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Finite-size scaling analysis of generalized mean-field theories

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Abstract. We investigate families of generalized mean-field theories that can be formulated using the Peierls–Bogoliubov inequality. For test Hamiltonians describing mutually non-interacting subsystems of increasing size, the thermodynamics of these mean-field-type systems approaches that of the infinite, fully interacting system except in the immediate vicinity of their respective mean-field critical points. Finite-size scaling analysis of this mean-field critical behaviour allows us to extract the critical exponents of the fully interacting system. It turns out that this procedure amounts to the coherent anomaly method (CAM) proposed by Suzuki, which is thus given a clear interpretation in terms of conventional renormalization group ideas. Moreover, given the geometry of approximating systems, we can identify the family of approximants which is optimal in the sense of the Peierls–Bogoliubov inequality. In the case of the 2D Ising model it turns out that, surprisingly, this optimal family gives rise to a spurious singularity in the thermodynamic functions.

1. Introduction

Standard wisdom has it that closed form approximations and renormalization group methods play complementary roles in the analysis of the thermodynamic behaviour of many-particle systems. The former usually generate mean-field-type theories and, as such, often provide efficient tools to obtain a good *qualitative* picture of a given system's thermodynamics. Equations of state and qualitatively correct phase diagrams are relatively easily calculated. Well known examples of such approaches are the van der Waals theory of imperfect gases and the Weiss self-consistent theory of ferromagnetism. With respect to a *quantitative* description of phase transitions, however, these theories invariably fail and produce the wrong critical exponents. Renormalization group ideas, on the other hand, provide a satisfactory theoretical description of critical phenomena and the interplay of critical exponents. Except for the determination of critical exponents, renormalization group calculations are rather involved and do not easily allow us to obtain a picture of the system's thermodynamic properties.

In the course of time various refinements of the standard mean-field theory have been proposed; for an overview see [1]. A precedent was set after the first such attempt due to Bethe [2]: short-range correlations of the dynamic variables are taken into account by considering small clusters. Equations of state are generated in the form of *self-consistency* equations which impose certain physically plausible constraints, such as homogeneity of the order parameter. This inclusion of short-range correlations, hence of additional phase space, leads to improved (i.e. lower) estimates of the critical temperature; but it fails to produce

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improved critical exponents—the reason being that critical phenomena are dominated by *long-range* correlations.

An alternative, more systematic construction of mean-field-type theories is derived from a *variational* scheme based on the Peierls–Bogoliubov (PB) inequality [3]. This inequality is based on convexity arguments and states that, given a system with Hamiltonian $\mathcal{H}$, its free energy F can be approximated from above by the trial 'free energy' Φ as

$$F \leqslant \Phi := F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 = \langle \mathcal{H} \rangle_0 - TS_0. \tag{1.1}$$

Here, $\mathcal{H}_0$ is an arbitrary test Hamiltonian for the system in question which depends on some set $\{h_\alpha\}$ of variational parameters, $\langle \ldots \rangle_0$ denotes the average over the Gibbs distribution generated by $\mathcal{H}_0$, and F_0 and S_0 denote the corresponding free energy and entropy. The idea is to choose $\mathcal{H}_0$ such that the corresponding Gibbs distribution is analytically or numerically tractable and to determine the variational parameters h_α so as to minimize the right-hand side of (1.1). The resulting minimization conditions replace the above self-consistency equations and generate the system's equations of state. To state an example, let $\mathcal{H}$ describe the Ising spin system on a lattice in d space dimensions. The simplest approximating $\mathcal{H}_0$ then describes a system of non-interacting spins in a mean field h_0, that is, $\mathcal{H}_0 = -h_0 \sum_i S_i$. Minimizing the corresponding trial free energy with respect to h_0 generates the conventional Weiss mean-field equation of state. For a recent application of the variational method to $CsNiF_3$ chains see [4].

Short-range correlations can now be taken into account by choosing a system of mutually independent *clusters* of spins, which together make up the whole system. Increasing the size of these clusters, one obtains a scheme of approximations that should systematically approach the thermodynamics of the underlying, fully interacting (spin) system.

Despite the fact that every PB system of finite (or quasi one-dimensional) geometry exhibits mean-field-type critical behaviour, the true critical exponents of the underlying system can be extracted by invoking finite-size scaling (FSS) ideas. Thermodynamic functions can be evaluated as functions of cluster size. We will show that this procedure is equivalent to Suzuki's coherent anomaly method (CAM) [5, 6]. CAM is thus demonstrated to be firmly rooted in the FSS philosophy and hence in conventional renormalization group ideas.

Within the general PB scheme, and for a given cluster geometry, various families of approximating systems can be constructed which differ in number, symmetries or even nature of their variational parameters. Of all of these, the optimal family—in the sense of minimal trial free energy—is the one with the largest set of independent variational parameters compatible with the symmetries of the system.

In this paper we will explore a collection of approximating sequences for the 2D Ising model. Two families will prove to be of special interest: cyclically 'closed' strips that display Suzuki's coherent anomaly, and 'open' strips of lower symmetry that can be identified as the optimal PB sequence. Surprisingly, this optimal family gives rise to a spurious singularity of thermodynamic functions making any extrapolation to the full 2D model based on the open strip's mean-field critical behaviour impossible. Thus, for open strips our attempt to use renormalization group (RG) ideas to extract asymptotic critical exponents does *not* lead to useful results.

