Analytic properties of the Ruelle ζ–function for mean field models of phase transition

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Abstract. We evaluate by analytical means the Ruelle ζ–function for a spin model with global coupling. The implications of the ferromagnetic phase transitions for the analytical properties of the ζ–function are discussed in detail. In the paramagnetic phase the ζ–function develops a single branch point. In the low–temperature regime two branch points appear which correspond to the ferromagnetic state and the metastable state. The results are typical for any Ginsburg–Landau type phase transition.

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1. Introduction

Spectral properties of linear operators play an important role in quite diverse fields of theoretical physics, e.g. the time evolution operator in dynamical systems theory, the Hamiltonian in quantum mechanics, and transfer operators in equilibrium statistical mechanics. Various types of ζ–functions have been introduced as a tool to evaluate the spectrum of linear operators [1]. Roughly speaking ζ–functions provide an intelligent way for writing down the characteristic equation of a linear operator. In particular there exist suitable expansion and approximation schemes for evaluating ζ–functions in a systematic way (cf. e.g. the seminal article [2] on cycle expansions of dynamical systems). Evaluating the analytic behaviour one is able to determine e.g. ergodic properties of dynamical systems, spectral properties like the density of states in quantum physics, or the partition function and spatial correlations in statistical physics (cf. [3] and references theirin for a comprehensive overview).

The analytical properties of ζ–functions are therefore of great interest. Only in simple cases, like uniformly hyperbolic dynamical systems or statistical mechanics in the high–temperature phase, one has to some extent an overview over the analytical structure. Qualitative changes like bifurcations in dynamical systems or thermodynamic phase transitions in statistical physics are reflected by qualitative changes of the spectrum of the corresponding linear operator and thus leave characteristic fingerprints in the analytic properties of ζ–functions. Classical examples are intermittent motion which causes branch points [4], phase transition behaviour in spin chains caused by long range interactions [5, 6], or anomalous transport in low–dimensional deterministic dynamical systems [7]. But there are only a small number of examples available where the ζ–function can be evaluated by analytical means.

Here we compute the ζ–function for a simple model of equilibrium statistical physics, a spin model with global coupling. Such a mean field model exhibits a phase transition in the thermodynamic limit if the strength of the coupling constant exceeds a certain threshold. We will discuss in detail how the analytical properties of the ζ–function reflect the phase transition. We keep our analysis elementary so that the whole presentation is completely self–contained.

2. Mean field spin model

If Z_N denotes the partition function of a system with N particles then the corresponding ζ–function is defined through the relation

$$\zeta(z) = \exp\left(\sum_{N=1}^{\infty} \frac{z^N}{N} Z_N\right) \quad . \tag{2.1}$$

The complex valued argument z plays the role of a fugacity–like quantity. Since the asymptotic behaviour of the partition function is given by $Z_N \sim \exp(-Nf)$ for large N, where f denotes essentially the free energy per particle, the expression (2.1) develops a singularity at $z = \exp(f)$. Actually this singularity is the singularity with smallest modulus in z.

The logarithm of the ζ–function, $\ln\zeta(z)$, is obviously the formal integral of the grand partition function with respect to z. But contrary to the grand partition function the ζ–function directly relates to the properties of transfer operators [2]. Thus ζ–functions play a prominent role when spectral properties of linear operators are at stake, like in quantum chaos, ergodic theory, or equilibrium statistical mechanics. The analytical properties of the ζ–function, i.e poles and other singularities, directly reflect the spectrum of the corresponding linear operator. Of particular interest are cases when qualitative changes are involved, e.g. in the vicinity of phase transition points.

To investigate the analytical properties of eq.(2.1) we resort to a simple spin system which displays a phase transition in the thermodynamic limit. Consider the globally coupled Ising Hamiltonian

$$\beta\mathcal{H} = -H\sum_{\nu=1}^{N}\sigma_\nu - \frac{J}{2N}\sum_{\nu,\mu=1}^{N}\sigma_\nu\sigma_\mu \tag{2.2}$$

where $\sigma_\nu = \pm 1$ denotes the single site spin variable and $J \geq 0$ the coupling constant. It is standard textbook knowledge that the system undergoes a second order phase transition at $H = 0$ and $J = J_c = 1$. For simplicity we have absorbed the temperature β in the parameters of the model. Evaluation of the partition function for finite N is standard and yields (to keep our presentation self–contained we have summarised the main computational steps in Appendix A, although the calculation can be found in most textbooks on statistical mechanics)

$$Z_N = 2^N\sqrt{\frac{N}{\pi}}\int_{-\infty}^{\infty}\exp\left(-Ng(u)\right)\,du \tag{2.3}$$

where

$$g(u) = u^2 - \ln\cosh\left(u\sqrt{2J} + H\right) \quad . \tag{2.4}$$

Combining eqs.(2.1) and (2.3) we obtain for the ζ–function

$$\ln\zeta(z) = \sum_{N=1}^{\infty}\frac{z^N}{N}Z_N = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\mathrm{Li}_{1/2}\left[2z\exp\left(-g(u)\right)\right]\,du \tag{2.5}$$

where we have used the polylogarithm‖ [8, 9]

$$\mathrm{Li}_s\left[z\right] = \sum_{N=1}^{\infty}\frac{z^N}{N^s} \tag{2.6}$$

which is a generalisation of Eulers dilogarithm (cf. e.g. [10] for a recent application of the polylogarithm in statistical mechanics). We are thus left with the discussion of the analytical properties of the integral (2.5).

