Free Energy and Correlations of the Number-Theoretical Spin Chain

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Abstract

We analyze the number-theoretical spin chain with partition function $Z(\beta) = \zeta(\beta - 1)/\zeta(\beta)$ using the polymer model technique. The finite (grand) canonical chains give bounds for the limit free energy and internal energy. The correlation functions for inverse temperature $\beta = -1$ are products of two-point functions. A combinatorial result for general interval graphs is derived.

1 Introduction

The simplest kind of number theory consists in adding integers and observing the regularities that arise. For example, one may add integers at neighbouring positions in a row and write the results in the next row. If one starts with the row no. $k = 0$ containing a single one, then the result is Pascal's triangle (Fig. 1a)), with the binomial coefficient $\binom{k}{l}$ at position (k, l). The defining relations of the binomial coefficients are thus

$$\binom{0}{l} := \delta_0(l) \quad \text{and} \quad \binom{k+1}{l} := \binom{k}{l-1} + \binom{k}{l}.$$

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Although Pascal's triangle was already described in the 1303 book 'The Precious Mirror of the Four Elements' by Chu Shih-chieh and thus has a rather long history, there are still many unsolved questions connected with it. Anybody who is now and then summing series knows some non-trivial identities met by the binomial coefficients.

Now we change the defining rule a bit. Instead of simply forgetting the values written in the k-th row, we copy them to the row no. $k+1$, thus obtaining *Pascal's triangle with memory.*

We want 2^k instead of $2^{k+1}-1$ entries in each row. Thus we consider these entries as being circularly ordered. For practical purposes we write a second copy of the first entry 1 at the end of the row but encircle it in order to mark its identification with the first entry (Fig. 1b)).

The 2^k entries can be indexed by the base 2 k-digit numbers $0\ldots0$, $0\ldots01$, …, $1\ldots1$, writing them in ascending order. Thus we may consider these entries as the values of a function $\mathbf{h}_k^C : \mathbf{G}_k \to \mathbb{N}$ with the k-fold cartesian product group $\mathbf{G}_k := \mathbb{Z}_2^k$, $\mathbb{Z}_2 = (\{0,1\},+)$ being the two-element group in additive notation. A moment's thought shows that these functions can be defined by $\mathbf{h}_0^C := 1$,

$$\mathbf{h}_{k+1}^C(\sigma_1,\ldots,\sigma_{k+1}) := \mathbf{h}_k^C(\sigma_1,\ldots,\sigma_k) + \sigma_{k+1}\cdot\mathbf{h}_k^C(1-\sigma_1,\ldots,1-\sigma_k). \quad (1)$$

If one defines the *energy function* $\mathbf{H}_k^C : \mathbf{G}_k \to \mathbb{R}$ of the *canonical ensemble* by $\mathbf{H}_k^C = \ln(\mathbf{h}_k^C)$, then the functions

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

can be interpreted as partition functions, the superscript C referring to the canonical ensemble. It turns out that they converge for $\mathrm{Re}(\beta) > 2$ to

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

which is the quotient

$$Z(\beta) := \frac{\zeta(\beta-1)}{\zeta(\beta)} = \sum_{n=1}^{\infty} \varphi(n)\cdot n^{-\beta}$$

of Riemann zeta functions. Here $\varphi(n) := |\{l\in\{1,\ldots,n\} \mid \gcd(l,n)=1\}|$ is Euler's totient function.

$$
\begin{array}{lcccccccccc}
a) & & & & & & l=0 & & & & \\
k=0 & & & & & 1 & & l=1 & & & \\
k=1 & & & & 1 & & 1 & & l=2 & & \\
k=2 & & & 1 & & 2 & & 1 & & l=3 & \\
k=3 & & 1 & & 3 & & 3 & & 1 & & l=4 \\
k=4 & 1 & & 4 & & 6 & & 4 & & 1 &
\end{array}
$$

$$
\begin{array}{lcccccccccccccccccc}
b) & & & & & & & & & & & & & & & & & \\
k=0 & 1 & & & & & & & & & & & & & & & & 1 \\
k=1 & 1 & & & & & & & & 2 & & & & & & & & 1 \\
k=2 & 1 & & & & 3 & & & & 2 & & & & 3 & & & & 1 \\
k=3 & 1 & & 4 & & 3 & & 5 & & 2 & & 5 & & 3 & & 4 & & 1 \\
k=4 & 1 & 5 & 4 & 7 & 3 & 8 & 5 & 7 & 2 & 7 & 5 & 8 & 3 & 7 & 4 & 5 & 1
\end{array}
$$

Figure 1: Pascal's triangle a) without memory and b) with memory.

In [8] one of us showed 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 $1/(r-l)^2$.

The dual group $\mathbf{G}_k^*$ of $\mathbf{G}_k$ being isomorphic to $\mathbf{G}_k$, the Fourier transform of $f : \mathbf{G}_k \to \mathbb{R}$ is given by

$$(\mathcal{F}_k f)(t) := 2^{-k} \sum_{\sigma \in \mathbf{G}_k} f(\sigma) \cdot (-1)^{\sigma \cdot t} \tag{2}$$

and thus $j_k^C = -\mathcal{F}_k \mathbf{H}_k^C$. In [8] the interaction was shown to be weakly ferromagnetic in the sense that $j_k^C(t) \geq 0$ for $t \neq 0$.

It turned out to be useful to introduce the *grand canonical* energy functions $\mathbf{H}_k^G : \mathbf{G}_k \to \mathbb{R}$, $\mathbf{H}_k^G := \ln(\mathbf{h}_k^G)$, the values

$$\mathbf{h}_k^G(\sigma) := \mathbf{h}_{k+1}^C(\sigma, 1) \tag{3}$$

being the new elements appearing in each row of Fig 1b). They have the 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 [10] the existence of the thermodynamic limit $F(\beta):=\lim_{k\to\infty}F_k^C(\beta)$ of the free energy $F_k^C(\beta):=-(\beta\cdot k)^{-1}\ln(Z_k^C(\beta))$ was shown (due to the lack of strict translation invariance of the interaction standard estimates cannot be applied here).

In [9] thermodynamic expectations

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

of quantities like the internal energy $U_k^C:=\left\langle\frac{1}{k}\mathbf{H}_k^C\right\rangle_k^C$ and magnetization $M_k:=\left\langle\frac{1}{k}\sum_{l=1}^k(-1)^{\sigma_l}\right\rangle_k^C$ 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 $U(\beta):=\lim_{k\to\infty}U_k^C(\beta)$ 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

$$\frac{\ln 2-\beta\ln(3/2)}{2-\beta}\le U(\beta)\le\ln(3/2) \tag{4}$$

were derived.

The corresponding grand canonical quantities are defined similarly.

In [11] 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 [12] by one of us.

In [2] Contucci and Knauf showed that there exists only one phase transition, at $\beta = 2$. There the magnetization jumps from 1 to 0. The phase transition is at most of second order.

In a forthcoming paper [3] the relations between number theory and polymer models are treated.

The same partition function (but without the interpretation as coming from a spin chain) was discussed by Artuso, Cvitanović and Kenny in [1]. See also the related work [5] by Feigenbaum and the overview [4] by Cvitanović.

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.

For example, a interpretation of the functional equation of Z in terms of a Wannier-type duality of polymer model interpretations would be welcome.