The outline of our paper is as follows. In section 2 we introduce a collection of variational trial systems for the 2D Ising system based on the PB inequality. Test Hamiltonians will be defined on $M \times \infty$ strips which may be open or closed in the M direction. We show that, quite generally, all but one of the extremization conditions for the variational parameters can be solved explicitly, leaving only one non-trivial condition as the equation of state. In section 3 we use FSS to derive the scaling of the mean-field critical temperatures T_M with strip width M. For test ensembles based on cyclically closed strips (subsection 3.1), this provides a first method to extract the susceptibility exponent γ of the underlying, fully interacting system. The second method uses the mean-field susceptibilities and their scaling with strip width M. The coherent anomaly, which is the basis of this method, is given a simple explanation as a standard FSS phenomenon. Subsection 3.2 is devoted to an analysis of variational approximants defined on open strips. These were identified in section 2 as the best sequence of variational approximants of strip geometry in the framework of the PB inequality. Contrary to expectations, a FSS analysis of these 'optimal' variational approximants predicts a spurious singularity of thermodynamic functions that precludes any extrapolation attempt to the two-dimensional system. Section 4 is a discussion of the results.

2. Variational approximants for the 2D Ising model

We now introduce a collection of approximating systems for the 2D Ising model based on the PB inequality. Let

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i \tag{2.1}$$

describe the fully interacting system on a square lattice of $N' \times N$ Ising spins, and let us assume periodic boundary conditions in both directions. As a test ensemble we use a system of mutually *non-interacting* strips of size $M \times N$ with periodic boundary conditions in the 'longitudinal' N direction, and either free or periodic boundary conditions in the 'transverse' M direction.

2.1. Test ensembles based on closed strips

Let us first consider the version which is cyclically closed in *both* directions. A simple Hamiltonian for a single strip of width M, which exhibits full translational invariance in both directions, is given by

$$\mathcal{H}^{c}_{M,N} = -h_T \sum_{\langle ij \rangle_T} s_i s_j - h_L \sum_{\langle ij \rangle_L} s_i s_j - (H + h) \sum_i s_i \tag{2.2}$$

where we have introduced three variational parameters $\{h_\alpha\} := \{h_T, h_L, h\}$: a coupling h_T for transverse nearest neighbours $\langle ij \rangle_T$, a coupling h_L for longitudinal nearest neighbours $\langle ij \rangle_L$ and a variational field h. The trivial effect of the external field H has been absorbed into the definition of h.

Let us denote the free energy density of an isolated strip with Hamiltonian (2.2) by $f^c_M = f^c_M(T, H, \{h_\alpha\})$. Assuming N' to be an integer multiple of M, the PB inequality for this set-up states that

$$F \leqslant \Phi^c_M(T, H, \{h_\alpha\}) =: N'N\phi^c_M(T, H, \{h_\alpha\}) = N'N\Bigg\{ f^c_M + \left(J\left(1 - \frac{1}{M}\right) - h_T \right) \frac{\partial f^c_M}{\partial h_T} + (J - h_L)\frac{\partial f^c_M}{\partial h_L} - \left(J\frac{1}{M}\frac{\partial f^c_M}{\partial h} + h \right) \frac{\partial f^c_M}{\partial h} \Bigg\} \tag{2.3}$$

Here we have used the fact that $\langle s_i s_j\rangle_0$ is given by $(-\partial f_M^{\rm c}/\partial h_{\rm T})$ for transverse nearest neighbours and by $(-\partial f_M^{\rm c}/\partial h_{\rm L})$ for longitudinal nearest neighbours *within* a strip, while $\langle s_i s_j\rangle_0 = \langle s_i\rangle_0\langle s_j\rangle_0 = (-\partial f_M^{\rm c}/\partial h)^2 =: (m_M^{\rm c})^2$ for spins belonging to *different* strips. Here $m_M^{\rm c}$ denotes the magnetization of a strip of width M.

From (2.3) the minimization conditions are obtained in the form

$$\varphi_\alpha := \frac{\partial \phi_M^{\rm c}}{\partial h_\alpha} = \sum_\beta \frac{\partial^2 f_M^{\rm c}}{\partial h_\alpha \partial h_\beta}\psi_\beta = 0 \tag{2.4}$$

with $h_\alpha \in \{h_{\rm T}, h_{\rm L}, h\}$, and

$$\{\psi_\beta\} = \left\{J\left(1-\frac{1}{M}\right) - h_{\rm T},\, J - h_{\rm L},\, J\frac{2}{M}m_M^{\rm c} - h\right\}. \tag{2.5}$$

Due to the concavity of $f_M^{\rm c}$ as a function of h_α—the Hessian $(\partial^2 f_M^{\rm c}/\partial h_\alpha \partial h_\beta)_{\alpha,\beta}$ is a strictly negative definite matrix—the solution of (2.4) can be read off immediately: it is $\psi_\beta = 0$, i.e.

$$h_{\rm T} = J\left(1-\frac{1}{M}\right) \tag{2.6}$$

$$h_{\rm L} = J \tag{2.7}$$

$$h = J\frac{2}{M}m_M^{\rm c} = -J\frac{2}{M}\frac{\partial f_M^{\rm c}}{\partial h}. \tag{2.8}$$

Of these, only (2.8) is a non-trivial transcendental equation with a solution that varies with temperature T and external field H. It determines the mean field $h = h(T, H)$. The variational (mean-field) free energy density computed within this approach is then

$$f_M^{\rm mf}(T, H) = \phi_M^{\rm c}(T, H, h_{\rm T}, h_{\rm L}, h(T, H)) \tag{2.9}$$

with variational parameters $\{h_\alpha\}$ determined by (2.6)–(2.8).

