Phases of the Number-Theoretical Spin Chain

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Abstract

We present numerical and analytical evidence for a first-order phase transition of the ferromagnetic spin chain with partition function $Z(\beta) = \zeta(\beta - 1)/\zeta(\beta)$ at the inverse temperature $\beta_{\mathrm{cr}} = 2$.

KEY WORDS: Riemann zeta function, spin chain, phase transition.

In a recent paper [6] we established a link between analytic number theory and classical statistical mechanics by interpreting the quotient

$$Z(s) = \zeta(s-1)/\zeta(s)$$

of Riemann zeta functions as the partition function of an infinite spin chain with ferromagnetic interactions. For $\mathrm{Re}(s) > 2$ the quotient has the Dirichlet series representation

$$Z(s) = \sum_{n=1}^{\infty} \varphi(n) \cdot n^{-s} \tag{1}$$

where for $n \geq 1$ the Euler totient function $\varphi(n)$ is defined to be the number of positive integers not exceeding n which are relatively prime to n (that is, $\varphi(n) = \#\{i \in \{1, \ldots, n\} \mid \gcd(i,n) = 1\}$). Now on any half-plane of the form $\mathrm{Re}(s) > 2 + \varepsilon$, $\varepsilon > 0$, Z is uniformly approximated by partition functions

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

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with $\mathbf{G}_k := (\{0,1\})^k$, $k \in \mathbf{N}_0$ and canonical energy function $\mathbf{H}_k^C := \ln \mathbf{h}_k^C$. The coefficients $\mathbf{h}_k^C(\sigma)$, $\sigma = (\sigma_1, \ldots, \sigma_k) \in \mathbf{G}_k$, are defined inductively by setting $\mathbf{h}_0^C(0) := 1$,

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

with $1 - \sigma \equiv (1 - \sigma_1, \ldots, 1 - \sigma_k)$.

For example, for $k = 3$ we have $\mathbf{h}_3^C(000) = 1$, $\mathbf{h}_3^C(001) = \mathbf{h}_3^C(111) = 4$, $\mathbf{h}_3^C(010) = \mathbf{h}_3^C(110) = 3$, $\mathbf{h}_3^C(011) = \mathbf{h}_3^C(101) = 5$ and $\mathbf{h}_3^C(100) = 2$.

Writing

$$Z_k(s) = \sum_{n=1}^{\infty} \varphi_k(n) \cdot n^{-s} \qquad \text{with } \varphi_k(n) = \#\{\sigma \in \mathbf{G}_k \mid \mathbf{h}_k^C(\sigma) = n\},$$

we have $\varphi_k(n) \leq \varphi_{k+1}(n) \leq \varphi(n)$.

For functions f on the additive group $\mathbf{G}_k$ we define the Fourier transform $\mathcal{F}_k f$ by

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

We call the coefficients

$$j_k^C(t) := -(\mathcal{F}_k \mathbf{H}_k^C)(t)$$

of the Fourier transform of $-\mathbf{H}_k^C$ the canonical interaction coefficients. Then the canonical energy function $\mathbf{H}_k^C$ is the negative inverse Fourier transform of j_k^C:

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

We use the unconventional spin values $\sigma_i \in \{0, 1\}$ instead of $(-1)^{\sigma_i} \in \{1, -1\}$ since then the strings $\sigma = (\sigma_1, \ldots, \sigma_k)$ can be interpreted as the dyadic representations of the integers between 0 and $2^k - 1$, see [6].

Similarly, we consider the grand canonical interaction coefficients $j_k^G(t) := -(\mathcal{F}_k \mathbf{H}_k^G)(t)$ of the grand canonical energy functions $\mathbf{H}_k^G(\sigma) := \mathbf{H}_{k+1}^C(\sigma, 1)$.

Let $\#_k(t) := \#\{i \in \{1, \ldots, k\} \mid t_i = 1\}$ denote the number of ones appearing in $t = (t_1, \ldots, t_k)$. Then the coefficients $j_k^C(t)$ with $\#_k(t) = 1$ describe the couplings of the individual spins to an external magnetic field, and for $\#_k(t) = 2$ the interaction coefficients are the strengths of the pair interactions.

In [6] we proved several results on the form of the interaction:

1. The multibody interactions (i.e., $\#_k(t) > 2$) are non-zero in general. Nevertheless, for the grand canonical ensemble we have
$$j_k^G(t) = 0 \qquad \text{for } \#_k(t) = \text{ odd}.$$
In particular, there is no external magnetic field for the grand canonical ensemble.