‖ Usually one reserves the notion polylogarithm for eq.(2.6) with integer s. For non integer values of s one sometimes calls eq.(2.6) Joncquiéres function which is closely related to the Lerch transcendent.

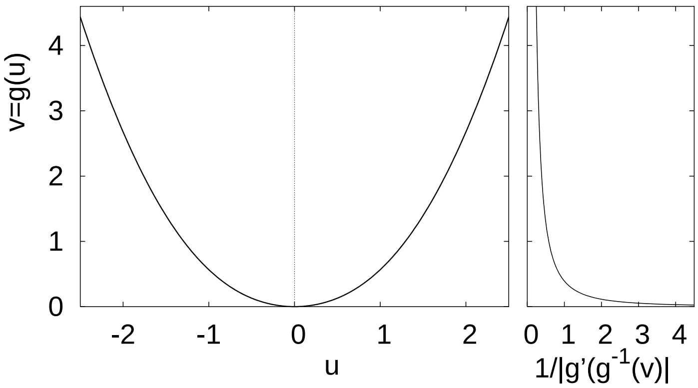

Figure 1. Left: potential (2.4) in the high–temperature regime for $J = 0.5$. Right: modulus of the derivative of the inverse branch, $1/|g'(g_1^{-1}(v))|$, (cf. eq.(3.2)).

3. Analytical properties of the ζ–function

As a simple exercise let us first consider the case without interaction $J = 0$. Because of eq.(2.4) the inverse of $g(u)$ has two branches $g_{1,2}^{-1}(v) = \pm\sqrt{v + \ln(\cosh(H))}$ and substitution yields

$$\begin{aligned}\ln\zeta(z) &= \frac{1}{\sqrt{\pi}}\int_{-\ln\cosh(H)}^{\infty}\frac{1}{\sqrt{v+\ln(\cosh(H))}}\mathrm{Li}_{1/2}\left[2z\exp(-v)\right]\,dv\\ &= \frac{1}{\sqrt{\pi}}\int_{0}^{\infty}\frac{1}{\sqrt{v}}\mathrm{Li}_{1/2}\left[2z\cosh(H)\exp(-v)\right]\,dv\\ &= -\ln\left(1-2z\cosh(H)\right) \quad .\end{aligned} \tag{3.1}$$

For the last step we used the identities (B.3) and (B.2) of the polylogarithm. Thus the ζ–function has a simple pole at $z = 1/(2\cosh(H)) = \exp(f)$.

Let us now consider a non vanishing coupling but let us focus on the case without external field, $H = 0$. In the high–temperature regime $J < J_c = 1$ eq.(2.4) yields a symmetric convex function with a minimum at the origin (cf. figure 1). Thus the inverse consists of two branches $g_1^{-1}(v) = -g_2^{-1}(v) \geq 0$ like in the case of vanishing coupling. Using substitution eq.(2.5) reads

$$\ln\zeta(z) = \frac{2}{\sqrt{\pi}}\int_0^{\infty}\frac{1}{|g'(g_1^{-1}(v))|}\mathrm{Li}_{1/2}\left[2z\exp(-v)\right]\,dv \quad . \tag{3.2}$$

Since the first factor of the kernel, $1/|g'(g_1^{-1}(v))|$, has a square root singularity at $v = 0$ and is otherwise analytic (cf. figure 1) the analytical properties of the whole expression are inferred by applying the asymptotic property (B.5) of the polylogarithm. Thus using

$$g'(u) = 2(1-J)u\left(1+\mathcal{O}(u^2)\right) \tag{3.3}$$

$$g_1^{-1}(v) = \sqrt{\frac{v}{1-J}}\left(1+\mathcal{O}(v)\right) \tag{3.4}$$

we obtain form eqs.(3.2) and (B.5) the asymptotic result

$$\ln\zeta(z) \simeq -\frac{1}{\sqrt{1-J}}\ln(1-2z) \quad . \tag{3.5}$$

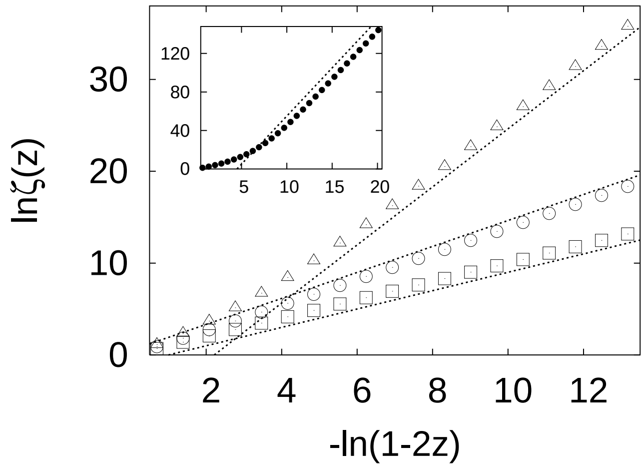

Figure 2. Numerical evaluation of the ζ–function (2.5) for $z < 1/2$ and different values of the coupling: squares $J = 0$, circles $J = 0.5$, triangles $J = 0.9$. Dotted lines indicate the slope according to the analytically obtained asymptotic behaviour (3.5). Inset: the same data for $J = 0.99$.

