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The Critical Behavior of Kac-Type Models for Semi-Infinite Systems

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The critical behavior of the layer magnetizations and local susceptibilities of the D-vector lattice models with Kac-type ferromagnetic interactions for a semi-infinite system is studied. These local quantities behave less singularly than the bulk ones, showing that this is not peculiar to the two-dimensional Ising model. Moreover, the limiting form (at the critical point) of the magnetization profile can be obtained, which, when properly scaled, satisfies the minimum condition in the Landau theory for a semi-infinite continuous system. Landau-type critical behavior is thus recovered.

KEY WORDS: Kac-type interactions; semi-infinite systems; critical behavior; local quantities; functional equation.

1. INTRODUCTION

A great deal of interest has been devoted recently to the study of the critical behavior of semi-infinite systems, especially via scaling or renormalization group arguments (see, e.g., Ref. 1, and references therein). The main prediction concerning semi-infinite systems is that local thermodynamic quantities near the surface (for instance, the magnetization of the boundary layer in ferromagnetic lattice spin systems) should have critical indices different from the corresponding bulk quantities. The only rigorous result in this direction has been obtained for the two-dimensional Ising model with nearest-neighbor interactions by McCoy and Wu,[(2)] who have found that the boundary row magnetization vanishes as $(T_c - T)^{1/2}$, in contradistinction to the $(T_c - T)^{1/8}$ behavior of the bulk spontaneous magnetization.

In order to lend support to the fact that such peculiar behavior is

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general, it is interesting to see whether it can be put into evidence on other rigorously tractable models. In this paper, we shall consider a class of mean-field models sensitive to the geometry of the system for which a complete description of the critical behavior can be obtained.

We shall briefly describe the models under consideration following Pearce.[3] Consider the D-vector model Hamiltonian with Kac–Helfand interaction[4] for a rectangular array of $N \times n$ spins of length $D^{1/2}$:

$$\mathcal{H}^{(n)}_{D,\gamma,N} = -\frac{\gamma}{4} \sum_{\mu,\nu=1}^{N} e^{-\gamma|\mu-\nu|} \sum_{i,j=1}^{n} J^{(n)}_{ij} \mathbf{S}_{\mu i} \mathbf{S}_{\nu j} - \sum_{\mu=1}^{N} \sum_{i=1}^{n} \mathbf{H}_i \mathbf{S}_{\mu i} \tag{1}$$

where $J^{(n)}_{ij} = 4\delta_{ij} + \delta_{i,j+1} + \delta_{i,j-1}$, $1 \leqslant i, j \leqslant n$, and $\mathbf{H}_i$ has equal components H_i in the spin space. Denote

$$\psi^{(n)}_D(\beta; \{H_i\}) = \lim_{\gamma \searrow 0} \lim_{N\to\infty} \left(-\frac{1}{\beta N n D}\right) \log \operatorname{Tr} \exp\left(-\beta \mathcal{H}^{(n)}_{D,\gamma,N}\right)$$

$\psi^{(n)}_D(\beta; \{H_i\})$ will be taken as the free energy per spin and per spin component, defining the Kac-type D-vector model for a slab with n layers. Its $D \to \infty$ limit, $\psi^{(n)}_\infty$, defines the Kac-type spherical model. (Let us remark that the order of the $D \to \infty$ and $\gamma \searrow 0$ limits can be reversed, as seen by combining arguments in Refs. 3 and 5.) The existence of the $\gamma \searrow 0$ limit is proved in Ref. 3, where, as expected from the $D = 1$ case,[6] the following expression is obtained:

$$\beta\psi^{(n)}_D(\beta; \{H_i\}) = \min_{m \in R^n} \frac{1}{n} \left[\frac{\beta}{2}(m, J^{(n)}m) - \sum_{i=1}^{n} \mathcal{F}_D\left(\beta(J^{(n)}m)_i + \beta H_i\right) \right] \tag{2}$$

where

$$\mathcal{F}_1(H) = \log(2\cosh H) \tag{3}$$

$$\mathcal{F}_D(H) = \frac{1}{D} \log \int_{S_D} e^{(\mathbf{H},\mathbf{S})}\, d\mu_D(\mathbf{S})$$

$$= \frac{1}{D} \log \frac{1}{B(1/2, (D-1)/2)} \int_0^\pi e^{DH\cos\theta} \sin^{D-2}\theta\, d\theta,$$

$$2 \leqslant D < \infty \tag{3'}$$

$$\mathcal{F}_\infty(H) = \tfrac{1}{2}\left\{(1+4H^2)^{1/2} - 1 - \log \tfrac{1}{2}\left[1 + (1+4H^2)^{1/2}\right]\right\} \tag{3''}$$

[In (3′), S_D is the sphere of radius $D^{1/2}$ in R^D, $d\mu_D$ its natural (normalized) measure, and $B(.,.)$ is the beta function.]