   The grand canonical ensemble is mirror-symmetric, that is,
$$j_k^G(t_1, \ldots, t_k) = j_k^G(t_k, \ldots, t_1).$$

2. The interaction coefficients are asymptotically translation invariant in the sense that the difference $j_{k+1}^G(0,t) - j_{k+1}^G(t,0)$ is small in absolute value if both l and $k-r$ are large for $t \in \mathbf{G}_k^*$ of the form
$$t \equiv (t_1, \ldots, t_k) = (0, \ldots, 0, 1, t_{l+1}, \ldots, t_{r-1}, 1, 0, \ldots, 0):$$
$$|j_{k+1}^G(0,t) - j_{k+1}^G(t,0)| < (2^{-r} + 2^{l-(k+1)}) \ln 2.$$

3. The interaction stabilizes in the thermodynamic limit $k \to \infty$, namely for $t \in \mathbf{G}_{k+1} \setminus \{0\}$ with an even number $\#_{k+1}(t)$ of ones and
$$t \equiv (t_1, \ldots, t_{k+1}) = (t_1, \ldots, t_{r-1}, 1, 0, \ldots, 0)$$
we have
$$|j_{k+1}^G(t_1, \ldots, t_{k+1}) - j_k^G(t_2, \ldots, t_{k+1})| < 2^{1-r} \cdot \ln 2.$$

4. The individual canonical interaction coefficients are bounded from above by
$$j_k^C(t) \le 2^{-(r-l)+1} \cdot \ln 2 \qquad \text{for } \#_k(t) = \text{ even}$$
and
$$j_k^C(t) \le 2^{-(k-l)} \cdot \ln 2 \qquad \text{for } \#_k(t) = \text{ odd},$$
respectively. So the odd canonical interactions are small except for those involving only spins near the right edge of the chain. The canonical interaction coefficients for an even number of spins decay exponentially with the maximal distance $r-l$ of spins involved.

5. This exponential decay estimate is not enough to guarantee the existence of a thermodynamic limit of the free energy, since the number of interaction coefficients grows with the same exponential rate. To describe the fall-off of the potential, we consider for $l, r, k \in \mathbf{N}$ and $1 \le l < r \le k$ the functions
$$A_k^G(l,r) := \sum_{(t_{l+1}, \ldots, t_{r-1})} j_k^G(0, \ldots, 0, 1, t_{l+1}, \ldots, t_{r-1}, 1, 0, \ldots, 0)$$
and similarly for the canonical ensemble. We obtain the estimate
$$A_k^G(l,r) \le \left(\frac{1}{r-l}\right)^2, \qquad (2)$$
that is, a quadratic decay with the maximal distance of spins involved.

   Generally speaking, for one-dimensional spin systems we need a decay rate which is faster than $(r-l)^{-1}$ in order to guarantee for the existence of a thermodynamic limit.

   On the other hand, extending a result of van Hove, Ruelle [8] showed that for systems with a faster than second power decay of the potential no phase transition occurs (the Gibbs measure depending continuously on the temperature). So w.r.t. phase transitions we are in a borderline situation.

6. The system is ferromagnetic in the sense that for all $k \in \mathbf{N}_0$
$$j_k^C(t) \ge 0 \text{ and } j_k^G(t) \ge 0 \qquad \text{for all } t \ne 0.$$
This fact is remarkable insofar much more is known about ferromagnetic spin systems than about non-ferromagnetic ones (GKS inequalities, Lee-Yang theorem, etc.). So there is some hope that one may prove new results on Riemann's zeta function by applying ideas from statistical mechanics.

The interested reader should consult [6] and [7] for more information. See also the related work [3] of Bost and Connes on Hecke C^*-algebras and the Riemann zeta function.

Among the thermodynamical quantities describing a spin chain of length k there are the density F_k of the free energy, the expectation value U_k of the energy density and the mean magnetization M_k. These quantities are defined by

$$F_k(\beta) := -\frac{1}{\beta \cdot k} \ln\left(Z_k(\beta)\right),$$

$$U_k(\beta) := \frac{1}{k}\left\langle \mathbf{H}_k^C \right\rangle_k (\beta)$$

and

$$M_k(\beta) := \left\langle \frac{1}{k}\sum_{i=1}^{k} \mu_i \right\rangle_k (\beta)$$

with $\mu_i := (-1)^{\sigma_i}$ and

$$\langle G\rangle_k(\beta) := \frac{1}{Z_k(\beta)} \cdot \sum_{\sigma\in\mathbf{G}_k} G(\sigma)\exp\left(-s\cdot \mathbf{H}_k^C(\sigma)\right)$$

denoting the expectation of a variable G for the Gibbs ensemble of the spin chain of length k at inverse temperature β.