In Sect. 2 we calculate the Fourier transforms of the functions $\mathbf{h}_k^C$ and $\mathbf{h}_k^G$. This leads directly to expressions for the correlation functions at $\beta = -1$.

The polymer model technique is then used in Sect. 3 in order to derive a formula for the interaction coefficients. They and not the free energy are described using connected multi-polymers.

Like any Dirichlet series with an Euler product the number-theoretical spin chain itself has an interpretation as a polymer model (see [3]), but this interpretation is not well-adapted to the peculiarities of this chain. So we would like to see another such interpretation in the spirit of Sect. 3.

Sect. 4 deals with general interval graphs, that is, graphs whose vertices correspond to intervals and which are connected by an edge if the corresponding intervals overlap. These types of graphs are used in our context.

In Sect. 5 the limit free energy is estimated from above and below using the k-spin (grand) canonical ensembles.

This result and a polymer inequality finally leads in Sect. 6 to inequalities for the internal energy.

2 Correlation Functions at $\beta = -1$

In this section we analyze the Fourier transforms (see (2)) $J_k^C := \mathcal{F}_k(\mathbf{h}_k^C)$, $J_k^G := \mathcal{F}_k(\mathbf{h}_k^G)$ of the exponentiated (grand) canonical energy functions $\mathbf{h}_k^C$ resp. $\mathbf{h}_k^G$ inductively defined in (1) and (3). Using the shorthand $|s| := \sum_{i=1}^{l} s_i$ for $s \in \mathbf{G}_l$, we have

Lemma 1 $J_0^C = 1$, *and for* $t = (t_1, \ldots, t_{k+1}) \in \mathbf{G}_{k+1}^*$

$$J_{k+1}^C(t_1, \ldots, t_{k+1}) = \tfrac{1}{2}\left(1 + (-1)^{t_{k+1}} + (-1)^{|t|}\right) J_k^C(t_1, \ldots, t_k). \qquad (5)$$

The grand canonical Fourier coefficients are given by

$$J_{k+1}^G(t) = \left(1 + (-1)^{|t|}\right) J_k^C(t), \qquad (t \in \mathbf{G}_k^*). \qquad (6)$$

Proof. If $k = 0$, then $|\mathbf{G}_k| = 1$ and $J_0^C = \mathbf{h}_0^C = 1$. To show the inductive formula (5), we use the abbreviation $t' := (t_1, \ldots, t_k) \in \mathbf{G}_k^*$. Then

$$\begin{aligned}
J_{k+1}^C(t) &= 2^{-k-1} \sum_{\sigma \in \mathbf{G}_{k+1}} \mathbf{h}_{k+1}^C(\sigma) \cdot (-1)^{\sigma \cdot t} \\
&= 2^{-k-1} \sum_{\sigma' \in \mathbf{G}_k} \left(\mathbf{h}_{k+1}^C(\sigma', 0) + (-1)^{t_{k+1}} \mathbf{h}_{k+1}^C(\sigma', 1)\right) \cdot (-1)^{\sigma' \cdot t'} \\
&= \tfrac{1}{2} 2^{-k} \textstyle\sum_{\sigma' \in \mathbf{G}_k} \mathbf{h}_k^C(\sigma') \cdot (-1)^{\sigma' \cdot t'} + \\
&\quad \tfrac{1}{2} (-1)^{t_{k+1}} 2^{-k} \textstyle\sum_{\sigma' \in \mathbf{G}_k} \left(\mathbf{h}_k^C(\sigma') + \mathbf{h}_k^C(1 - \sigma')\right) \cdot (-1)^{\sigma' \cdot t'} \\
&= \tfrac{1}{2}\left(1 + (-1)^{t_{k+1}} + (-1)^{|t|}\right) J_k^C(t'),
\end{aligned}$$

using the iterative definition (1) of $\mathbf{h}_k^C$ and the relation

$$\sum_{\sigma' \in \mathbf{G}_k} \mathbf{h}_k^C(1 - \sigma') \cdot (-1)^{\sigma' \cdot t'} = (-1)^{|t'|} \sum_{\sigma' \in \mathbf{G}_k} \mathbf{h}_k^C(\sigma') \cdot (-1)^{\sigma' \cdot t'}.$$

Eq. (6) follows from the definition $\mathbf{h}_k^G(\sigma) = \mathbf{h}_{k+1}^C(\sigma, 1)$ of $\mathbf{h}_k^G$ and (5), since this implies

$$\begin{aligned}
J_k^G(t) &= 2^{-k} \sum_{\sigma \in \mathbf{G}_k} \mathbf{h}_{k+1}^C(\sigma, 1) \cdot (-1)^{\sigma \cdot t} \\
&= 2^{-k} \sum_{\sigma \in \mathbf{G}_k} \left(\mathbf{h}_k^C(\sigma) + \mathbf{h}_k^C(1 - \sigma)\right) \cdot (-1)^{\sigma \cdot t} \\
&= (1 + (-1)^{|t|}) J_k^C(t). \square
\end{aligned}$$

The above formulas allow us to write the Fourier coefficients as products over contributions from so-called polymers. The set

$$P_k := \{p_{l,r}, p_l \in \mathbf{G}_k^* \mid 1 \le l, r \le k;\ l < r\}$$

of *polymers* in $\mathbf{G}_k^*$ is given by

$$p_{l,r}(i) := \delta_l(i) + \delta_r(i), \quad p_l(i) := \delta_l(i) \qquad (i = 1, \ldots, k). \tag{7}$$

We define their *support* by $\mathrm{supp}(p_{l,r}) := \{i \mid l \leq i \leq r\}$ for the *even* polymers and $\mathrm{supp}(p_l) := \{i \mid l \leq i \leq k\}$ for the *odd* ones. Two polymers $\gamma_1, \gamma_2 \in P_k$ are called overlapping or *incompatible* if $\mathrm{supp}(\gamma_1) \cap \mathrm{supp}(\gamma_2) \neq \emptyset$. So in particular all the odd polymers p_l, $1 \leq l \leq k$, are mutually incompatible.

Now an arbitrary group element $t = (t_1, \ldots, t_k) \in \mathbf{G}_k^*$ can be uniquely decomposed into the sum of $n := [\frac{1}{2}(|t| + 1)]$ compatible polymers:

$$t = \begin{cases} \sum_{i=1}^{n} p_{l_i,r_i} & , |t| \text{ even} \\ \sum_{i=1}^{n-1} p_{l_i,r_i} + p_{l_n} & , |t| \text{ odd.} \end{cases} \tag{8}$$

whose indices l_i, r_i may be assumed to be increasing in i and are determined by $t_{l_i} = t_{r_i} = 1$. As an example $(0,1,0,1,1,0) = p_{2,4} + p_5 \in \mathbf{G}_6^*$.

We write this decomposition in the short form $t = \sum_{i=1}^{n} \gamma_i$ and set the activity of a polymer $\gamma \in \mathbf{G}_k^*$ equal to $z(\gamma) := -3^{-|\mathrm{supp}(\gamma)|}$.