Thus the ζ–function develops a branch point $(1-2z)^{-1/\sqrt{1-J}}$. The exponent of the branch point changes continuously when changing the coupling strength J. The actual value of the exponent is determined by the prefactors of our asymptotic expansion and thus depends on the coupling strength. Overall, even in the high–temperature phase the ζ–function develops a nontrivial analytical behaviour in contrast to spin chains with finite range interaction, where meromorphic behaviour prevails. The exponent of the branch point tends to minus infinity when the phase transition point $J = J_c = 1$ is approached. The analytical result may be confirmed by numerical evaluation of the integral (2.5) (cf. figure 2)¶.

In the ferromagnetic case $J > J_c = 1$, $H = 0$ the potential (2.4) develops minima $v_{\min} = g(\pm u_{min})$ at $u = \pm u_{min}$. In the range $v_{min} \le v \le 0$ two additional branches of the inverse exist, $g_3^{-1}(v) = -g_4^{-1}(v) \ge 0$ (cf. figure 3). Using appropriate substitutions the ζ–function (2.5) splits into two different contributions and thus reads

$$\ln\zeta(z) = \ln\zeta_1(z) + \ln\zeta_2(z) \tag{3.6}$$

where we have introduced the abbreviations

$$\ln\zeta_1(z) = \frac{2}{\sqrt{\pi}}\int_{v_{min}}^{\infty} \frac{1}{|g'(g_1^{-1}(v))|}\mathrm{Li}_{1/2}\left[2z\exp(-v)\right]\,dv \tag{3.7}$$

$$\ln\zeta_2(z) = \frac{2}{\sqrt{\pi}}\int_{v_{min}}^{0} \frac{1}{|g'(g_3^{-1}(v))|}\mathrm{Li}_{1/2}\left[2z\exp(-v)\right]\,dv \quad . \tag{3.8}$$

Because of the different inverse branches the ζ–function develops as usual a product structure $\zeta(z) = \zeta_1(z)\zeta_2(z)$ where the analytical properties of the two factors are determined by the expressions (3.7) and (3.8). As in the previous case the factor

¶ Numerical evaluation of the polylogarithm and of the corresponding integrals has been achieved with Mathematica®.

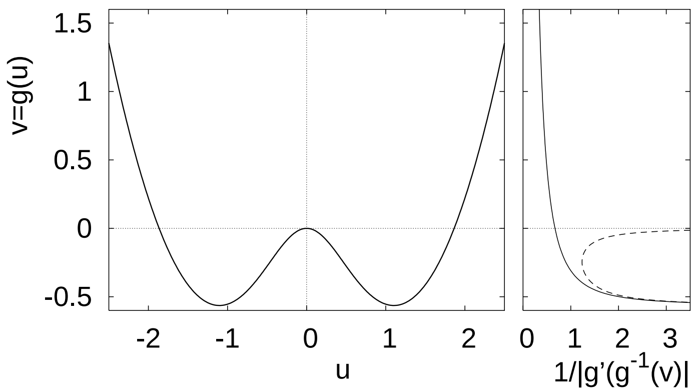

Figure 3. Left: potential (2.4) in the low–temperature regime for $J = 2.5$. Right: modulus of the derivative of the two inverse branches, $1/|g'(g_1^{-1}(v))|$ (full line) and $1/|g'(g_3^{-1}(v))|$ (broken line), (cf. eqs.(3.7) and (3.8)).

$\zeta_1(z)$ has a branch point for $2z\exp(-v_{min}) = 1$ since in this limit the two square root singularities of the kernel collide. Using the expansions

$$g'(u) \quad = g''(u_{min})(u - u_{min})\left(1 + \mathcal{O}\left((u - u_{min})^2\right)\right) \tag{3.9}$$

$$g_1^{-1}(v) = u_{min} + \sqrt{\frac{2}{g''(u_{min})}}\sqrt{v - v_{min}}\left(1 + \mathcal{O}\left(v - v_{min}\right)\right) \tag{3.10}$$

eq.(3.7) yields

$$\ln\zeta_1(z) \simeq -\sqrt{\frac{2}{g''(u_{min})}}\ln(1 - 2z\exp(-v_{min})) \tag{3.11}$$

when taking the asymptotic result (B.5) into account. For the factor $\zeta_2(z)$ we expect at least two branch points to occur, at $2z\exp(-v_{min}) = 1$ and at $2z = 1$ since the first factor of the kernel provides square root singularities at $v = v_{min}$ and at $v = 0$. The leading branch point, i.e. that with smallest modulus, can be obtained using the expansions (3.9) and

$$g_3^{-1}(v) = u_{min} - \sqrt{\frac{2}{g''(u_{min})}}\sqrt{v - v_{min}}\left(1 + \mathcal{O}\left(v - v_{min}\right)\right) \quad . \tag{3.12}$$

We hence obtain

$$\ln\zeta_2(z) \simeq -\sqrt{\frac{2}{g''(u_{min})}}\ln(1 - 2z\exp(-v_{min})) \quad . \tag{3.13}$$

Thus the ζ–function develops a leading branch point $z = \exp(v_{min})/2$ with exponent $-2\sqrt{2/g''(u_{min})}$ and a branch point at $z = 1/2$ which is apparently much more difficult to evaluate.