Note that the ferromagnetic property and the GKS inequalities imply

$$M_k(\beta) \geq 0 \text{ and } \frac{d}{d\beta}M_k(\beta) \geq 0 \quad \text{for all } k\in\mathbf{N}.$$

Moreover, for $\beta > 2$ we have for $i \in \{1,\ldots,k\}$ the k-independent estimate

$$\langle \mu_i\rangle_k(\beta) > 1 - \frac{2}{\beta-2}(i+1)^{2-\beta}, \tag{3}$$

which follows from

$$\begin{aligned}\langle \mu_i\rangle_k(\beta) &= 1 - 2\frac{\sum_{\rho\in\mathbf{G}_{i-1}}\sum_{\tau\in\mathbf{G}_{k-i}}\exp(-\beta\mathbf{H}_k^C(\rho,1,\tau))}{Z_k(\beta)}\\ &\geq 1 - 2\sum_{n=i+2}^{\infty}\varphi(n)\cdot n^{-\beta} > 1 - 2\sum_{n=i+2}^{\infty} n^{1-\beta}\\ &> 1 - 2\int_{n=i+1}^{\infty} n^{1-\beta}\,dn\end{aligned}$$

since $Z_k(\beta) \geq 1$ and $\varphi_k(n) \leq \varphi(n) \leq n$.

For $\beta > 2$ both $F_k(\beta)$ and $U_k(\beta)$ tend to zero in the thermodynamic limit $k\to\infty$, since the series (1) is absolutely convergent and since $U_k(\beta) = \frac{d}{d\beta}(\beta F_k(\beta))$. Estimate (3) implies

$$M(\beta) := \lim_{k\to\infty} M_k(\beta) = 1. \tag{4}$$

On the other hand, in the large temperature limit we have

$$\lim_{\beta\searrow 0}\beta\cdot F_k(\beta) = -\ln 2 \tag{5}$$

independent of k. So at least for one inverse critical temperature $\beta_{\rm cr}$ with $0 < \beta_{\rm cr} \leq 2$ a phase transition (i.e., point of non-analyticity of the free energy) occurs.

We can easily obtain a better lower estimate for $\beta_{\rm cr}$ by the following argument.

$$-\beta F_k(\beta) = \frac{1}{k}\ln\left(1 + \sum_{l=0}^{k-1} Z_l^G(\beta)\right)$$

with grand canonical partition function

$$Z_l^G(\beta) := \sum_{\sigma\in\mathbf{G}_l}\exp(-\beta\mathbf{H}_l^G(\sigma)) = \sum_{\sigma\in\mathbf{G}_l}(\mathbf{h}_l^G(\sigma))^{-\beta}$$

for $\mathbf{h}_l^G(\sigma) := \exp(\mathbf{H}_l^G(\sigma))$. Moreover,

$$\mathbf{h}_l^G(\sigma) = \mathbf{h}_{l+1}^C(\sigma,1) = \mathbf{h}_l^C(\sigma) + \mathbf{h}_l^C(1-\sigma), \tag{6}$$

$$\mathbf{h}_{l+1}^G(\sigma,0) = 2\mathbf{h}_l^C(\sigma) + \mathbf{h}_l^C(1-\sigma), \tag{7}$$

and

$$\mathbf{h}_{l+1}^G(\sigma,1) = \mathbf{h}_l^C(\sigma) + 2\mathbf{h}_l^C(1-\sigma). \tag{8}$$

In [7] we proved the existence of the thermodynamic limit

$$F(\beta) := \lim_{k\to\infty} F_k(\beta).$$

By concavity of $\beta\cdot F(\beta)$ the thermodynamic limit $U(\beta)$ of $U_k(\beta)$ exists for almost all β and is monotone decreasing.

We already know that $F(\beta) = 0$ for $\beta \geq 2$. Thus for $\beta > 2$ we have $U(\beta) = 0$, too. In other words, the system is in a frozen state for low temperatures, having mean magnetization $M(\beta) = 1$ by (4).

For high temperatures ($\beta < 2$) the analytic continuation of $Z(\beta)$ cannot be directly interpreted as the partition function of the infinite chain. There, $\lim_{k\to\infty} Z_k(\beta) = \infty$ so that the partition functions of the finite chains do not converge to $Z(\beta)$.

Nevertheless, the free energy $F(\beta)$ of the infinite chain *is* well-defined.