The detailed study of the minimum in Eq. (2) will be performed in Section 2, with the result that the minimum is attained in a unique point

$m^{(n)}(\beta, H) \in R_+^{(n)}$ $(R_+ = [0, \infty))$; $m_i^{(n)}$ can be identified with the layer magnetizations, i.e.,

$$m_i^{(n)}(\beta, H) = \lim_{\gamma \to 0} \lim_{N \to \infty} \langle S_{\mu i}^{\alpha} \rangle$$

Different properties of the magnetizations and susceptibilities $\chi_{ij}^{(n)} = \partial m_i^{(n)} / \partial H_j$ in zero magnetic field will also be given. The argument follows partially, though with some simplifications, that previously given for the $D = 1$ case.[7]

The semi-infinite system is obtained in Section 3 (restricting attention to $H = 0$) as a limit of slabs of finite thickness. Namely, it will be shown that $\lim_{n\to\infty} m_i^{(n)} = m_i$, $\lim_{n\to\infty} \chi_{ij}^{(n)} = \chi_{ij}$, and $\lim_{n\to\infty} \sum_{j=1}^{n} \chi_{ij}^{(n)}$ do exist. These local quantities are to be compared to the global (bulk) quantities: $\lim_{n\to\infty}(1/n)\sum_{i=1}^{n} m_i^{(n)} = m_B$ and $\lim_{n\to\infty}(1/n)\sum_{i,j=1}^{n} \chi_{ij}^{(n)} = \chi_B$. As expected, $m_B = \lim_{i\to\infty} m_i$ and $\chi_B = \lim_{i\to\infty} \sum_{j=1}^{\infty} \chi_{ij}$. The surface free energy exists and can be obtained explicitly in terms of m_i.

Section 4 is devoted to the critical behavior of the above-mentioned quantities. We find that the local quantities, such as m_i, χ_{ij}, or $\sum_{j=1}^{\infty} \chi_{ij}$ are less singular than the global ones. While the critical indices of the local quantities appear to be independent of the distance from the boundary, the magnitudes of their leading asymptotic terms go to infinity with this distance, showing that the two limits cannot be interchanged. The way in which the boundary critical behavior turns into bulk critical behavior deep into the bulk is explicitly shown to be

$$m_k \simeq m_B \tanh\left[\sqrt{3}\left(\frac{\beta - \beta_c}{\beta_c}\right)^{1/2} k\right], \qquad \text{where } m_B \simeq \left(\frac{\beta - \beta_c}{\beta_c}\right)^{1/2}$$

This is in fact the scaling ansatz usually made in studying the critical behavior of systems with surfaces.

It should be noted that this expression of the layer magnetization valid in the critical region, is precisely the same as that obtained in Landau-type theory in the limit of the "extrapolation length" λ, going to zero. (In our case the interaction constants in the surface and the bulk are the same. For an exposition of Landau theory for semi-infinite systems see, for instance, Ref. 1.d.) This shows that the correspondence between Kac-type theory and Landau theory does work not only for "global" critical behavior, but also for the "local" one. However, we have not been able to get the magnetization profile outside the critical region to check this correspondence any further. Actually, obtaining the magnetization profile for lattice models even in the critical region is not a trivial problem and there is little hope to solve it for any temperature in the ferromagnetic phase.

Section 5 is devoted to a discussion of some problems which we leave for future study and of possible contacts with other approaches.

2. THE DESCRIPTION OF THE FINITE SLAB

In order to study the minimum in Eq. (2), some properties of the functions $\mathcal{F}_D(\cdot)$ will be needed. These will follow easily by remarking that $\mathcal{F}_D(H)$ is (up to factors) the free energy of a single D-dimensional spin in an external magnetic field **H** with equal components H.

Proposition 2.1. $\mathcal{F}_D$: $R \to R$ are nonnegative, even C^∞ functions, and

(i)	$\mathcal{F}'_D(x) > 0$	for $x > 0$,	and $\lim_{x\to\infty} \mathcal{F}'_D(x) = 1$
(ii)	$\mathcal{F}''_D(x) > 0$,	$\forall x \in R$,	and $\mathcal{F}''_D(0) = 1$
(iii)	$\mathcal{F}'''_D(x) < 0$	for $x > 0$.	