Thermodynamic functions are obtained by differentiation of $f_M^{\rm mf}(T, H)$ along the solution manifold given by (2.8). This yields

$$m_M^{\rm mf} = -\left(\frac{{\rm d}f_M^{\rm mf}(T, H)}{{\rm d}H}\right)_{\varphi,T} = -\frac{\partial \phi_M^{\rm c}}{\partial H} - \sum_\alpha \frac{\partial \phi_M^{\rm c}}{\partial h_\alpha}\left(\frac{{\rm d}h_\alpha}{{\rm d}H}\right)_{\varphi,T} \tag{2.10}$$

where the subscripts φ, T denote differentiation along the manifold $\varphi_\alpha = 0$ at constant T. Partial differentials are taken as usual. With the help of (2.9) and $\partial\phi_M^{\rm c}/\partial h_\alpha \equiv 0$ one obtains the mean-field magnetization

$$m_M^{\rm mf} = -\frac{\partial f_M^{\rm c}}{\partial H}. \tag{2.11}$$

In a similar vein the mean-field susceptibility is found to be

$$\begin{aligned}\chi_M^{\rm mf} &= \left(\frac{{\rm d}m_M^{\rm mf}(T, H)}{\partial H}\right)_{\varphi,T} = \frac{\partial m_M^{\rm mf}}{\partial H} + \sum_\alpha \frac{\partial m_M^{\rm mf}}{\partial h_\alpha}\left(\frac{{\rm d}h_\alpha}{{\rm d}H}\right)_{\varphi,T} \\ &= -\frac{\partial^2 f_M^{\rm c}}{\partial H^2} + J\frac{2}{M}\frac{(\partial^2 f_M^{\rm c}/\partial H \partial h)^2}{1 + J\frac{2}{M}\partial^2 f_M^{\rm c}/\partial h^2}.\end{aligned} \tag{2.12}$$

That is, magnetization and mean-field susceptibility can be expressed in terms of *free* partial derivatives of the strip free energy f_M^c of a strip, the strip being described by the Hamiltonian $\mathcal{H}_{M,N}^c$ evaluated at parameter values given by (2.6)–(2.8).

In principle, one may try to improve the approximation by introducing additional variational parameters that represent 'generalized' couplings beyond the ones already contained in (2.2) which generate interaction terms added to $\mathcal{H}_{M,N}^c$ in a translationally invariant way. To be specific, we modify $\mathcal{H}_{M,N}^c$ according to

$$\mathcal{H}_{M,N}^c \to \mathcal{H}_{M,N}^c - \sum_{\omega\subseteq\Omega} h_\omega \sum_i \left(\prod_{j\in\omega} s_{j+i}\right) \tag{2.13}$$

where Ω denotes a collection of subsets of the $M\times N$ strip which are mutually non-equivalent under translation. It turns out that such an enlarged space of variational parameters does *not* actually improve the variational free energy because the enlarged set of minimization conditions is solved by (2.6)–(2.8) and $h_\omega = 0$ for all of the added $\omega \subseteq \Omega$. To see this, note that the modification (2.13) implies a corresponding replacement

$$\langle\mathcal{H}_0\rangle_0 \to \langle\mathcal{H}_0\rangle_0 + NN' \sum_{\omega\subseteq\Omega} h_\omega \frac{\partial f_M^c}{\partial h_\omega} \tag{2.14}$$

where f_M^c is now the free energy corresponding to the modified Hamiltonian (2.13). Hence the enlarged set of minimization conditions can be formulated in a complete analogy to (2.4), albeit with an enlarged set of variational parameters, $h_\alpha \in \{h_\mathrm{T}, h_\mathrm{L}, h, \{h_\omega\}_{\omega\subseteq\Omega}\}$ and

$$\{\psi_\beta\} = \left\{J\left(1-\frac{1}{M}\right) - h_\mathrm{T},\, J - h_\mathrm{L},\, J\frac{2}{M}m_M^c - h,\, \{-h_\omega\}_{\omega\subseteq\Omega}\right\}. \tag{2.15}$$

Due to the concavity of $f_M^c(T, H, \{h_\alpha\})$ the assertion follows, that is $h_\omega = 0$ for all $\omega \subseteq \Omega$.