Finally, at the critical point $J = J_c = 1$, $H = 0$ the potential has two inverse branches only $g_1^{-1}(v) = -g_2^{-1}(v)$ so that eq.(2.5) reduces again to eq.(3.2) where now

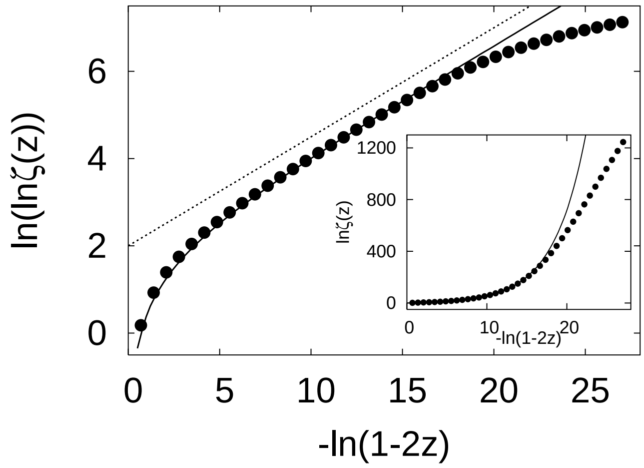

Figure 4. The double logarithm of the ζ–function in dependence on $-\ln(1-2z)$ for $J = 0.9999$ (symbols). Full line: asymptotic behaviour for $J = J_c$ according to eq.(3.16a), dotted line: linear graph with slope 1/4 (cf. eq.(3.16b)). Inset: the same data in a double logarithmic plot (cf. figure 2). Crossover to normal behaviour appears at about $z = 20$ since $J < J_c = 1$.

the expansions

$$g'(u) \;= \frac{g^{IV}(0)}{3!} u^3 \left(1 + \mathcal{O}\left(u^2\right)\right) \tag{3.14}$$

$$g_1^{-1}(v) = \left(\frac{4!}{g^{IV}(0)} v\right)^{1/4} \left(1 + \mathcal{O}(\sqrt{v})\right) \tag{3.15}$$

are valid. Using the asymptotic formula (B.3) and (B.4) respectively, eq.(3.2) evaluates to

$$\ln\zeta(z) \simeq \frac{\sqrt[4]{3}}{2\sqrt{\pi}} \Gamma(1/4) \mathrm{Li}_{s=3/4}[2z] \tag{3.16a}$$

$$\simeq \frac{\sqrt[4]{3}}{2\sqrt{\pi}} \left(\Gamma(1/4)\right)^2 (1-2z)^{-1/4} \quad . \tag{3.16b}$$

Thus the ζ–function in the critical case develops an essential singularity at $z = 1/2$. A triple logarithmic plot clearly displays the critical exponent $-1/4$ (cf. figure 4). Furthermore, the asymptotic formula (3.16a) is even able to capture the z–dependence in a large region of the complex plane.

4. Discussion

We have analysed the analytical properties of the Ruelle ζ–function of the globally coupled spin model in the high– and low–temperature regime as well as at the critical point $J = J_c = 1$. In the high–temperature phase $J < J_c$ the ζ–function has a branch point at $z = 1/2$ with asymptotic expansion (cf. eq.(3.5))

$$\zeta(z) \simeq (z - 1/2)^{-1/\sqrt{1-J}}, \qquad (J < J_c, z \to 1/2) \quad . \tag{4.1}$$

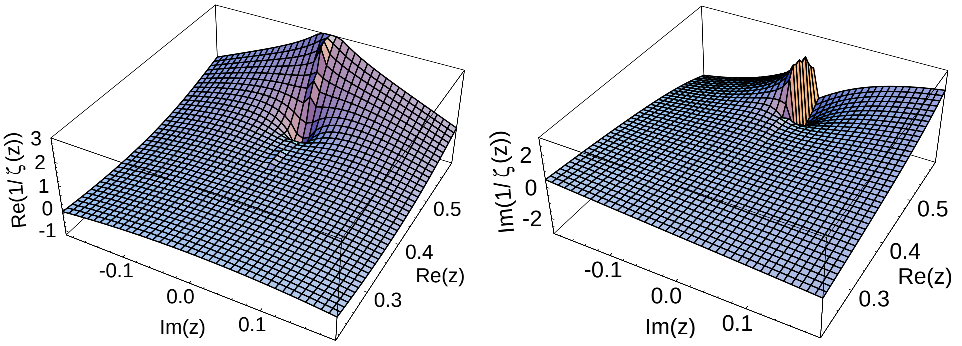

Figure 5. Inverse ζ–function in dependence on z in the ferromagnetic phase ($J = 2$), left: real part, right: imaginary part. Branch points occur at $z = \exp(f) = 0.3607\ldots$ and $z = 1/2$ causing a cut along the real axis. The inverse ζ–function takes small values along this cut between $z = \exp(f)$ and $z = 1/2$ (cf. figure 6). Apparently no further singularities are visible.

