lambda_-} \frac{\lambda_- \lambda_-^{-k+1}}{1 - \lambda_-^{-1}} \\
&= 1 + Z_{k-1}^G(\beta) \left[\frac{\lambda_-^{-k+1}}{(\lambda_- - 1)} + \frac{1}{k} \frac{(1 - \lambda_-^{-k})(1 - 2\lambda_-^{-1})}{(1 - \lambda_-^{-1})^2} \right].
\end{aligned}
$$

With the lower bound (24) for $Z_k(\beta)$ we obtain

$$
M_k(\beta) \leq \left((Z_{k-1}^G(\beta))^{-1} + \frac{\lambda_-^{-k-1}}{(\lambda_- - 1)} + \frac{1}{k} \frac{1}{(1 - \lambda_-^{-1})^2} \right) \Big/ \left(\frac{1 - \lambda_+^{-k}}{1 - \lambda_+^{-1}} \right);
$$

since by (21) $\lim_{k \to \infty} Z_{k-1}^G(\beta) = \infty$, and $\lambda_- > 1$ this implies $\limsup_{k \to \infty} M_k(\beta) \leq 0$. $\square$

3 Discussion of the Results

Putting together the lemmata of the last section and the results of [11], we obtain

Proposition 10 *The free energy F is real-analytic in $\mathbb{R}^+ \setminus \{2\}$, and*

- *the magnetization $M(\beta) = 1$ and $F(\beta) = 0$ for $\beta > \beta_{\rm cr} := 2$*
- *$M(\beta) = 0$ and*

$$\left(\frac{\beta}{2} - 1\right) \ln(2) \leq \beta F(\beta) \leq \beta \ln(3/2) - \ln(2)$$

  for $\beta < \beta_{\rm cr}$.
- *In addition $\beta F(\beta) \leq -\frac{1}{4}(\beta_{\rm cr} - \beta)^2$ for $1 \leq \beta < \beta_{\rm cr}$.*

Proof. Real analyticity of the free energy in $(0, 2)$ follows from Lemma 7 and Lemma 8. For $\beta > 2$ the Dirichlet series of the partition function $Z(\beta)$ converges absolutely so that $F(\beta) = 0$. It was shown in [11] that $M(\beta) = 1$ for these inverse temperatures.

For $\beta < 2$ the lower bound $(\frac{\beta}{2} - 1)\ln(2) \leq \beta F(\beta)$ follows from concavity of $\beta F(\beta)$, $F(2) = 0$ and $\lim_{\beta \to 0} \beta F(\beta) = -\ln(2)$, the last limit being a consequence of $Z_k(0) = 2^k$.

The linear upper bound $\beta F(\beta) \leq \beta \ln(3/2) - \ln(2)$ was derived in [11].

Thus we need only show the quadratic bound $\beta F(\beta) \leq -\frac{1}{4}(\beta_{\rm cr} - \beta)^2$ in the subinterval $[\beta_2, 2)$ of $[1, 2)$ where $\frac{1}{4}(\beta_{\rm cr} - \beta)^2 \geq \ln(2) - \beta \ln(3/2)$, $\beta_1 \approx 0.75$ and $\beta_2 := 2 \cdot (1 - \log(3/2) + \sqrt{\ln(2) - 2\ln(3/2) + \ln^2(3/2)}) \approx 1.6209$ being the solutions of the corresponding quadratic equation.

We showed in Lemma 6 and Lemma 8 that for $1 \leq \beta < 2$

$$\beta F(\beta) \leq -\ln\left(1 + c\frac{2 - \beta}{Z(4 - \beta)}\right)$$

with $c = (1 - \ln(2)) \exp(-\pi^2/48) \approx 0.2498$.

Thus we must show that

$$\ln\left(1 + c\frac{2 - \beta}{Z(4 - \beta)}\right) \geq \frac{1}{4}(2 - \beta)^2, \qquad (\beta_2 \leq \beta < 2). \tag{25}$$

First of all $(Z(4-\beta))^{-1} = \frac{\zeta(4-\beta)}{\zeta(3-\beta)}$, and $\beta \mapsto \zeta(4-\beta)$ is monotone increasing.