2.2. *Test ensembles based on open strips*

An alternative sequence of test systems is defined by considering 'open' $M \times N$ strips with free boundary conditions in the transverse M direction. While such strips retain the full translational invariance in the closed N direction, they exhibit only a reflection symmetry $j \to M + 1 - j$ in the open M direction. This reduced symmetry group allows us to introduce a considerably larger set of independent variational parameters. A simple Hamiltonian respecting these symmetries is given by

$$\begin{aligned}\mathcal{H}_{M,N}^o = -\sum_{i=1}^{N} \Bigg\{ &\sum_{j=1}^{\mu} h_{\mathrm{T},j} \sum_{\kappa\in\{j,M-j\}} s_{i,\kappa}s_{i,\kappa+1} + \sum_{j=1}^{\mu'} h_{\mathrm{L},j} \sum_{\kappa\in\{j,M+1-j\}} s_{i,\kappa}s_{i+1,\kappa} \\ &+ \sum_{j=1}^{\mu'} (H + h_j) \sum_{\kappa\in\{j,M+1-j\}} s_{i,\kappa} \Bigg\}\end{aligned} \tag{2.16}$$

where $\mu = [M/2]$ and $\mu' = [(M + 1)/2]$ with the convention that $[k]$ denotes the largest integer less than or equal to k. We have also introduced a two-dimensional notation to label the vertices of the strip. Note that the variational fields and couplings vary from row to row, but respect the reflection invariance of the open strip in the M direction. The total number of independent variational parameters is $3M/2$ for even M and $(3M+1)/2$ for odd M.

Denoting the free energy density of an isolated (open) strip with Hamiltonian (2.16) by $f_M^\circ = f_M^\circ(T, H, \{h_{\mathrm{T},j}\}, \{h_{\mathrm{L},j}\}, \{h_j\})$ and assuming N' to be an integer multiple of M, we conclude by PB inequality that

$$F \leqslant \Phi_M^\circ(T, H, \{h_{\mathrm{T},j}\}, \{h_{\mathrm{L},j}\}, \{h_j\})$$
$$= N'N\Bigg\{f_M^\circ + \sum_{j=1}^{\mu}(J - h_{\mathrm{T},j})M\frac{\partial f_M^\circ}{\partial h_{\mathrm{T},j}} + \sum_{j=1}^{\mu'}(J - h_{\mathrm{L},j})M\frac{\partial f_M^\circ}{\partial h_{\mathrm{L},j}}$$
$$- \sum_{j=2}^{\mu'} h_j M\frac{\partial f_M^\circ}{\partial h_j} - \left(J\frac{M}{2}\frac{\partial f_M^\circ}{\partial h_1} + h_1\right)M\frac{\partial f_M^\circ}{\partial h_1}\Bigg\}. \tag{2.17}$$

The minimization conditions are formally the same as (2.4), with f_M^c replaced by f_M°, with $h_\alpha \in \{\{h_{\mathrm{T},j}\}, \{h_{\mathrm{L},j}\}, \{h_j\}\}$, and

$$\{\psi_\beta\} = \{\{J - h_{\mathrm{T},j}\}, \{J - h_{\mathrm{L},j}\}, \{-h_j\}_{j=2,\ldots,\mu'}, Jm_{M,1}^\circ - h_1\}. \tag{2.18}$$

Here $m_{M,1}^\circ = \langle s_{i,1}\rangle_0 = -(M/2)\partial f_M^\circ/\partial h_1$. Again, due to concavity, the solutions of the minimization conditions are $\psi_\beta = 0$, or

$$h_{\mathrm{T},j} = J \tag{2.19}$$

$$h_{\mathrm{L},j} = J \tag{2.20}$$

$$h_j = 0 \qquad \text{for } j = 2, \ldots, \mu' \tag{2.21}$$

$$h_1 = Jm_{M,1}^\circ = -J\frac{M}{2}\frac{\partial f_M^\circ}{\partial h_1}. \tag{2.22}$$

That is, all variational couplings are equal to the coupling J of the underlying system, and all variational fields except for the boundary field h_1 vanish.

Thermodynamic functions are obtained as before. In particular, the mean-field magnetization of an 'open' strip of width M is given by

$$m_M^{\mathrm{mf}} = -\frac{\partial f_M^\circ}{\partial H} \tag{2.23}$$

and the mean-field susceptibility by

$$\chi_M^{\mathrm{mf}} = -\frac{\partial^2 f_M^\circ}{\partial H^2} + J\frac{M}{2}\frac{(\partial^2 f_M^\circ/\partial H\partial h_1)^2}{1 + J\frac{M}{2}\partial^2 f_M^\circ/\partial h_1^2}. \tag{2.24}$$

As above, thermodynamic functions can be expressed in terms of the *free* partial derivatives of the free energy of a single strip of corresponding geometry, described by the Hamiltonian (2.16) with parameter values given by (2.19)–(2.22).

As in the case of closed approximants, any attempt to enlarge the space of variational parameters by adding further (multi-spin) interactions to $\mathcal{H}_{MN}^\circ$ does not lead to any improvement of the variational approximations: the minimization condition requires the corresponding coupling constants to be zero. In particular, an extra variational coupling $h_{\mathrm{T},M}$ which would *close* the strip in the transverse M direction will have to vanish, rendering the strip open again at optimally chosen variational parameters. Therefore, within the framework of strip geometries, the test ensemble based on open strips with Hamiltonian (2.16) may be identified as *optimal* in the sense of the PB inequality. It uses the largest meaningful set of independent variational parameters compatible with the lowest symmetry of $M \times \infty$ strips. Hence, the minimum obtained by f_M° is the total minimum of the sensible trial free energies Φ.