Proof. For $D < \infty$, the inequalities in (i) and (ii) are nothing but Griffiths' first and second inequalities and, in fact, can be easily checked in Eqs. (3), from which $\lim \mathcal{F}'_D$ and $\mathcal{F}''_D(0)$ follow as well. Property (iii) is a GHS inequality and is proved by remarking that, changing the variable to $\sigma = \cos\theta$ in Eq. (3′), one gets the free energy of a continuous Ising spin with *a priori* distribution meeting the conditions of Ellis and Newman.[8] For $\mathcal{F}_\infty$ these follow by inspection. ■

As a consequence of the properties (i) and (ii), $\mathcal{F}_D(x)$ grows linearly for $|x| \to \infty$, so the function to be minimized in Eq. (2) has indeed a minimum point, which is necessarily one of its stationary points. Taking advantage of the invertibility of $J^{(n)}$, we can write the stationarity condition as

$$m_i = \mathcal{F}'_D\big(\beta(J^{(n)}m)_i + \beta H_i\big), \qquad \forall i = 1, \ldots, n \tag{4}$$

As $\perp \mathcal{F}'_D(x) \perp < 1$ from Proposition 2.1, all the solutions of Eq. (4) satisfy $|m_i| < 1$.

A more convenient form of these equations is obtained in terms of the function F_D: $(-1, 1) \to R$ defined as follows:

$$F_D(x) = (1/\beta)\mathcal{F}'^{-1}_D(x) - 4x \tag{5}$$

As a consequence of Proposition 2.1, F_D is a well-defined, odd C^∞ function and

$$F''_D(x) > 0 \quad \text{for } x > 0, \qquad \lim_{x \nearrow 1} F_D(x) = +\infty, \qquad F'_D(0) = (1/\beta) - 4 \tag{6}$$

The extremum condition—Eq. (4)—becomes

$$(A^{(n)}m)_i = F_D(m_i) - H_i, \qquad \forall i = 1, \ldots, n \tag{7}$$

where $A^{(n)}_{ij} = 1$ for $|i - j| = 1$, and 0 otherwise.

Proposition 2.2. Let $H \in R_+^n$ and D be given. Define

$$\beta_c^{(n)} = \frac{1}{\lambda_{\max}(J^{(n)})} = \left(4 + 2\cos\frac{\pi}{n+1}\right)^{-1} \tag{8}$$

Then, denoting $I = [0, 1)$ we have the following:

(i) For $H = 0$ and $\beta \leqslant \beta_c^{(n)}$, Eq. (7) has in I^n the unique solution $m^{(n)}(\beta, 0) = 0$. Otherwise, Eq. (7) has in $I^n \backslash \{0\}$ a unique solution $m^{(n)}(\beta, H)$, which, moreover, is in $\operatorname{Int} I^n$.

(ii) The function $m^{(n)}$: $(0, \infty) \times R_+^n \to I^n$ defined in (i) is continuous and increasing in (β, H) [with respect to the partial orders induced by the cone R_+^{n+1} for (β, H) and by the cone $\{0\} \cup \operatorname{Int} R_+^n$, for $\mathrm{m}^{(n)}$].

(iii) The absolute minimum in Eq. (2) is attained at $m^{(n)}(\beta, H)$ defined in (i). If $H \neq 0$, it is attained only at $m^{(n)}(\beta, H)$, while if $H = 0$, it is attained only at $\pm m^{(n)}(\beta, H)$.

Proof. (i) We start by remarking that every nonzero solution in I^n of Eq. (7) for $H \in R_+^n$ is, in fact, in $\operatorname{Int} I^n$. Indeed, if $m_i = 0$ for some i, then, as $F_D(0) = 0$, Eq. (7) implies $m_{i-1} + m_{i+1} + H_i = 0$, so $m_{i-1} = m_{i+1} = H_i = 0$, etc.

We shall construct solutions in $\operatorname{Int} I^n$ of the system (7), by reducing it to a single equation, via successive elimination of the unknowns. The following elementary remarks will prove useful.