Theorem 2 *With the above decomposition (8) of $t \in \mathbf{G}_k^*$*

$$J_k^C(t) = (3/2)^k \prod_{i=1}^{n} z(\gamma_i) \tag{9}$$

and

$$J_k^G(t) = \left(1 + (-1)^{|t|}\right) (3/2)^k \prod_{i=1}^{n} z(\gamma_i). \tag{10}$$

Proof. We proceed by induction in the number k of spins. For $k = 0$ eq. (9) gives $J_0^C = 1$, as in Lemma 1.

- If $|t|$ is even and $t_{k+1} = 0$, then the polymers of the representation (8) of $(t_1, \ldots, t_{k+1})$ coincide with the polymers of $(t_1, \ldots, t_k)$.

  So by (9) $J_{k+1}^C(t_1, \ldots, t_{k+1}) = \frac{3}{2} J_k^C(t_1, \ldots, t_k)$, in accordance with (5).

- If $|t|$ is even and $t_{k+1} = 1$, then $(t_1, \ldots, t_{k+1})$ contains the additional polymer p_{k+1} so that both (5) and (9) imply

  $$J_{k+1}^C(t_1, \ldots, t_{k+1}) = -\tfrac{1}{2} J_k^C(t_1, \ldots, t_k).$$

- If $|t|$ is odd, then the odd polymer p_{l_n} in the decomposition (8) of $(t_1,\ldots,t_k)$ has activity $z(p_{l_n}) = -3^{l_n-k-1}$.

  If $t_{k+1}=0$, then the polymer decomposition for $(t_1,\ldots,t_{k+1})$ remains the same, but now $z(p_{l_n}) = -3^{l_n-k-2}$. If $t_{k+1}=1$, the odd polymer p_{l_n} is changed into the even polymer $p_{l_n,k+1}$ which, too, has activity $z(p_{l_n,k+1}) = -3^{l_n-k-2}$. So both (5) and (9) predict $J^C_{k+1}(t_1,\ldots,t_{k+1}) = \frac{1}{2}J^C_k(t_1,\ldots,t_k)$, independent of whether $t_{k+1}=0$ or 1.

The corresponding equation (10) for the grand canonical coefficients $J^G_k(t)$ follows directly from (9) and (6). □

Theorem 2 has the following corollary concerning the (grand) canonical expectations

$$\langle f\rangle^{C/G}_k(\beta) = \frac{\sum_{\sigma\in\mathbf{G}_k} f(\sigma)e^{-\beta\mathbf{H}^{C/G}_k(\sigma)}}{Z^{C/G}_k(\beta)}$$

of $f:\mathbf{G}_k\to\mathbb{R}$ at inverse temperature β:

Corollary 3 *For $1\le i_1<\ldots<i_{2l}\le k$ the even (grand) canonical correlation functions at inverse temperature $\beta=-1$ equal*

$$\left\langle \prod_{m=1}^{l} \sigma_{i_{2m-1}}\sigma_{i_{2m}} \right\rangle^{C/G}_k(-1) = \prod_{m=1}^{l} \left\langle \sigma_{i_{2m-1}}\sigma_{i_{2m}} \right\rangle^{C/G}_k(-1),$$

whereas the grand canonical correlation functions between an odd number of spins vanish for any $\beta\in\mathbb{R}$.

Proof. Using (9) resp. (10) we obtain for $|t|$ even the general identity

$$\left\langle \prod_{i:t_i=1} \sigma_i \right\rangle^{C/G}_k(-1) = \frac{J^{C/G}_k(t)}{J^{C/G}_k(0)} = \prod_{i=1}^{n} z(\gamma_i)$$

for the correlation functions, proving the product formula. The odd grand canonical correlation functions vanish identically since by (10) $J^G_k(t)=0$ for $|t|$ odd. □

3 Polymers and Interaction Coefficients

Now we will express the (grand) canonical interaction coefficients

$$\mathbf{j}_k^{C/G}(t) = -\mathcal{F}_k(\mathbf{H}_k^{C/G})(t), \qquad (t \in \mathbf{G}_k^*)$$

in terms of the Fourier transforms $J_k^{C/G}(t) = \mathcal{F}_k(\mathbf{h}_k^{C/G})(t)$ of the exponentiated energy functions $\mathbf{h}_k^{C/G} = \exp(\mathbf{H}_k^{C/G})$ (observe that for historical reasons the $\mathbf{j}_k^{C/G}(t)$ are the *negative* Fourier coefficients).

Our motivation for considering that functional relationship is the existence of the explicit formulae (9) and (10) for J_k^C resp. J_k^G.

The technique we apply stems from the theory of polymer models whose general setting we now recall (see, e.g., Gallavotti, Martin-Löf and Miracle-Solé [6], Simon [13] and Glimm and Jaffe [7]).

In an abstract setting one starts with a denumerable set P whose elements are called *polymers.* Two given polymers $\gamma_1, \gamma_2 \in P$ may or may not overlap (be *incompatible*). Incompatibility is assumed to be a reflexive and symmetric relation on P.

Thus one may associate to a *k-polymer* $X := (\gamma_1, \ldots, \gamma_k) \in P^k$ an undirected graph $G(X) = (V(X), E(X))$ without loops with vertex set $V(X) := \{1, \ldots, k\}$, vertices $i \neq j$ being connected by the edge $\{\gamma_i, \gamma_j\} \in E(X)$ if γ_i and γ_j are incompatible. Accordingly the k-polymer X is called *connected* if $G(X)$ is path-connected and *disconnected* if it has no edges ($E(X) = \emptyset$).

The corresponding subsets of P^k are called C^k resp. D^k, with $D^0 := P^0 := \{\emptyset\}$ consisting of a single element. Moreover $P^\infty := \bigcup_{k=0}^\infty P^k$ with the subsets $D^\infty := \bigcup_{k=0}^\infty D^k$ and $C^\infty := \bigcup_{k=1}^\infty C^k$. We write $|X| := k$ if $X \in P^k$.

Statistical weights or activities $z : P \to \mathbb{C}$ of the polymers are multiplied to give the activities $z^X := \prod_{i=1}^k z(\gamma_i)$ of k-polymers.

Finally, in order to work with finite sums, we use finite subsets $P_\Lambda \subset P$ of polymers, which are thought of being geometrically enclosed in a finite region $\Lambda \subset S$.

A system of statistical mechanics is called *polymer model* if its partition functions Z_Λ have the form

$$Z_\Lambda = \sum_{X \in D_\Lambda^\infty} \frac{z^X}{|X|!}. \tag{11}$$

Then, up the normalization factor $|\Lambda|^{-1}$, the free energy is given by

$$\ln(Z_\Lambda) = \sum_{X \in C_\Lambda^\infty} \frac{n(X)}{|X|!} z^X, \tag{12}$$

with $n(X) := n_+(X) - n_-(X)$, $n_\pm(X)$ being the number of subgraphs of $G(X)$ connecting the vertices of $G(X)$ with an even resp. odd number of edges (see Gallavotti et al. [6]).

In the present context we argue as follows: Our polymers are elements of the abelian group

$$\mathbf{G}_\infty^* := \bigoplus_{n=1}^{\infty} \mathbb{Z}_2 \subset \bigotimes_{n=1}^{\infty} \mathbb{Z}_2$$

which is the direct sum of the $\mathbb{Z}_2$ groups and thus consists of those infinite sequences $t = (t_1, t_2, \ldots) \in \otimes_{n=1}^\infty \mathbb{Z}_2$ which have only finitely many entries $t_i \neq 0$. The set P of polymers and their supports is defined similarly to the set P_k (see (7)) except that now $k = \infty$.