3. Finite-size scaling (FSS) analysis of variational approximants

We now turn to an evaluation of thermodynamic functions computed within the variational approximation schemes described in section 2. The dependence of the thermodynamic behaviour of mean-field test strips on their width M will be extracted by the use of FSS. Wherever possible we will determine critical exponents.

In both cases only one variational parameter turned out to be non-trivial. In the case of test ensembles living on closed strips, this parameter is a variational field h acting *homogeneously* on all spins and determined by (2.8),

$$h = J\frac{2}{M}m_M^{\mathrm{c}}$$

whereas in the case of test ensembles based on open strips, it is a *boundary* field h_1 acting only on the first and the Mth row of each strip and which is determined by (2.22),

$$h_1 = Jm_{M,1}^{\mathrm{o}}.$$

In both versions of the variational scheme, the approximation T_M of the critical point T_{c} is signalled by the appearance of non-zero solutions of the variational field h or h_1 respectively. As the temperature T is lowered, the bifurcation from the zero solution occurs when (setting $J = 1$)

$$1 = \frac{2}{M}\frac{\partial m_M^{\mathrm{c}}}{\partial h}(T, H = 0, h = 0) \tag{3.1}$$

in the 'closed' variant, and when

$$1 = \frac{\partial m_{M,1}^{\mathrm{o}}}{\partial h_1}(T, H = 0, h_1 = 0) \tag{3.2}$$

in the 'open' variant. The solutions of these equations define the mean-field critical temperatures T_M. In the following, we discuss the scaling analysis of these equations and of the corresponding divergence of the mean-field susceptibilities (2.12) and (2.24). The two different cases will be considered separately.

3.1. *Finite-size analysis of test ensembles based on closed strips*

Let us begin with the sequence of approximants based on closed homogeneously magnetized strips. In this case both the variational field h and the external field H act homogeneously on all spins. As we have chosen $\mathcal{H}_{M,N}^{\mathrm{c}}$ to depend on these fields through their sum $H + h$, the free energy f_M^{c} is a function of $(H + h)$ only, and we can replace partial derivatives of f_M^{c} with respect to h by partial derivatives with respect to H and *vice versa*. Denoting the 'free' susceptibility of a closed strip of circumference M by

$$\chi_M^{\mathrm{c}}(T, h) = -\frac{\partial^2 f_M^{\mathrm{c}}}{\partial H^2}(T, H = 0, h) \tag{3.3}$$

we can formulate the critical condition (3.1) as

$$1 = \frac{2}{M}\chi_M^{\mathrm{c}}(T_M, 0) \tag{3.4}$$

and the expression (2.12) for the mean-field susceptibility according to

$$\begin{aligned}\chi_M^{\mathrm{mf}}(T, H=0) &= \chi_M^{\mathrm{c}}(T,h) + \frac{2}{M}\frac{(\chi_M^{\mathrm{c}}(T,h))^2}{1-\frac{2}{M}\chi_M^{\mathrm{c}}(T,h)} \\ &= \frac{\chi_M^{\mathrm{c}}(T,h)}{1-\frac{2}{M}\chi_M^{\mathrm{c}}(T,h)}.\end{aligned} \tag{3.5}$$

These two expressions are now directly amenable to analysis by FSS [7].

Analysis of (3.4) will give the asymptotic behaviour of the reduced mean-field critical temperatures $t_M := (T_M - T_c)/T_M$. Let us first recall the finite-size behaviour of the free energy of an Ising strip of width M in a zero field. Close to the critical temperature T_c of the 2D Ising system, the singular part of its zero-field susceptibility is given by the finite-size scaling expression

$$\chi_M(T) \sim \chi_\infty(T)\mathcal{Q}\left(\frac{\xi_\infty(T)}{M}\right) \sim |t|^{-\gamma}\mathcal{Q}_{\mathrm{hom}}\left(\frac{|t|^{-\nu}}{M}\right) \tag{3.6}$$

where $t = (T - T_c)/T_c$. This expression holds for open and closed strips alike, albeit with different scaling functions. The behaviour of the scaling function $\mathcal{Q}_{\mathrm{hom}}(z)$ in the limits $z := (|t|^{-\nu}/M) \to 0$ and $z \to \infty$ can be easily determined. These limits correspond to the cases $M \to \infty$ at non-critical temperature $T \neq T_c$, or $|t| \to 0$ at finite size $M < \infty$ respectively. Regularity of the left-hand side of (3.6) in these cases implies the power laws $\mathcal{Q}_{\mathrm{hom}}(z) \sim 1$ for $z \to 0$ and $\mathcal{Q}_{\mathrm{hom}}(z) \sim z^{-\gamma/\nu}$ for $z \to \infty$.