Moreover, by Theorem 12.21 of Apostol [3]

$$\zeta(s) = \frac{s}{s-1} - s\int_1^\infty \frac{x-[x]}{x^{s+1}}dx \quad \text{for } s > 1.$$

$$\int_1^\infty \frac{x-[x]}{x^{s+1}}dx = \frac{1-2^{1-s}}{s-1} - \frac{1-2^{-s}}{s} + \int_2^\infty \frac{x-[x]}{x^{s+1}}dx,$$

and

$$\int_2^\infty \frac{x-[x]}{x^{s+1}}dx \geq \tfrac{1}{2}\int_{5/2}^\infty x^{-(s+1)}dx = \tfrac{(2/5)^s}{2s},$$

so that

$$\zeta(s) \leq \frac{s+1}{s-1}2^{-s} + 1 - \tfrac{1}{2}(2/5)^s.$$

Therefore

$$(\zeta(3-\beta))^{-1} \geq (2-\beta)/h(\beta)$$

with $h(\beta) := (4-\beta)2^{\beta-3} + (2-\beta)\left(1+\frac{1}{2}(2/5)^{3-\beta}\right)$.

Inspection of the terms in $h'(\beta)$ shows that $h|_{[1,2]}$ is monotone decreasing.

Thus

$$(Z(4-\beta))^{-1} = \frac{\zeta(4-\beta)}{\zeta(3-\beta)} \geq c_1\cdot(2-\beta) \qquad \text{for } \beta_2 \leq \beta < 2$$

with $c_1 := \zeta(4-\beta_2)/h(\beta_2) \approx 1.0338$.

The estimate $\ln(1+x) \geq x - x^2/2$ for $x \geq 0$ implies for $\beta_2 \leq \beta < 2$

$$\begin{aligned}
\ln\left(1 + c\frac{2-\beta}{Z(4-\beta)}\right) &\geq \ln\left(1 + c\cdot c_1\cdot(2-\beta)^2\right) \\
&\geq cc_1(1-\tfrac{1}{2}cc_1(2-\beta_2)^2)\cdot(2-\beta)^2 \\
&\approx 0.2534\cdot(2-\beta)^2,
\end{aligned}$$

proving (25).

So the free energy $F(\beta) < 0$ for $\beta < 2$ or, equivalently, the eigenvalue $\lambda(\beta)$ of the Perron-Frobenius operator is strictly larger than 1. Therefore, by Lemma 9 the mean magnetization $M(\beta) = 0$ in this regime. □

Corollary 11 *The internal energy* $U(\beta) = 0$ *for* $\beta > \beta_{\rm cr}$*, and*

$$\frac{\ln(2) - \beta \ln(3/2)}{2-\beta} \leq U(\beta) \leq \ln(3/2) \qquad (0 < \beta < 2).$$

Moreover, $U(\beta) \geq \frac{1}{4}(\beta_{\rm cr} - \beta)$ *for* $1 \leq \beta < \beta_{\rm cr}$ *(See Figure 1).*

Proof. That $U(\beta) = 0$ in the frozen state was shown in [11], and similarly the upper bound $U(\beta) \leq \ln(3/2)$. To prove the lower bounds we use that $U(\beta) = \frac{d}{d\beta}\beta \cdot F(\beta)$, and that $\beta \mapsto U(\beta)$ is monotone decreasing. So

$$-\beta \cdot F(\beta) = \int_\beta^2 U(b)db \leq U(\beta) \cdot (2-\beta),$$

since $F(2) = 0$, or $U(\beta) \geq -\beta F(\beta)/(2-\beta)$. Then the estimates follow from the above proposition. □

The lower bound on U shows that the phase transition is at most of second order. One cannot exclude from the upper bound a first-order phase transition, but we conjecture that U is continuous in β.

The mechanism of this Thouless type phase transition becomes very clear if one considers the logarithmic energy density $D(E)$.

We compare with the Ising chain $H_k : \{-1,1\}^k \to \mathbb{R}$, $H_k(\sigma) := -\sum_{i=1}^k \sigma_i$. There one has

$$D(E) = -\tfrac{1}{2}\left((1+E)\ln(1+E) + (1-E)\ln(1-E)\right), \qquad (E \in (-1,1))$$

so that $D'(E) = \frac{1}{2}\ln(\frac{1-E}{1+E})$ has limits $\lim_{E\to\pm1} D'(E) = \mp\infty$. Moreover, the smooth function D is strictly concave, so that the internal energy $U(\beta) = (dD/dE)^{-1}(\beta) = -\tanh(\beta)$ is smooth in $\beta \in \mathbb{R}$.