This infinite volume case is then approximated by considering the set P_k of polymers in the finite subset $\Lambda = \{1, \ldots, k\} \subset \mathbb{N}$. The group $\mathbf{G}_k^*$ is identified with the subgroup of those $t \in \mathbf{G}_\infty^*$ with $t_n = 0$ for $n > k$.

Then the map $D_k^\infty \to \mathbf{G}_k^*$, $(\gamma_1, \ldots, \gamma_n) \mapsto \sum_{i=1}^n \gamma_i$ is an isomorphism between the disconnected multi-polymers in $\{1, \ldots, k\}$ and the abelian group $\mathbf{G}_k^*$.

We will now use this isomorphism to calculate the interaction coefficients.

For the canonical ensemble formula (9) in Theorem 2 implies

$$\begin{aligned} j_k^C(t) &= -2^{-k} \sum_{\sigma \in \mathbf{G}_k} \mathbf{H}_k^C(\sigma) \cdot (-1)^{\sigma \cdot t} \\ &= -2^{-k} \sum_{\sigma \in \mathbf{G}_k} \ln \left[\sum_{s \in \mathbf{G}_k^*} J_k^C(s) \cdot (-1)^{s \cdot \sigma} \right] \cdot (-1)^{\sigma \cdot t} \\ &= -\delta_{t,0} \cdot k \ln(3/2) - 2^{-k} \sum_{\sigma \in \mathbf{G}_k} \ln \left[\sum_{X \in D_k^\infty} \tilde{z}_\sigma^X \right] \cdot (-1)^{\sigma \cdot t} \end{aligned} \tag{13}$$

where the redefined single-polymer activities $\tilde{z}_\sigma(\gamma)$, $\gamma \in P_k$ are given by $\tilde{z}_\sigma(\gamma) := z_\sigma(\gamma) \cdot (-1)^{\sigma \cdot \gamma}$, that is

$$\tilde{z}_\sigma(p_{l,r}) := z(p_{l,r}) \cdot (-1)^{\sigma_l + \sigma_r}, \qquad \tilde{z}_\sigma(p_l) := z(p_l) \cdot (-1)^{\sigma_l}.$$

By (12) we get

$$\begin{aligned}
& j_k^C(t) + \delta_{t,0} \cdot k \ln(3/2) \\
&= -2^{-k} \sum_{\sigma \in \mathbf{G}_k} \sum_{X \in C_k^\infty} \frac{n(X)}{|X|!} \tilde{z}_\sigma^X \cdot (-1)^{\sigma \cdot t} \\
&= - \sum_{X=(\gamma_1,\ldots,\gamma_{|X|}) \in C_k^\infty} \frac{n(X)}{|X|!} z^X \cdot 2^{-k} \sum_{\sigma \in \mathbf{G}_k} (-1)^{\sigma \cdot (t + \sum_{i=1}^{|X|} \gamma_i)} \\
&= - \sum_{\substack{X=(\gamma_1,\ldots,\gamma_{|X|}) \in C_k^\infty \\ \sum_{i=1}^{|X|} \gamma_i = t}} \frac{n(X)}{|X|!} z^X, \qquad (14)
\end{aligned}$$

using the identity $\sum_{\sigma \in \mathbf{G}_k} (-1)^{\sigma \cdot s} = 2^k \delta_{s,0}$.

For the grand canonical ensemble $j_k^G(t) = 0$ if $|t|$ is odd. If $|t|$ is even, then by (10) and a similar derivation as above

$$j_k^G(t) = -\delta_{t,0} \cdot (\ln(2) + k \ln(3/2)) - \sum_{\substack{X=(\gamma_1,\ldots,\gamma_{|X|}) \in C_k^{\infty,e} \\ \sum_{i=1}^{|X|} \gamma_i = t}} \frac{n(X)}{|X|!} z^X \qquad (15)$$

where now $C_k^{\infty,e}$ contains precisely those multi-polymers $X = (\gamma_1, \ldots, \gamma_{|X|})$ consisting only of even polymers γ_i of the form $p_{l,r}$ and not the odd polymers p_l.

4 Combinatorics of Interval Graphs

The graphs $G(X)$ of the connected multi-polymers $X \in C_k^\infty$ resp. $C_k^{\infty,e}$ occurring in (14) resp. (15) have a special structure which enables us to obtain a simple explicit formula for the combinatorial factor $n(X)$.

The supports of the even polymers $p_{l,r}$ were of the form $\{l, \ldots, r\}$, whereas for the odd polymers p_l one had $\mathrm{supp}(p_l) = \{l, \ldots, k\}$. Polymers in P_k with overlapping supports were called incompatible.

These definitions imply that the graph $G(X)$ of a multi-polymer is a so-called interval graph. In general, a graph $G = (V, E)$ is called *interval graph* if there exists an isomorphism $I : V \to \bar{V}$ between the set V of vertices and a set $\bar{V}$ of intervals in $\mathbb{R}$ such that $v_i, v_j \in V$ are connected by the edge

$\{v_i, v_j\} \in E$ precisely if the corresponding intervals $I(v_i)$ and $I(v_j)$ have non-empty intersection.

By renaming the vertices we can assume that $V = V_r := \{v_1, \ldots, v_r\}$, $I(v_i) = [a_i, b_i]$ and $a_i \le a_j$ for $i < j$. Then $G_i := (V_i, E_i)$ with $E_i := E \cap (V_i \times V_i)$ is the induced subgraph of G on the first i vertices, $1 \le i \le r$.

Theorem 4 *For interval graphs G with the above notation*

$$n(G) = \prod_{i=1}^{r-1} (|E_i| - |E_{i+1}|).$$

Proof. We prove the formula by induction in the number $|V|$ of vertices.

If $|V| = 1$, the index set of the product is empty so that the product gives 1. But $n(G) = n_+(G) - n_-(G) = 1$, too, since $n_+(G) = 1$ and $n_-(G) = 0$.

The subgraphs G_i of G are themselves interval graphs. We assume that $n(G_{l-1}) = \prod_{i=1}^{l-2}(|E_i| - |E_{i+1}|)$ and show that

$$n(G_l) = \prod_{i=1}^{l-1}(|E_i| - |E_{i+1}|) = n(G_{l-1}) \cdot (|E_{l-1}| - |E_l|) = -n(G_{l-1}) \cdot |\hat{E}_l|, \quad (16)$$

where $\hat{E}_l := E_l - E_{l-1}$ is the set of edges in G_l connecting the vertex v_l with the subgraph G_{l-1}. The set $\mathcal{C}_l$ of connected subgraphs of G_l is the disjoint union

$$\mathcal{C}_l = \dot{\bigcup}_{\hat{E} \subset \hat{E}_l} \mathcal{C}_l(\hat{E})$$

of $\mathcal{C}_l(\hat{E}) := \{(V_l, \tilde{E}) \in \mathcal{C}_l \mid \tilde{E} \cap \hat{E}_l = \hat{E}\}$, i.e., the subsets of those connected graphs where the edges in $\hat{E}$ emanate from the vertex v_l. So

$$n(G_l) = \sum_{\hat{E} \subset \hat{E}_l} \sum_{(V_l, \tilde{E}) \in \mathcal{C}_l(\hat{E})} (-1)^{|\tilde{E}|}. \quad (17)$$

We will show now that in fact

$$n(G_l) = \sum_{\substack{\hat{E} \subset \hat{E}_l \\ |\hat{E}| = 1}} \sum_{(V_l, \tilde{E}) \in \mathcal{C}_l(\hat{E})} (-1)^{|\tilde{E}|}, \quad (18)$$

that is, only subgraphs with exactly one edge adjacent to v_l contribute.