This can be applied to the strips considered above. At temperatures at and above the mean-field critical temperature T_M no variational field is present. Under the assumption that the temperatures T_M are sufficiently close to T_c for large M, standard FSS holds, and (3.4) becomes

$$1 \sim \frac{t_M^{-\gamma}}{M}\mathcal{Q}_{\mathrm{hom}}\left(\frac{t_M^{-\nu}}{M}\right). \tag{3.7}$$

As $M \to \infty$ the argument $z_M := (t_M^{-\nu}/M)$ of the scaling function at $T = T_M$ can either vanish, converge to a non-zero constant, or diverge. The latter two cases lead to contradictions ($\gamma \neq \nu$ assumed), leaving $z_M \to 0$ as the only possibility. Hence $\mathcal{Q}_{\mathrm{hom}}(z_M) \sim 1$ as $M \to \infty$, and by (3.7) the mean-field critical temperatures T_M asymptotically scale as

$$t_M = (T_M - T_c)/T_c \sim M^{-1/\gamma}. \tag{3.8}$$

Note that γ is the true susceptibility exponent of the underlying 2D Ising model so that (3.8) can be used to determine both T_c and γ.

The same analysis applied to (3.5) gives the behaviour of the mean-field susceptibility χ_M^{mf} in the vicinity of the mean-field critical temperatures T_M. Expanding the denominator in small temperature differences $t - t_M = (T - T_M)/T_c$ above T_M gives

$$1 - \frac{2}{M}t^{-\gamma}\mathcal{Q}_{\mathrm{hom}}(z) \simeq (t - t_M)\frac{2}{M}t_M^{-\gamma-1}[\gamma\mathcal{Q}_{\mathrm{hom}}(z_M) + \nu z_M \mathcal{Q}'_{\mathrm{hom}}(z_M)]. \tag{3.9}$$

The second term in the square brackets can be neglected, as $z_M \to 0$ and $\mathcal{Q}'_{\mathrm{hom}} \to 0$ for $M \to \infty$. We substitute $M \propto t_M^{-\gamma}$, cancel $\chi_M^{\mathrm{c}}(T_M, 0) \propto t_M^{-\gamma}\mathcal{Q}_{\mathrm{hom}}(z_M)$, and finally arrive at

$$\chi_M^{\mathrm{mf}}(T) \propto \frac{1}{(t - t_M)}\frac{1}{t_M^{\gamma-1}}. \tag{3.10}$$

Equation (3.10) exhibits the usual mean-field divergence of the susceptibility $\chi_M^{\mathrm{mf}}(T) \propto (t - t_M)^{-1}$ as $t \to t_M$. Note that the prefactor $t_M^{-(\gamma-1)}$ itself diverges as $M \to \infty$, a phenomenon for which Suzuki coined the term *coherent anomaly* [5]. Obviously, the coherent anomaly provides a second opportunity to extract the asymptotic susceptibility exponent γ of the underlying system from the sequence of mean-field approximations. Our considerations clearly show that this method is entirely rooted in the FSS philosophy, hence in conventional RG ideas. This relationship has hitherto been much less clear in the literature on this topic.

The dependence of the mean-field critical temperatures T_M on the strip width M is displayed in figure 1. The convergence to the asymptotic value is fairly slow, as can be anticipated from (3.8). Nevertheless, good extrapolation algorithms (see for instance [8]) predict $T_M \to T_\infty = 2.26 \pm 0.01$, which is reasonably close to the exact value of $T_c \simeq 2.269$. Setting $T_c = T_\infty$ in (3.8) we obtain an estimate for γ, that is $\gamma \to 1.77 \pm 0.03$ as $M \to \infty$. While not extraordinary, this result is also not too far from the exact value.

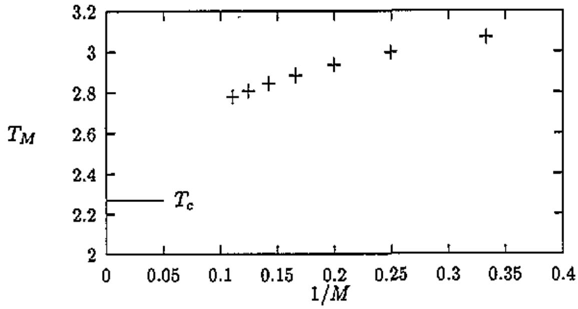

Figure 1. Mean-field critical temperature T_M of closed approximants as a function of the inverse strip width $1/M$.

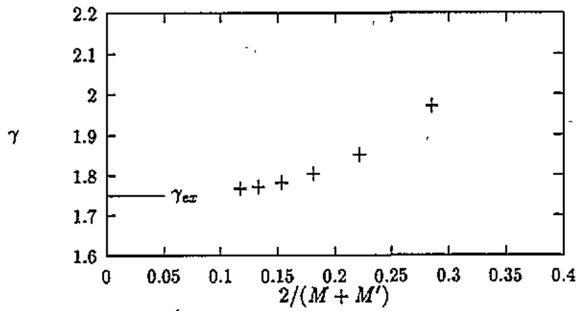

Figure 2. Estimate of the susceptibility exponent γ derived from the ratio of prefactors $\bar{\chi}_M$ of the mean-field susceptibility for two successive strip widths M and $M' = M + 1$ as a function of $2/(M + M')$.