In Figure 2 we show a numerical approximation to the logarithmic energy density $D(E)$ of the number-theoretical spin chain. In [10] we derived the sharp estimates $1 \leq \mathbf{h}_k^C \leq F(k+2)$, $F(k)$ being the kth Fibonacci number. So the energy per particle is bounded by $0 \leq \frac{1}{k}\mathbf{H}_k^C \leq \frac{1}{k}\ln(F(k+2))$, and we consider $D(E)$ on the interval $[0, \ln(g)]$, $g := \frac{1}{2}(1+\sqrt{5})$ being the golden mean.

The phase transition at $\beta_{\rm cr} = 2$ corresponds to an initial slope $D'(0) = \beta_{\rm cr}$. For $\beta > \beta_{\rm cr}$ there is no energy E with $D'(E) = \beta$, so that $U(\beta) = 0$. It seems that $\lim_{E\searrow 0} D''(E) = 0$ which would imply $\lim_{\beta\nearrow\beta_{\rm cr}} U'(\beta) = -\infty$.

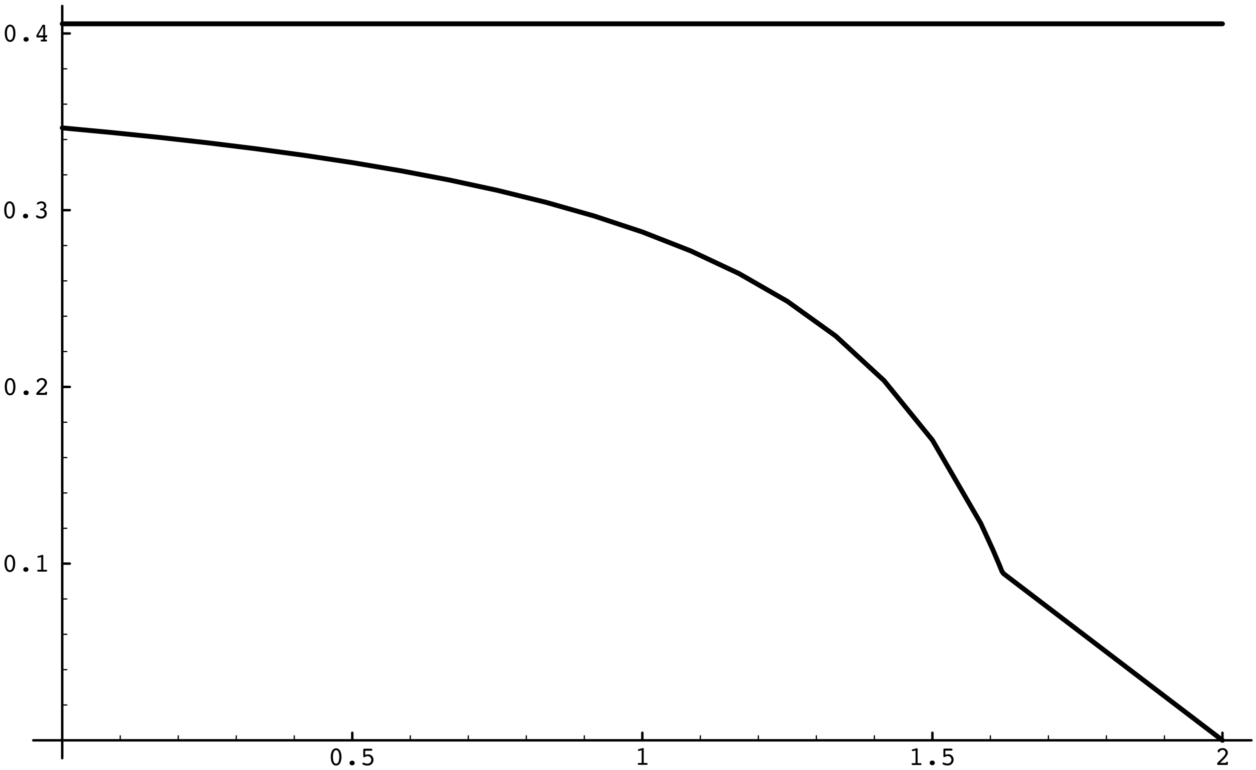

Figure 1: Upper and lower bounds for the energy density $U(\beta)$

Figure 2: The logarithmic energy density $D(E)$, with a line of slope $\beta_{\rm cr} = 2$

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