The exponent diverges when the critical point is approached. In the low–temperature phase $J > J_c$ the ζ–function develops two branch points at $z = \exp(f)$ and at $z = 1/2$ where $f < -\ln 2$ denotes the mean field free energy per particle. While the leading branch point corresponds to the thermodynamic equilibrium the non leading branch point is generated by the metastable state. The leading term of the asymptotic expansion reads (cf. eqs.(3.11) and (3.13))

$$\zeta(z) \simeq (z - \exp(f))^{-2\sqrt{2/g''(u_{min})}}, \qquad (J > J_c, z \to \exp(f)) \tag{4.2}$$

where the exponent is essentially determined by the mean field magnetic susceptibility. We suspect that in both cases, the high– and the low–temperature phase, no further singularities appear, apart from those mentioned above. But a real proof requires a more sophisticated discussion of the integral (2.5). However, a direct numerical evaluation (cf. figure 5) confirms such a conjecture. Eqs.(4.1) and (4.2) can be obtained simply by inserting the saddle point approximation of the partition function (2.3) into the definition (2.1). But such a reasoning misses the non leading branch point of the low–temperature phase.

To unveil the nature of the nonleading singularity at $z = 1/2$ we consider a slice along the lower edge of the cut, $z = x - i0+$

$$\zeta(x) = r(x)\exp(i\varphi(x)) = \lim_{\varepsilon \to 0+} \zeta(x - i\varepsilon) \quad . \tag{4.3}$$

Figure 6 clearly reveals the leading singularity at $z = \exp(f)$ and the nonleading branch point at $z = 1/2$. The modulus $\mathrm{Re}(\ln\zeta(x)) = \ln r(x)$ shows logarithmic behaviour and the complex phase $\mathrm{Im}(\ln\zeta(x)) = \phi(x)$ simultaneously develops a discontinuity at the leading singularity. Actually such a property is not a coincidence as both quantities are tied together by a Kramers–Kronig type relation (cf. Appendix D). For the nonleading branch point the role of modulus and phase are seemingly interchanged as logarithmic behaviour appears for the phase and the discontinuity for the modulus. Since the leading

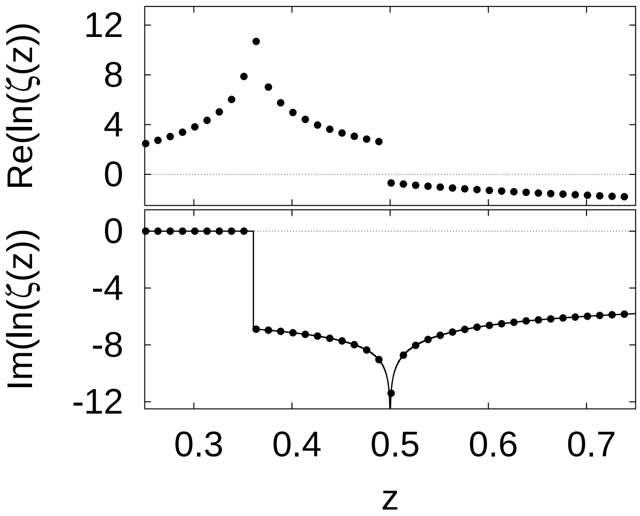

Figure 6. Real and imaginary part of the logarithm of the ζ–function along the real axis, $z = x - i0+$, for $J = 2$. Symbols: evaluation of eq.(2.5), line: evaluation of eq.(4.6). Singularities at $z = \exp(f) = 0.3607\ldots$ and at $z = 1/2$ are clearly visible (cf. figure 5).

branch point of $\ln\zeta(z)$ is of the type $(z - \exp(f))^a$ we conjecture that the nonleading branch point is a power law with imaginary exponent $(z - 1/2)^{i\alpha}$. In fact

$$\ln\,(z - 1/2)^{i\alpha}\big|_{z=x-i0+} = i\alpha \ln|x - 1/2| - \alpha\phi \qquad (4.4)$$

holds where the complex phase ϕ of $z-1/2 = x-1/2-i0+$ jumps from $\phi = \pi$ to $\phi = 2\pi$ when x changes from $x < 1/2$ to $x > 1/2$. Thus eq.(4.4) reproduces all the analytical features visible in figure 6 at the second branch point. Accordingly the imaginary part of the exponent, α, can be obtained e.g. from the scaling behaviour of $\varphi(x)$ at $x = 1/2$.

Fortunately eq.(C.4) eventually provides us with a simple analytical expression for $\varphi(x)$. By virtue of $\zeta(x + i\varepsilon) = (\zeta(x - i\varepsilon))^*$ we have

$$-2i\varphi(x) = \lim_{\varepsilon\to 0+} \left(\ln\zeta(x + i\varepsilon) - \ln\zeta(x - i\varepsilon)\right) \quad . \qquad (4.5)$$

Using eqs.(2.5) and (C.4) we just obtain

$$\varphi(x) = -\int_{u\geq 0,\,\ln(2x)\geq g(u)} \frac{2}{\sqrt{\ln(2x) - g(u)}}\,du \quad . \qquad (4.6)$$

Although this integral cannot be solved by elementary methods its asymptotic properties for $x \to 1/2$ can be obtained quite straightforwardly (cf. Appendix E). We end up with

$$\varphi(x) \simeq \sqrt{\frac{2}{-g''(0)}}\ln|x - 1/2| = \frac{1}{\sqrt{J-1}}\ln|x - 1/2| \quad . \qquad (4.7)$$

Comparison with eqs.(4.3) and (4.4) yields for the imaginary part of the exponent $\alpha = 1/\sqrt{J-1}$ so that the singular part of the ζ–function at $z = 1/2$ is inferred to be

$$\zeta(z) \simeq (z - 1/2)^{i/\sqrt{J-1}}, \qquad (J > J_C, z \to 1/2) \quad . \qquad (4.8)$$

Such a result nicely complies with the high–temperature behaviour, eq.(4.1), since the formally negative susceptibility of the metastable state causes a branch point with imaginary exponent in the low–temperature phase.