Figure 2 shows the values of γ obtained from the ratio of prefactors $\bar{\chi}_M = t_M^{-(\gamma-1)}$ of the mean-field susceptibility (3.10) for two successive strip widths M and $M' = M + 1$. Assuming $T_c = T_\infty$, we extrapolate this sequence of γ values to $\gamma_\infty = 1.765 \pm 0.01$, which produces a reasonably good agreement with the exact result $\gamma = 1.75$ for the susceptibility exponent. With the exact value for T_c the extrapolation yields a slightly better result, $\gamma_\infty = 1.751 \pm 0.01$, which gives the susceptibility exponent to within less than 1% of the exact result.

3.2. Finite-size analysis of test ensembles based on open strips

Much to our surprise, the approximation scheme breaks down in the case of the ensemble of open, inhomogeneously magnetized strips—the family of systems we identified as ideal in the sense of the PB inequality!

By concavity, we have singled out the boundary field h_1 as the only non-trivial variational parameter. It affects only two spins per column. The self-consistency equation is given by (2.22) and the critical condition by

$$1 = \frac{\partial m^o_{M,1}}{\partial h_1}(T_M, 0, 0). \tag{3.11}$$

Numerical values of T_M obtained by transfer matrix calculations are plotted in figure 3. Unexpectedly, as $M \to \infty$ they converge to a temperature $T_\infty \simeq 2.64$ which is *different* from the correct critical temperature $T_c \simeq 2.27$ of the 2D Ising model.

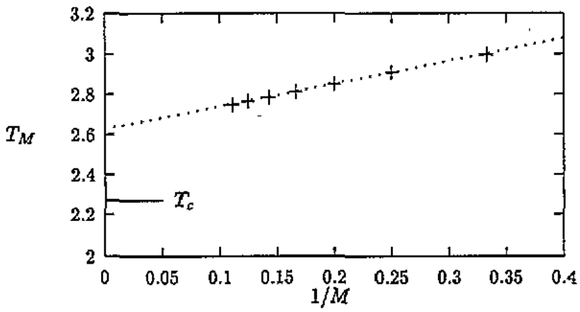

Figure 3. Mean-field critical temperature T_M of open approximants as a function of the inverse strip width $1/M$. Note that they do *not* extrapolate to T_c as $M \to \infty$.

For a qualitative explanation of this behaviour, we again refer to FSS analysis. We note that the susceptibility

$$\frac{\partial m^o_{M,1}}{\partial h_1}(T, 0, h_1) = -\frac{M}{2}\frac{\partial^2 f^o_M}{\partial h_1^2}(T, 0, h_1) =: \chi_{1,1}(T, h_1, M) \tag{3.12}$$

that appears in the critical condition (3.11) is well known in the theory of surface critical phenomena [9, 7]. It takes the scaling form

$$\chi_{1,1}(T, h_1, M) \sim \log|t|^{-1}\tilde{\mathcal{Q}}_1(h_1|t|^{-\Delta_1}, |t|^{-\nu}/M) + \tilde{\mathcal{Q}}_2(h_1|t|^{-\Delta_1}, |t|^{-\nu}/M) \tag{3.13}$$

where Δ_1 is the gap exponent corresponding to h_1 (see [10–12] for extensive treatments). In the limit $z = (|t|^{-\nu}/M) \to 0$, which corresponds to first taking the thermodynamic limit and then approaching the critical temperature, it diverges logarithmically:

$$\chi_{1,1}(T) \sim \log|t|^{-1}. \tag{3.14}$$

This fact is closely related to the anomalous logarithmic divergence of the specific heat occurring in the 2D Ising lattice. Consequently, at finite width and at the critical temperature ($z \to \infty$), the FSS behaviour of $\chi_{1,1}$ at a zero variational field is given by

$$\chi_{1,1}(T_c, M) \sim \log M. \tag{3.15}$$

With these results at hand, we can now return to the critical condition

$$1 \sim \chi_{1,1}(T_M, 0, M) \sim \log t_M^{-1} \tilde{Q}_1(0, z_M) + \tilde{Q}_2(0, z_M). \tag{3.16}$$

Again, the cases $z_M \to$ constant and $z_M \to \infty$ as $M \to \infty$ can be ruled out by (3.16) and (3.15) respectively. For $z_M \to 0$ (3.14) becomes $1 \sim \log t_M^{-1}$ or $t_M \sim 1$, which is consistent with $z_M \to 0$. We therefore conclude that

$$t_M = (T_M - T_c)/T_c \sim 1 \qquad (M \to \infty). \tag{3.17}$$

The critical temperatures of the sequence of test systems based on open inhomogeneously magnetized strips do *not* converge to T_c, which conforms to our above observation. Note that this result is not merely an anomaly of the 2D Ising lattice. It does not, as it might seem, depend on the logarithmic singularity of $\chi_{1,1}(T)$. A similar calculation for the case of a non-zero exponent $\gamma_{1,1}$ corresponding to $\chi_{1,1}$ gives just the same behaviour for the t_M's. It has tacitly been assumed that the edge itself cannot become critical at a temperature different from that of the bulk's T_c; this restricts the above argument to quasi-one-dimensional test systems.