It is obvious that $\mathcal{C}_l(\emptyset) = \emptyset$, since in that case the vertex v_l is disconnected.

So we are left to show that terms in (17) with $|\hat{E}| \geq 2$ give no contribution.

We choose two different edges $\{v_x, v_l\}, \{v_y, v_l\} \in \hat{E}$. Then the graph G_l contains the edge $e := \{v_x, v_y\}$, as we show now. Namely the intervals $[a_x, b_x] = I(v_x)$ and $[a_y, b_y] = I(v_y)$ both intersect the interval $[a_l, b_l] = I(v_l)$ so that $a_l \leq b_x, b_y$, and they have the additional property $a_x, a_y \leq a_l$ since $x, y \leq l$. Thus $a_l \in [a_x, b_x] \cap [a_y, b_y]$ showing that these intervals intersect.

The set $A := \{(V_l, \tilde{E}) \in \mathcal{C}_l(\hat{E}) \mid e \in \tilde{E}\}$ consists of the connected subgraphs containing the edge $e = \{v_x, v_y\}$. The map

$$J : A \to J(A), \quad (V_l, \tilde{E}) \mapsto (V_l, \tilde{E} - \{e\})$$

deletes the edge e and is obviously one-to-one. Moreover

$$\mathcal{C}_l(\hat{E}) = A \cup J(A),$$

since the graph $(V_l, \tilde{E} - \{e\})$ is still connected (v_x and v_y are connected by the edges $\{v_x, v_l\}$, $\{v_y, v_l\}$).

So if $|\hat{E}| \geq 2$ then

$$\sum_{(V_l, \tilde{E}) \in \mathcal{C}_l(\hat{E})} (-1)^{|\tilde{E}|} = \sum_{(V_l, \tilde{E}) \in A} \left((-1)^{|\tilde{E}|} + (-1)^{|\tilde{E} - \{e\}|} \right) = 0,$$

showing (18).

Now we resum (18):

$$n(G_l) = -\sum_{\hat{e} \in \hat{E}_l} \sum_{(V_l, \tilde{E}) \in \mathcal{C}_l(\{\hat{e}\})} (-1)^{|\tilde{E} - \{\hat{e}\}|}.$$

But the map K on $\mathcal{C}_l(\{\hat{e}\})$ given by $K((V_l, \tilde{E})) := (V_{l-1}, \tilde{E} - \{\hat{e}\})$ is one-to-one and $K(\mathcal{C}_l(\{\hat{e}\})) = \mathcal{C}_{l-1}$, that is, its image consists of the connected subgraphs on the first $l-1$ vertices (by removing $\hat{e}$ we disconnect the vertex v_l from the vertices $v_1, \ldots, v_{l-1}$, but we do not disconnect any of these). Thus

$$n(G_l) = -\sum_{\hat{e} \in \hat{E}_l} \sum_{(V_{l-1}, \tilde{E}) \in \mathcal{C}_{l-1}} (-1)^{|\tilde{E}|} = -n(G_{l-1}) \cdot |\hat{E}_l|,$$

proving (16). $\Box$

Remark. As the example of the graph $G = (V, E)$ of a square with $V :=$

$\{v_1, v_2, v_3, v_4\}$ and $E := \{\{v_1, v_2\}, \{v_2, v_3\}, \{v_3, v_4\}, \{v_4, v_1\}\}$ shows, an analogous result does not hold for general graphs. Namely here $n(G_3) = 1 - 0 = 1$ but $n(G) = 1 - 4 = -3$, although there are only two edges adjacent to the vertex v_4.

It was already shown in [8] that the (grand) canonical interaction is weakly ferromagnetic, i.e. that

$$j_k^C(t) \geq 0 \quad \text{and} \quad j_k^G(t) \geq 0 \qquad \text{for } t \in \mathbf{G}_k^* \setminus \{0\}.$$

That fact can now be easily seen to be a by-product of our above theorem for interval graphs $G = (V, E)$, since Theorem 4 implies

$$\mathrm{sign}(n(G)) = \begin{cases} 0 & G \text{ not connected} \\ -(-1)^{|V|} & G \text{ connected} \end{cases} .$$

On the other hand, the sign of the activity of a multi-polymer X is $\mathrm{sign}(z^X) = (-1)^{|X|}$. Thus all connected multi-polymers give a positive contribution to the interaction coefficients (14) and (15).

By estimating the contribution of the simplest multi-polymers, we may obtain more precise lower bounds for the interaction coefficients. As in [8] we denote the positions of the first resp. last one in $t = (t_1, \ldots, t_k) \in \mathbf{G}_k^* \setminus \{0\}$ by

$$P_k^l(t) := \min\{i \in \{1, \ldots, k\} \mid t_i = 1\}$$

and

$$P_k^r(t) := \max\{i \in \{1, \ldots, k\} \mid t_i = 1\}.$$

Corollary 5 *Let $t = (t_1, \ldots, t_k) \in \mathbf{G}_k^* \setminus \{0\}$.*

- *If $|t|$ is odd, then $j_k^G(t) = 0$ and $j_k^C(t) \geq 3^{-2s}$, with $s := k + 1 - P_k^l(t)$.*
- *If $|t|$ is even, then $j_k^G(t) \geq 3^{-2s}$ and $j_k^C(t) \geq 3^{-2s}$, with $s := P_k^r(t) + 1 - P_k^l(t)$.*

The grand canonical interaction coefficients increase under concatenation, that is,

$$j_{k+l}^G(s, t) \geq \delta_{t,0} \cdot j_k^G(s) + \delta_{s,0} \cdot j_l^G(t), \qquad (s \in \mathbf{G}_k^*, t \in \mathbf{G}_l^*). \tag{19}$$

Proof. We already stated that $j_k^G(t) = 0$ for $|t|$ odd. The other lower bounds are achieved by first decomposing t according to (8) into disconnected polymers $t = \sum_{i=1}^n p_{l_i,r_i}$ for $|t|$ even resp. $t = \sum_{i=1}^{n-1} p_{l_i,r_i} + p_{l_n}$ for $|t|$ odd. Then one remarks that for

- $|t|$ even the connected multi-polymer

$$X = (\gamma_1, \ldots, \gamma_n) := (p_{l_1,r_n}, p_{r_1,l_2}, \ldots, p_{r_{n-1},l_n}) \in C_n^{\infty,e}$$

  and for

- $|t|$ odd the connected multi-polymer

$$X = (\gamma_1, \ldots, \gamma_n) := (p_{l_1}, p_{r_1,l_2}, \ldots, p_{r_{n-1},l_n}) \in C_n^{\infty},$$

and their $n!$ different permutations have the property $\sum_{i=1}^n \gamma_i = t$. So they give contributions to $j_k^C(t)$ and $j_k^G(t)$ in (14) and (15).