Here we show that

$$-\beta F(\beta) \geq \ln 2 - \beta \cdot \ln 3/2 \tag{9}$$

which implies the existence of a phase transition at some

$$\beta_{\rm cr} \geq \frac{\ln 2}{\ln 3/2} \approx 1.709.$$

(9) follows from the inequality

$$\frac{Z_{l+1}^G(\beta)}{Z_l^G(\beta)} \geq 2 \cdot \left(\frac{3}{2}\right)^{-\beta}$$

which in turn follows from the estimates

$$\frac{(\mathbf{h}_{l+1}^G(\sigma,0))^{-\beta} + (\mathbf{h}_{l+1}^G(\sigma,1))^{-\beta}}{(\mathbf{h}_l^G(\sigma))^{-\beta}} \geq 2 \cdot \left(\frac{3}{2}\right)^{-\beta} \quad \text{for all } \sigma \in \mathbf{G}_l. \tag{10}$$

But by (6), (7) and (8) the l.h.s. of (10) has the form

$$f(d,\beta) := \frac{(2d+1)^{-\beta} + (d+2)^{-\beta}}{(d+1)^{-\beta}}$$

with $d := \mathbf{h}_l^C(\sigma)/\mathbf{h}_l^C(1-\sigma)$.

As a function of d, $f(d,\beta)$ has its absolute non-degenerate minimum at $d = 1$, and $f(1,\beta) = 2 \cdot (3/2)^{-\beta}$, proving (10).

The inequality (9) together with the concavity of $\beta F(\beta)$ and $F(2) = 0$ imply

$$U(\beta) = \frac{d}{d\beta}(\beta F(\beta)) \geq \frac{\ln 2 - \beta \ln(3/2)}{2 - \beta} \qquad \text{for } \beta \leq \frac{\ln 2}{\ln 3/2}. \tag{11}$$

On the other hand, (9), the concavity of $\beta F(\beta)$ and (5) imply

$$U(\beta) \leq U(0) \leq \ln 3/2 \approx 0.405.$$

Figure 1: The mean magnetization $M_k(\beta)$ as a function of the inverse temperature β for $k = 600$ spins

Numerically the first traces of a phase transition can be seen for chains of lengths ~ 100. Since there are 2^k configurations, the sums appearing in the above definitions of the thermodynamic quantities had to be evaluated approximately, using the Metropolis algorithm of the Monte Carlo method.

Interpreting the numerical results, it seems likely that for $\beta_{\rm cr} = 2$ a first order transition occurs, the magnetization $M(\beta)$ of the infinite chain going discontinuously from one to zero as one enlarges the temperature (Fig. 1).

Similarly, the energy density $U(\beta)$, being zero for $\beta > 2$, seems to rise sharply from zero to a positive value at $\beta_{\rm cr} = 2$ (Fig. 2).

In order to control the precision of the approximation a full temperature cycle from $\beta = 1.2$ up to $\beta = 2.7$ and then back to $\beta = 1.2$ was calculated. The two curves in Fig. 1 show no hysteresis so that the appearance of metastable states is unlikely.

Figure 3 shows two typical configurations (that is, configurations generated by the Metropolis algorithm) for temperatures just below respectively above the critical temperature. In the magnetic phase, the inverted spins with $\sigma_i = 1$ tend to concentrate on the l.h.s. of the spin chain (for $\beta = 2.05$

Figure 2: The density $U_k(\beta)$ of the inner energy and the lower bound (11)

the configuration shown has $\sigma_i = 0$ for $i > 99$.

In fact, the rightmost position r of a spin with $\sigma_r = 1$ can be interpreted as the particle number of that configuration in the grand canonical ensemble. In the thermodynamic limit, the expectation value of that particle number is finite for $\beta > 2$ but diverges as $\beta \searrow 2$.

The type of phase transition which is observed numerically is similar to the one discussed by Thouless [9] for the Anderson model and by Dyson [4, 5] for other ferromagnetic chains with long-range interactions.

More recently, Aizenman, J.T. Chayes, L. Chayes and Newman studied one-dimensional models with $1/(x-y)^2$ decay of the interaction [1, 2], proving discontinuity of the magnetization and giving bounds for the critical temperature. In our context, however, one must use the specific form of the energy function in order to prove the above conjectures on the phase transition.

a)

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111111111101100010001111101110110000100001111111110111000000
000000000000000000000000000000000011000000100101100000111111
001111101110000110100011111111111111111111111111111111111111
111111111111111111011111111111110111011100111110100000000110
111000000000000000000000000000100100110000000000000000000000
000000000011100011111010000111110111111111111111111000110111
111100000001110001111111111110000010010010111111001011111110
101110011111111110101101100000010101101111111111111101111111
111111111111111111111111111100001011110001000000000000000111
111110001111111101000000001111110111001111110000000000000000
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b)

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110100010000011100000001000100111101000010111010001000111110
101101001101111111111000111111111111101000000000000000000000
000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000000000000000000000000000
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Figure 3: Typical configurations for a) $\beta = 1.95$ and b) $\beta = 2.05$

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