We can finally use these results to investigate the scaling of the mean-field susceptibilities (2.24) with strip width M near the respective mean-field critical points T_M. Analogous to (3.5) we find the mean-field susceptibility

$$\chi_M^{\mathrm{mf}}(T) = \chi_M(T, h_1(T)) + J\frac{2}{M}\frac{(\chi_1(T, h_1(T)))^2}{1 - J\chi_{1,1}(T, h_1(T))}. \tag{3.18}$$

Here $\chi_M = \partial^2 f/\partial H^2$, $\chi_1 = -(2/M)\partial^2 f/\partial H \partial h_1$ and $\chi_{1,1} = -(2/M)\partial^2 f/\partial h_1^2$ are the 'bulk' susceptibility and the two 'surface' susceptibilities well known in the standard treatment of surface critical phenomena. The mean-field susceptibility $\chi_M^{\mathrm{mf}}(T)$ differs from the free susceptibility $\chi_M(T)$ of a strip of the same geometry in two ways: by the action of the variational boundary field $h_1(T)$ in the first term of the right-hand side of (3.18), and by an explicit mean-field divergence in the second term.

Both of these contributions can be shown to become irrelevant in the limit of large M. In this limit, $\xi_M(T_M)/M \to 0$ in view of (3.17), so that the two surface susceptibilities χ_1 and $\chi_{1,1}$ become independent of the strip width M. Setting them constant and expanding in small temperature differences above T_M we arrive at

$$\chi_M^{\mathrm{mf}}(T) \sim \chi_M(T, h_1(T)) + \frac{\text{constant}}{M}\frac{1}{T - T_M}. \tag{3.19}$$

Thus, in the limit of large width M the explicit mean-field contribution is suppressed by a factor $1/M$. Furthermore, the surface field $h_1(T)$ appearing below T_M does not affect the thermodynamic properties of the bulk at large M since the thermodynamic limit is *independent* of boundary conditions.

We thus encounter the paradoxical situation of a singularity in the 'open' mean-field approximants which become spurious as the limit $M \to \infty$ is taken. That is, even though thermodynamic functions exhibit a (suppressed) singularity at a temperature $T_M > T_c$, this singularity does *not* correspond to a change in the system's thermodynamic properties in the limit $M \to \infty$. Evidently, no useful information can be drawn from these mean-field singularities and any attempt to extrapolate to the underlying 2D Ising lattice must fail.

The true thermodynamic singularity of the mean-field susceptibility develops right at T_c in the *first* contribution to (3.18) by conventional reduction of the finite-size rounding of the bulk susceptibility χ_M as $M \to \infty$.

4. Conclusions

In this paper a generalized mean-field theory based on the PB inequality is used to define quasi-one-dimensional approximants for the 2D Ising lattice. By convexity arguments, all but one of the minimization conditions for the variational parameters can be solved explicitly, a finding that is not restricted to the Ising model but holds generally for systems with a scalar order parameter. Thereby a systematic classification of PB approximants is possible. We singled out two types of strip: periodically 'closed' strips with rotational symmetry in the direction transverse to the axis of infinite extent and 'open' strips of inhomogeneous magnetization.

By standard FSS the former are shown to display a coherent anomaly. Estimates of critical exponents of the underlying, fully interacting Ising system can be extracted. At this point it has to be stressed that the variational method presented above should not be advocated as a new, superior numerical tool for computing transition temperatures or critical exponents; the estimates calculated above are clearly inferior to those obtained by Hu *et al* [13]. In the original CAM scheme based on *ad hoc* self-consistency equations, mean-field critical temperatures behave like $(T_M^{\mathrm{CAM}} - T_c) \sim M^{-1/\nu}$, whereas (3.7) states $(T_M^{\mathrm{PB}} - T_c) \sim M^{-1/\gamma}$; that is, the convergence of the PB critical temperatures is slower than in the scheme of Hu *et al* (which in turn is slower than that of the conventional phenomenological RG procedure [14]). In the PB scheme the asymptotic regime of FSS power laws is reached only for very large strip width; corrections to scaling are, therefore, expected to play an important role.

Nevertheless, we believe that our findings are of interest in their own right, since the appearance of a coherent anomaly in the family of 'closed' approximants can be given a clear interpretation as an FSS phenomenon.

It is difficult to give an intuitive explanation for the different scalings of the mean-field critical temperatures in the CAM (Weiss and Bethe approximations [13]) and the PB schemes respectively. In both cases critical conditions can be expressed in terms of summed correlation functions. In the PB scheme a true susceptibility involving correlations between spins at *all* distances is compared with an expression of the order of the system size M, hence the appearance of the exponent γ. In the Weiss and Bethe critical conditions, on the other hand, correlations between spins at a *minimal* distance $\mathcal{O}(M)$ dominate. Therefore, the relation between the correlation length ξ and the linear dimension M of the cluster plays the decisive role. This is responsible for the appearance of the exponent ν in the corresponding scaling expression.

In sharp contrast to expectations, the 'open' strips, which are found to be the optimal family of approximants in the sense of the PB inequality, give rise to a spurious criticality at a temperature *different* from the 2D Ising critical temperature. Any extrapolation to the full two-dimensional system based on the mean-field critical behaviour of this family must therefore fail. This unexpected result clearly shows that variational descriptions of many-particle systems should be used with the utmost caution.

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