When approaching the critical point $J = J_c = 1$ the exponents of the high–temperature as well as the low–temperature behaviour (cf. eq.(4.1) respectively eqs.(4.2) and (4.8)) become singular. In particular the two branch points of the low–temperature phase (cf. figure 6) approach each other, the height of the discontinuities on the real axis increases (cf. eq.(4.4)), and the imaginary part of $\ln\zeta(z)$ finally displays a discontinuity with infinite jump. Thus, at the critical point $J = J_c$ the ζ–function develops an essential singularity at $z = 1/2$. The asymptotic expansion reads (cf. eq.(3.16b))

$$\zeta(z) \simeq \exp\left(C(1-2z)^{-1/4}\right), \qquad (J = J_c, z \to 1/2) \tag{4.9}$$

where the numerical value of C is approximately given by $C = 4.880199$.

Summarising the results, eqs.(4.1), (4.2), (4.8), and (4.9), we find a quite sophisticated analytical behaviour of the ζ–function. Even in the high–temperature phase the function is not meromorphic contrary to models with short range interaction. That is, however, not surprising since from a formal perspective a global interaction is never small, no matter what is the size of the coupling constant J. In the low–temperature phase we expect two branch points, one corresponding to the thermodynamic stable and one corresponding to the metastable state. The exponents are essentially determined by the square root of the respective formal susceptibilities. Our results have been entirely based on the properties of the potential (2.4). Thus any “double well” potential produces the same structure of the ζ–function, and our expansions yield the generic properties of ζ–functions for Ginsburg–Landau models.

We have studied in detail the influence of a mean field ferromagnetic phase transition on the analytical properties of the Ruelle ζ–function. Although our model is quite simple such a result may be useful to test the quality of approximation schemes when ζ–functions in the presence of phase transition points have to be evaluated. The dimensionality of the underlying lattice did not play any role in our considerations. Actually the definition of ζ–functions for higher–dimensional lattices is far from obvious and the question is far from being settled (cf. [11]). Thus our results may contribute as well to the question how to introduce appropriate ζ–functions in such a setup.

Appendix A. Partition function

If $S = \sum_\nu \sigma_\nu$ denotes the total magnetisation and g_S the multiplicity of states with magnetisation S then the partition function reads

$$\begin{aligned} Z_N &= \sum_S g_S \exp(HS + JS^2/(2N)) \\ &= \sum_S g_S \exp(HS) \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp\left(-y^2 + yS\sqrt{2J/N}\right) dy \end{aligned} \tag{A.1}$$

Using $S = -N + 2k$, $k = 0, \ldots, N$ and $g_S = \binom{N}{k}$ eq.(A.1) results in

$$\begin{aligned} Z_N &= \sqrt{\frac{N}{\pi}} \int_{-\infty}^{\infty} \exp\left(-Nx^2\right) \sum_{k=0}^{N} \binom{N}{k} \exp\left(-(x\sqrt{2J}+H)(N-2k)\right) dx \\ &= \sqrt{\frac{N}{\pi}} \int_{-\infty}^{\infty} \exp\left(-Nx^2\right) \exp\left(-N(x\sqrt{2J}+H)\right) \left(\exp\left(2x\sqrt{2J}+2H\right)+1\right)^N dx \\ &= 2^N \sqrt{\frac{N}{\pi}} \int_{-\infty}^{\infty} \exp\left(-Nx^2\right) \cosh^N\left(x\sqrt{2J}+H\right) dx \end{aligned} \tag{A.2}$$

which in fact coincides with eq.(2.3).

Appendix B. Polylogarithm

Analytical properties of the polylogarithm (2.6) are well known [8, 9]. Here we concentrate on a few essential features. The polylogarithm is analytic apart from $z = 1$. At that point the asymptotic relation

$$\mathrm{Li}_s[z] \simeq \frac{\Gamma(1-s)}{(1-z)^{1-s}}, \qquad (\mathrm{Re}s < 1) \tag{B.1}$$

holds while for $s = 1$ we obviously have

$$\mathrm{Li}_{s=1}[z] = -\ln(1-z) \quad . \tag{B.2}$$

In addition, by direct computation we obtain the identity

$$\begin{aligned} &\int_0^\infty x^\alpha \mathrm{Li}_s\left[z\exp(-x)\right] dx \\ &= \sum_{N=1}^{\infty} \int_0^\infty \frac{z^N}{N^{s+\alpha+1}} y^\alpha \exp(-y)\, dy \\ &= \mathrm{Li}_{s+\alpha+1}[z]\Gamma(1+\alpha) \qquad (\alpha > -1,\ |z| < 1) \quad . \end{aligned} \tag{B.3}$$