The factor $|X|! = n!$ in the denominator is cancelled by the multiplicity of the permutations. The graphs $G(X)$ are trees, namely all γ_i, $i > 1$ are only connected to γ_1. So $n(X) \equiv n(G(X)) = -(-1)^n$. The activities are $z^X = (-1)^n \cdot 3^{l_1-r_n-1} \cdot 3^{r_1-l_2-1} \ldots 3^{r_{n-1}-l_n-1}$ for $|t|$ even resp. $z^X = (-1)^n \cdot 3^{l_1-k-1} \cdot 3^{r_1-l_2-1} \ldots 3^{r_{n-1}-l_n-1}$ for $|t|$ odd. Thus multiplying these factors lead to the estimates of the corollary.

One obtains inequality (19) by noticing that in the grand canonical case the activities of the occurring (even) polymers are translation invariant. If both s and t are non-zero, then (19) simply states that $j_{k+l}^G(s,t) \geq 0$, i.e. the ferromagnetic property. If s or t is zero, then all connected multi-polymers contributing to the right hand side of (19) contribute to l.h.s., too (after a translation by k for the t-terms). $\square$.

Remark. Proposition 3 of [10] says that for non-zero $t \in \mathbf{G}_n^*$

$$j_{n+1}^C(t,0) \leq j_n^C(t) \leq j_{n+1}^C(0,t).$$

This implies in particular that the canonical interaction coefficients neither increase nor decrease under concatenation.

5 Estimates for the Free Energy

In this section we will show that the limit free energy is majorized by the canonical and minimized by the grand canonical k-spin free energies.

In order to derive these estimates, we compare the (grand) canonical energy values of the spin chain of length $k+l$ with the ones of the chains with lengths k and l. We state these inequalities for the exponentiated energies.

Lemma 6 *For $\sigma \in \mathbf{G}_k$, $\tau \in \mathbf{G}_l$ one has*

$$\mathbf{h}^G_{k+l}(\sigma,\tau) \leq \mathbf{h}^G_k(\sigma) \cdot \mathbf{h}^G_l(\tau), \tag{20}$$

$$\mathbf{h}^C_{k+l}(\sigma,\tau) + \mathbf{h}^C_{k+l}(1-\sigma,\tau) = \Big(\mathbf{h}^C_k(\sigma) + \mathbf{h}^C_k(1-\sigma)\Big) \cdot \mathbf{h}^C_l(\tau) \tag{21}$$

and

$$\Big|\mathbf{h}^C_{k+l}(\sigma,\tau) - \mathbf{h}^C_{k+l}(1-\sigma,\tau)\Big| \leq \Big|\mathbf{h}^C_k(\sigma) - \mathbf{h}^C_k(1-\sigma)\Big| \cdot \mathbf{h}^C_l(\tau). \tag{22}$$

Proof. As in [8] we use the auxiliary functions $\mathbf{r}_k(s_0,s_1) : \mathbf{G}_k \to \mathbb{R}$ with real parameters s_0, s_1 which are defined by $\mathbf{r}_1(s_0,s_1)(\sigma) := s_\sigma$ and

$$\begin{aligned}&\mathbf{r}_{k+1}(s_0,s_1)(\sigma_1,\ldots,\sigma_{k+1}) :=\\ &\quad \mathbf{r}_k(s_0,s_1)(\sigma_1,\ldots,\sigma_k) + \sigma_{k+1}\cdot \mathbf{r}_k(s_0,s_1)(1-\sigma_1,\ldots,1-\sigma_k).\end{aligned}$$

In particular we have $\mathbf{h}^C_k = \mathbf{r}_k(1,2)$, $k \in \mathbb{N}$ and $\mathbf{h}^G_k(\sigma) = \mathbf{h}^C_{k+1}(\sigma,1) = \mathbf{r}_{k+1}(1,2)(\sigma,1)$, $\sigma \in \mathbf{G}_k$.

By Lemma 4.6 of [8]

$$\mathbf{r}_{k+l}(s_0,s_1)(\sigma,\tau) = \mathbf{r}_{l+1}(\mathbf{r}_k(s_0,s_1)(\sigma), \mathbf{r}_k(s_0,s_1)(1-\sigma))(0,\tau).$$

Moreover we have for $\rho \in \mathbf{G}_l$

$$\mathbf{r}_{l+1}(s,s)(0,\rho) = \mathbf{r}_l(s,2s)(\rho),$$

since for $l=1$ both sides equal $s\cdot(1+\rho)$, whereas for $\rho' \in \mathbf{G}_l$, $\rho'' \in \mathbf{G}_1$ and $\rho = (\rho',\rho'') \in \mathbf{G}_{l+1}$

$$\begin{aligned}\mathbf{r}_{l+2}(s,s)(0,\rho) &= \mathbf{r}_{l+1}(s,s)(0,\rho') + \rho''\mathbf{r}_{l+1}(s,s)(1,1-\rho')\\ &= \mathbf{r}_l(s,2s)(\rho') + \rho''\mathbf{r}_{l+1}(s,s)(0,1-\rho')\\ &= \mathbf{r}_l(s,2s)(\rho') + \rho''\mathbf{r}_l(s,2s)(1-\rho')\\ &= \mathbf{r}_{l+1}(s,2s)(\rho).\end{aligned}$$

Now we apply these identities:

$$\begin{aligned}
\mathbf{h}^G_{k+l}(\sigma,\tau) &= \mathbf{r}_{k+l+1}(1,2)(\sigma,\tau,1) = \mathbf{r}_{l+2}\left(\mathbf{r}_k(1,2)(\sigma),\mathbf{r}_k(1,2)(1-\sigma)\right)(0,\tau,1)\\
&= \mathbf{r}_{l+2}\left(\mathbf{h}^C_k(\sigma),\mathbf{h}^C_k(1-\sigma)\right)(0,\tau,1)\\
&= \mathbf{h}^C_k(\sigma)\cdot\mathbf{r}_{l+2}(1,0)(0,\tau,1)+\mathbf{h}^C_k(1-\sigma)\cdot\mathbf{r}_{l+2}(0,1)(0,\tau,1)\\
&\le \left(\mathbf{h}^C_k(\sigma)+\mathbf{h}^C_k(1-\sigma)\right)\cdot\mathbf{r}_{l+2}(1,1)(0,\tau,1)\\
&= \mathbf{h}^G_k(\sigma)\cdot\mathbf{r}_{l+2}(1,1)(0,\tau,1)\\
&= \mathbf{h}^G_k(\sigma)\cdot\mathbf{r}_{l+1}(1,2)(\tau,1)\\
&= \mathbf{h}^G_k(\sigma)\cdot\mathbf{h}^G_l(\tau),
\end{aligned}$$

showing (20).