For the finite integral the leading singularity occurs at $z = 1$ since both factors x^α and $L_s[z\exp(-x)]$ become singular at $x = 0$ in this limit. Thus expression (B.3) is indeed valid as an asymptotic result for the finite integral as well. In connection with eqs.(B.1) and (B.2) we hence obtain for $z \simeq 1$

$$\int_0^c x^\alpha \mathrm{Li}_s\left[z\exp(-x)\right] dx \simeq \Gamma(-s-\alpha)\Gamma(1+\alpha)(1-z)^{s+\alpha}, \qquad (-s > \alpha > -1) \tag{B.4}$$

and

$$\int_0^c x^{-s} \mathrm{Li}_s\left[z\exp(-x)\right] dx \simeq -\Gamma(1-s)\ln(1-z), \qquad (s < 1) \quad . \tag{B.5}$$

Appendix C. Analytic continuation of $\mathbf{Li}_{1/2}(z)$

Using the obvious identity

$$\frac{1}{\sqrt{n}} = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{\exp(-nt)}{\sqrt{t}}\, dt \tag{C.1}$$

we obtain from the series (2.6)

$$\mathrm{Li}_{1/2}[z] = \frac{1}{\sqrt{\pi}} \int_0^\infty \sum_{n=1}^\infty z^n \frac{\exp(-nt)}{\sqrt{t}}\, dt = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{1}{\sqrt{t}} \frac{z}{\exp(t) - z}\, dt \qquad (C.2)$$

which is the well know integral representation of the polylogarithm. The integral converges for any complex z values apart from a cut along the real axis, $z > 1$. Thus eq.(C.2) yields the proper analytical continuation. It is precisely this main branch we are using throughout our analysis. Actually the main branch obeys $(\mathrm{Li}_{1/2}(z))^* = \mathrm{Li}_{1/2}(z^*)$.

The behaviour of the polylogarithm along the cut can be evaluated explicitly. Using eq.(C.2) we have

$$\begin{aligned}\mathrm{Li}_{1/2}[x + i\varepsilon] - \mathrm{Li}_{1/2}[x - i\varepsilon] &= \frac{2i}{\sqrt{\pi}} \int_0^\infty \frac{1}{\sqrt{t}} \frac{\varepsilon \exp(t)}{(\exp(t) - x)^2 + \varepsilon^2}\, dt \\ &= 2i\sqrt{\pi} \int_1^\infty \frac{1}{\sqrt{\ln y}} \frac{\varepsilon/\pi}{(y - x)^2 + \varepsilon^2}\, dy \quad . \qquad (C.3)\end{aligned}$$

As in the limit $\varepsilon \to 0+$ the second factor in the integral yields the δ–function we obtain for the difference of the polylogarithm between a point on the upper edge of the cut and a point of the lower edge of the cut the result

$$\Delta\mathrm{Li}_{1/2}(x) = \lim_{\varepsilon \to 0+} \left(\mathrm{Li}_{1/2}[x + i\varepsilon] - \mathrm{Li}_{1/2}[x - i\varepsilon]\right) = \begin{cases} 2i\sqrt{\dfrac{\pi}{\ln x}} & \text{if} \quad x > 1 \\ 0 & \text{if} \quad x \le 1 \end{cases} \quad . \qquad (C.4)$$

All these considerations are textbook knowledge [8] and can be generalised easily to other values of the parameter s.

Appendix D. Kramers–Kronig type relations

The real and imaginary part of $\mathrm{Li}_{1/2}[z]$ are related by a Kramers–Kronig type relation. A similar property can then be deduced for the logarithm of the ζ–function.

Thanks to the integral representation (C.2) $\mathrm{Li}_{1/2}[z]/z$ is analytic in the lower half plane and decays if $|z| \to \infty$. By Cauchy's integral formula we have for any point z in the interior of the lower half of the complex plane

$$\frac{\mathrm{Li}_{1/2}[z]}{z} = -\frac{1}{2\pi i} \oint_{\mathcal{C}} \frac{\mathrm{Li}_{1/2}[w]/w}{w - z}\, dw \qquad (D.1)$$

where we choose for the contour $\mathcal{C}$ the lower edge of the real axis, i.e. $w = y - i0+$, and a semicircle (of infinite radius) in the lower half of the complex plane. As the integration along the semicircle does not contribute to the integral we are left with

$$\frac{\mathrm{Li}_{1/2}[z]}{z} = -\frac{1}{2\pi i} \int_{-\infty}^\infty \frac{1}{y - z} \frac{\mathrm{Li}_{1/2}(y)}{y}\, dy \qquad (D.2)$$

where we use the shorthand notation $\mathrm{Li}_{1/2}(y) = \mathrm{Li}_{1/2}[y - i0+]$ to indicate the value of the polylogarithm on the lower edge of the real axis. Considering now $z = x - i\varepsilon$, taking the limit $\varepsilon \to 0+$, and using the usual identity $1/(y-x+i0+) = 1/(y-x) - i\pi\delta(y-x)$ we obtain

$$\frac{\mathrm{Li}_{1/2}(x)}{x} = \frac{i}{\pi} \fint_{-\infty}^{\infty} \frac{1}{y-x} \frac{\mathrm{Li}_{1/2}(y)}{y}\, dy \tag{D.3}$$

where $\fint$ denotes the Cauchy principal value. Considering real and imaginary part we end up with the Kramers–Kronig type relation mentioned at the beginning

$$\begin{aligned} \mathrm{Re}(\mathrm{Li}_{1/2}(x)) &= -\frac{1}{\pi} \fint_{-\infty}^{\infty} \frac{x}{y(y-x)} \mathrm{Im}(\mathrm{Li}_{1/2}(y))\, dy \\ \mathrm{Im}(\mathrm{Li}_{1/2}(x)) &= \frac{1}{\pi} \fint_{-\infty}^{\infty} \frac{x}{y(y-x)} \mathrm{Re}(\mathrm{Li}_{1/2}(y))\, dy \quad . \end{aligned} \tag{D.4}$$

These relations translate directly into corresponding conditions for the logarithm of the ζ–function when eq.(2.5) is employed and the convergence of the integrals is presupposed

$$\begin{aligned} \mathrm{Re}(\ln \zeta(x)) &= -\frac{1}{\pi} \fint_{-\infty}^{\infty} \frac{x}{y(y-x)} \mathrm{Im}(\ln \zeta(y))\, dy \\ \mathrm{Im}(\ln \zeta(x)) &= \frac{1}{\pi} \fint_{-\infty}^{\infty} \frac{x}{y(y-x)} \mathrm{Re}(\ln \zeta(y))\, dy \quad . \end{aligned} \tag{D.5}$$

The existence of such a relation is an analytical indicator that the logarithm of the ζ–function has no singularities off the real axis.

Appendix E. Asymptotic expansion of hyperelliptic integrals

Consider

$$I_1 = \int_d^c \frac{1}{\sqrt{-\varepsilon^2 + u^2 f(u)}}\, du \tag{E.1}$$

where $f(u)$ has a simple zero at say $u = c_0 > 0$, $f(u) > 0$ if $0 \le u < c_0$ and the limits of integration are the singularities of the kernel. That means

$$\varepsilon^2 = d^2 f(d) = c^2 f(c) \tag{E.2}$$

where $d \to 0$ and $c \to c_0$ if $\varepsilon \to 0$. To obtain the asymptotic properties of eq.(E.1) in such a limit take a small but fixed value $\delta > 0$ and split the integral into two parts

$$I_1 = \int_d^\delta \frac{1}{\sqrt{-\varepsilon^2 + u^2 f(u)}}\, du + \int_\delta^c \frac{1}{\sqrt{-\varepsilon^2 + u^2 f(u)}}\, du \quad . \tag{E.3}$$

The second term remains bounded, uniformly in ε, since the singularity at the upper limit stays integrable for $\varepsilon = 0$. Thus the asymptotic properties are determined by the first part

$$\begin{aligned} I_1 &\simeq \int_{d/\varepsilon}^{\delta/\varepsilon} \frac{1}{\sqrt{-1 + v^2 f(v\varepsilon)}}\, dv \\ &= \frac{1}{\sqrt{f(d)}} \int_1^{\delta\sqrt{f(d)}/\varepsilon} \frac{1}{\sqrt{-1 + y^2 f(\varepsilon y/\sqrt{f(d)})/f(d)}}\, dy \end{aligned}$$

$$\simeq \frac{1}{\sqrt{f(d)}} \int_1^{\delta/d} \frac{1}{y} \sqrt{\frac{f(d)}{f(yd)}}\, dy$$
$$= \frac{1}{\sqrt{f(d)}} \int_1^{\delta/d} \frac{1}{y}\, dy + \frac{1}{\sqrt{f(d)}} \int_1^{\delta/d} \frac{1}{y} \frac{\sqrt{f(d)} - \sqrt{f(yd)}}{\sqrt{f(yd)}}\, dy \tag{E.4}$$

where we have used $0 \leq \varepsilon y \sqrt{f(d)} = yd \leq \delta$ (cf. eq.(E.2)). As $d \to 0$ when $\varepsilon \to 0$ the second term remains at least bounded when we impose Lipschitz continuity on f. Hence the asymptotic behaviour of the integral (E.1) is given by

$$I_1 \simeq \frac{1}{\sqrt{f(0)}} \ln\left(\frac{\delta}{d}\right) \simeq -\frac{\ln \varepsilon}{\sqrt{f(0)}} \quad . \tag{E.5}$$

If we now choose $\varepsilon^2 = -\ln(2x)$ and $u^2 f(u) = -g(u)$ and observe that $\varepsilon^2 \simeq 2(1/2 - x)$ and $-g''(0) = 2f(0)$ we obtain from eq.(E.5) the result (4.7) for $x < 1/2$.

For the opposite case consider

$$I_2 = \int_0^c \frac{1}{\sqrt{\varepsilon^2 + u^2 f(u)}}\, du \tag{E.6}$$

and follow a similar reasoning. Splitting, as before, the integral into two parts the asymptotic properties are given by

$$I_2 \simeq \int_0^{\delta/\varepsilon} \frac{1}{\sqrt{1 + v^2 f(\varepsilon v)}}\, dv$$
$$= \frac{1}{\sqrt{f(d)}} \int_0^{\delta\sqrt{f(d)}/\varepsilon} \frac{1}{\sqrt{1 + y^2 f(\varepsilon y/\sqrt{f(d)})/f(d)}}\, dy$$
$$\simeq \frac{1}{\sqrt{f(d)}} \int_1^{\delta/d} \frac{1}{y} \sqrt{\frac{f(d)}{f(yd)}}\, dy$$
$$\simeq -\frac{\ln \varepsilon}{\sqrt{f(0)}} \quad . \tag{E.7}$$

Choosing $\varepsilon^2 = \ln(2x)$ and $u^2 f(u) = -g(u)$ eq.(E.7) yields the result (4.7) for $x > 1/2$.

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