Similarly

$$\mathbf{h}^C_{k+l}(\sigma,\tau)=\mathbf{h}^C_k(\sigma)\cdot\mathbf{r}_{l+1}(1,0)(0,\tau)+\mathbf{h}^C_k(1-\sigma)\cdot\mathbf{r}_{l+1}(0,1)(0,\tau)$$

so that

$$\begin{aligned}
&\mathbf{h}^C_{k+l}(\sigma,\tau)+\mathbf{h}^C_{k+l}(1-\sigma,\tau)\\
&\quad= \left(\mathbf{h}^C_k(\sigma)+\mathbf{h}^C_k(1-\sigma)\right)\cdot\left(\mathbf{r}_{l+1}(1,0)(0,\tau)+\mathbf{r}_{l+1}(0,1)(0,\tau)\right)\\
&\quad= \left(\mathbf{h}^C_k(\sigma)+\mathbf{h}^C_k(1-\sigma)\right)\cdot\mathbf{r}_{l+1}(1,1)(0,\tau)\\
&\quad= \left(\mathbf{h}^C_k(\sigma)+\mathbf{h}^C_k(1-\sigma)\right)\cdot\mathbf{r}_{l}(1,2)(\tau),
\end{aligned}$$

which implies (21).

The difference

$$\begin{aligned}
&\left|\mathbf{h}^C_{k+l}(\sigma,\tau)-\mathbf{h}^C_{k+l}(1-\sigma,\tau)\right|\\
&\quad= \left|\mathbf{h}^C_k(\sigma)-\mathbf{h}^C_k(1-\sigma)\right|\cdot\left|\mathbf{r}_{l+1}(1,0)(0,\tau)-\mathbf{r}_{l+1}(0,1)(0,\tau)\right|\\
&\quad\le \left|\mathbf{h}^C_k(\sigma)-\mathbf{h}^C_k(1-\sigma)\right|\cdot\mathbf{h}^C_l(\tau),
\end{aligned}$$

which is (22). □

Theorem 7 *For inverse temperature $\beta>0$ the limit free energy $F(\beta)$ is bounded by the k-spin free energies, $k\in\mathbb{N}$:*

$$F^C_k(\beta)\le F(\beta)\le F^G_k(\beta).$$

(See Fig. 2, where $k=15$).

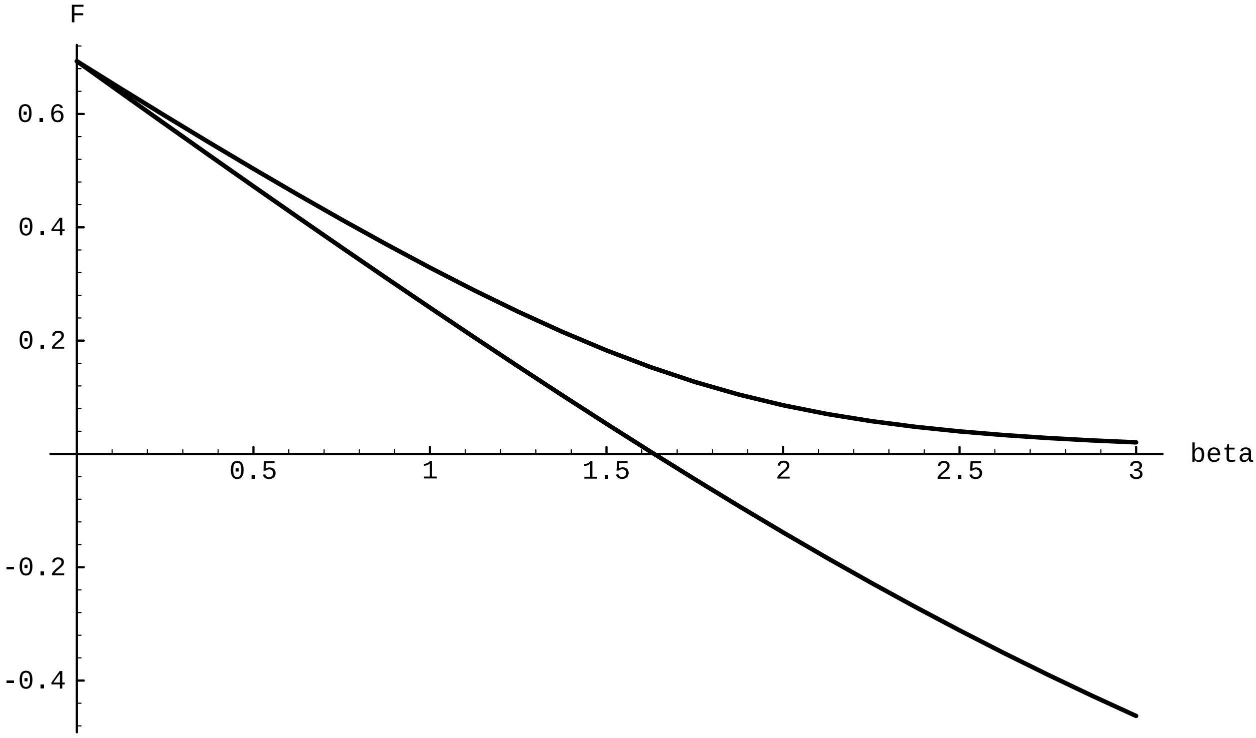

Figure 2: Upper and lower bounds on the free energy $F(\beta)$

Proof. We have for $n \in \mathbb{N}$

$$F_{nk}^G(\beta) = -\frac{1}{\beta k} \ln \left(Z_{nk}^G(\beta) \right)^{1/n} \leq -\frac{1}{\beta k} \ln \left(Z_k^G(\beta) \right) = F_k^G(\beta),$$

since by (20)

$$\begin{aligned} Z_{k+l}^G(\beta) &= \sum_{\sigma \in \mathbf{G}_k} \sum_{\tau \in \mathbf{G}_l} \left(\mathbf{h}_{k+l}^G(\sigma, \tau) \right)^{-\beta} \\ &\geq \sum_{\sigma \in \mathbf{G}_k} \sum_{\tau \in \mathbf{G}_l} \left(\mathbf{h}_k^G(\sigma) \cdot \mathbf{h}_l^G(\tau) \right)^{-\beta} = Z_k^G(\beta) \cdot Z_l^G(\beta). \end{aligned}$$

So $F(\beta) = \lim_{n \to \infty} F_{nk}^G(\beta) \leq F_k^G(\beta)$.

To show the lower estimate we need the converse inequality

$$Z_{k+l}^C(\beta) \leq Z_k^C(\beta) \cdot Z_l^C(\beta) \tag{23}$$

which then implies $F(\beta) = \lim_{n \to \infty} F_{nk}^C(\beta) \geq F_k^C(\beta)$.

To show (23), we use (21) and (22). For $a, b, c, d > 0$, $a + b = c + d$ and $|a - b| \leq |c - d|$ the convexity of the function $x \mapsto x^{-\beta}$ implies $a^{-\beta} + b^{-\beta} \leq$

$c^{-\beta}+d^{-\beta}$. Thus

$$\left(\mathbf{h}^C_{k+l}(\sigma,\tau)\right)^{-\beta}+\left(\mathbf{h}^C_{k+l}(1-\sigma,\tau)\right)^{-\beta}\leq\left(\mathbf{h}^C_k(\sigma)^{-\beta}+\mathbf{h}^C_k(1-\sigma)^{-\beta}\right)\cdot\mathbf{h}^C_l(\tau)^{-\beta}$$

which after summation over σ and τ leads to (23). $\Box$

6 The Internal Energy

From the estimates for the free energy we will derive upper and lower bounds for the internal energy per particle

$$U(\beta)=\lim_{k\to\infty}\frac{1}{k}\left\langle\mathbf{H}^C_k\right\rangle^C_k(\beta)=\lim_{k\to\infty}\frac{1}{k}\left\langle\mathbf{H}^G_k\right\rangle^G_k(\beta).$$

The first thing to say is that in general the k-spin energy expectation $\langle H_k\rangle(\beta)$ is *not* a monotone increasing function of the energy values $H_k(\sigma)$. But if

$$H_k(\sigma)=-\sum_{t\in\mathbf{G}^*_k}j(t)\cdot(-1)^{\sigma\cdot t}$$

is weakly ferromagnetic ($j(t)\geq 0$ for $t\neq 0_k$), then by the first and second GKS inequality for $\beta\geq 0$ and $s\in\mathbf{G}^*_k$

$$\frac{\partial\langle H_k\rangle}{\partial j(s)}=-\langle\chi_s\rangle-\beta\sum_{t\in\mathbf{G}^*_k}j(t)(\langle\chi_s\chi_t\rangle-\langle\chi_s\rangle\langle\chi_t\rangle)\leq 0 \tag{24}$$

with the character functions $\chi_s:\mathbf{G}_k\to\{-1,1\}$,

$$\chi_s(\sigma):=(-1)^{\sigma\cdot s}=\prod_{i:s_i=1}(-1)^{\sigma_i}.$$

Theorem 8 *For $\beta\geq 0$ and $k\in\mathbb{N}$*

$$U(\beta)\leq\frac{1}{k}\left\langle\mathbf{H}^G_k\right\rangle^G_k(\beta).$$

Proof. We start from the inequality (19)

$$j^G_{k+l}(s,t)\geq\delta_{t,0}\cdot j^G_k(s)+\delta_{s,0}\cdot j^G_l(t),\qquad(s\in\mathbf{G}^*_k,t\in\mathbf{G}^*_l)$$

for the interaction coefficients. Thus by (24)

$$\left\langle \mathbf{H}^G_{k+l} \right\rangle^G_{k+l} \le \left\langle \mathbf{H}^G_k \right\rangle^G_k + \left\langle \mathbf{H}^G_l \right\rangle^G_l .$$

In particular we have $\frac{1}{n}\left\langle \mathbf{H}^G_{nk} \right\rangle^G_{nk} \le \left\langle \mathbf{H}^G_k \right\rangle^G_k$ so that the theorem follows. $\Box$

We can also use the concavity of the function $\beta \mapsto \beta F(\beta)$ and our knowledge of the two values $\lim_{\beta\searrow 0} \beta F(\beta) = -\ln 2$ and $\beta_{\rm cr} F(\beta_{\rm cr}) = 0$ for the inverse critical temperature $\beta_{\rm cr} = 2$.

Theorem 9 *For* $0 < \beta < \beta_{\rm cr} = 2$ *and* $k \in \mathbb{N}$

$$\frac{-\beta F^G_k(\beta)}{2-\beta} \le U(\beta) \le \frac{\ln(2) + \beta F^G_k(\beta)}{\beta}.$$

Proof. In the above inverse temperature range the free energy is real-analytic, as shown in [2]. Thus we can write the internal energy in the form

$$U(\beta) = \frac{d}{d\beta}(\beta F(\beta)).$$

By concavity of the function $\beta \mapsto \beta F(\beta)$ the derivative is bounded by the slope of the secants:

$$\frac{\beta_{\rm cr} F(\beta_{\rm cr}) - \beta F(\beta)}{\beta_{\rm cr} - \beta} \le U(\beta) \le \frac{\beta F^G_k(\beta) - (-\ln(2))}{\beta - 0}.$$

The bounds then follow from this and Theorem 7. $\Box$

In Fig. 3 we show the different bounds on the internal energy $U(\beta)$ for $k = 15$. Although for this number k of spins Thm. 9 leads to a better upper bound than Thm. 8, only the latter estimate converges in the thermodynamic limit $k \to \infty$.

Since the methods used here are high-temperature expansions, the lower estimate for the internal energy derived in [2] is better near the critical temperature $\beta = 2$ but worse near $\beta = 0$.

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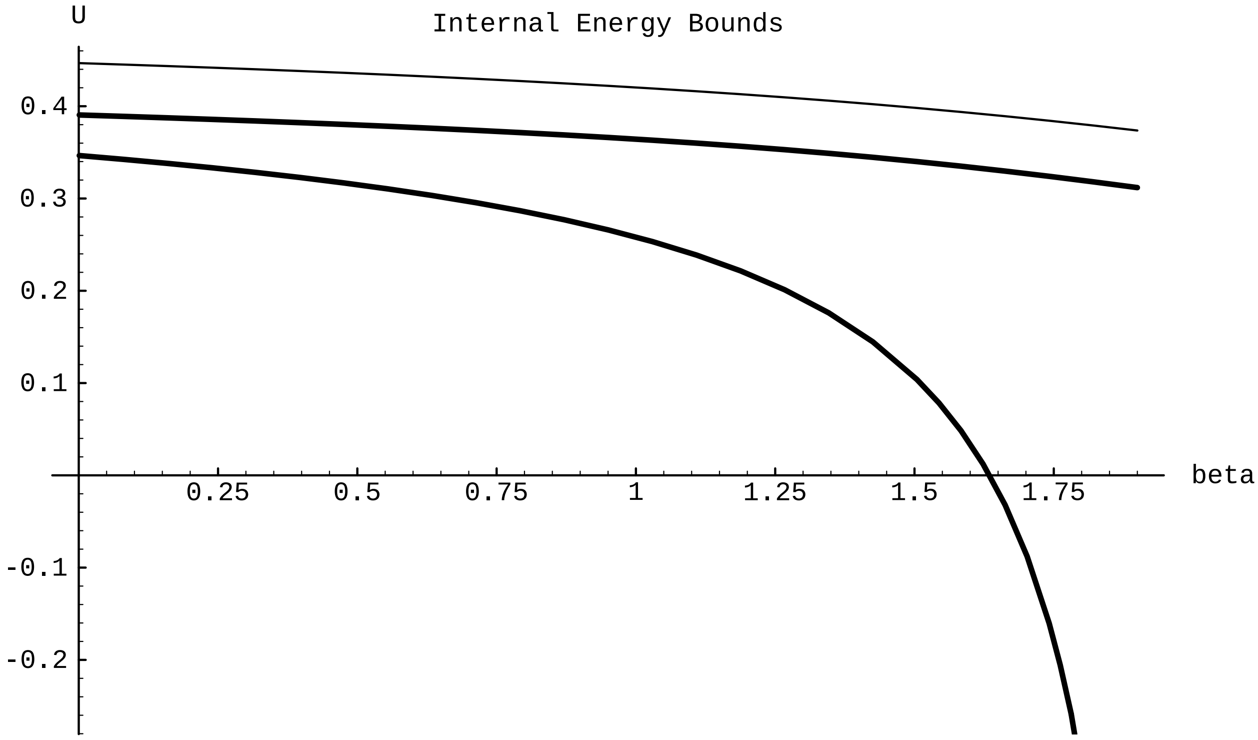

Figure 3: Upper and lower bounds on the internal energy $U(\beta)$ (bold: Thm. 9)

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