Lemma 2.3. Let $\mathcal{C}$ be the convex cone consisting of all continuous functions f: $I \to R$ which are C^∞ and strictly convex on $\operatorname{Int} I$ and have $f(0) \leqslant 0$, $\lim_{x \to 1} f(x) = \infty$. Every $f \in \mathcal{C}$ is either nonnegative and strictly increasing, or has a strictly positive root, which is unique and beyond which f is positive and strictly increasing; in both cases, denote f^{-1}: $I \to R_+$ the restriction to I of the inverse of the positive part of f. Then f^{-1} is C^∞ strictly increasing and strictly concave on $\operatorname{Int} I$. Moreover, for $f, g \in \mathcal{C}$

$$f \leqslant g \quad \text{implies} \quad -f^{-1} \leqslant -g^{-1} \tag{9}$$

$$x, y \in I, \quad x > f(y) \quad \text{implies} \quad f^{-1}(x) > y \tag{10}$$

irrespective of the sign of $f(y)$.

We shall adhere in the following to the notations established in Lemma 2.3.

Let us define $f_i \in \mathcal{C}$, $i = 1, 2, \ldots,$ by

$$f_1(x) = F_D(x) - H_1, \qquad f_i(x) = F_D(x) - H_i - f_{i-1}^{-1}(x), \quad i \geqslant 2 \tag{11}$$

Let us note that, in view of Eq. (9), and of the explicit dependence on (β, H) exhibited in Eqs. (11) and (5), $f_i(x)$ is a decreasing function of (β, H) for every $x \in I$.

In terms of these functions the system (7) can be written on $\mathrm{Int}\, I^n$ as $m_{i+1} = f_i(m_i)$, $i = 1, \ldots, n-1$, the nth equation being $f_n(m_n) = 0$. Thus, if $m \in \mathrm{Int}\, I^n$ is a solution of Eq. (7), m_n is the unique positive root of f_n. Conversely, if f_n has a root $m_n > 0$, then $m_{n-i} = f_{n-i}^{-1}(m_{n-i+1})$, $i = 1, \ldots, n-1$, are all strictly positive and $m = (m_1, \ldots, m_n)$ satisfies Eq. (7).

Thus Eq. (7) has at most one solution in $\mathrm{Int}\, I^n$, and it has one if and only if f_n has a strictly positive root. This in turn is ensured either by $f_n(0) < 0$ (which settles the existence for $H \neq 0$), or by $\lim_{x \to 0} f_n'(x) \equiv a_n < 0$. So, suppose $f_n(0) = 0$. Then, from the definition (11), $H = 0$ and $f_i^{-1}(0) = 0$ for $i = 1, \ldots, n-1$. In particular, $f_i(0) = 0$, and $a_i = F_D'(0) - 1/a_{i-1}$ can be calculated inductively. Remembering the relation of $\beta_c^{(n)}$ with the greatest eigenvalue of $J^{(n)}$, Eq. (8), the result is $a_n = \det(1/\beta - J^{(n)})/\det(1/\beta - J^{(n-1)})$ for $\beta < \beta_c^{(n-1)}$. This is negative for $\beta > \beta_c^{(n)}$ and nonnegative for $\beta \leqslant \beta_c^{(n)}$. As the f_i are decreasing in β, this settles the existence for $H = 0$ and all $\beta > \beta_c^{(n)}$. We are thus left with the case $H = 0$ and $\beta \leqslant \beta_c^{(n)}$, where no solution in $I^n \backslash \{0\}$ exists, because $a_n \geqslant 0$; in this case, however, the construction above (or direct inspection) gives $m = 0$ as a solution. This completes the proof of (i).

(ii) The monotonicity of $m^{(n)}(\beta, H)$ follows easily from the construction above and from the monotonicity of f_i^{-1}. As $\lim_{H \to 0} m^{(n)}(\beta, H) \in I^n$ satisfies Eq. (7), continuity follows from uniqueness.

(iii) Let us define $G_D\colon (-1, 1) \times R_+ \to R$ by

$$G_D(x, y) = \tfrac{1}{2} x \mathfrak{F}_D'^{-1}(x) - \mathfrak{F}_D\big(\mathfrak{F}_D'^{-1}(x)\big) - \tfrac{1}{2}\beta x y \tag{12}$$

$G_D(x, y) \geqslant G_D(|x|, y)$ and $G_D(x, y)$ is strictly decreasing in x on I at fixed y. Indeed, because $\mathfrak{F}_D'$ is strictly concave and $\mathfrak{F}_D'(0) = 0$, we have $\mathfrak{F}_D'(x)/x > \mathfrak{F}_D''(x)$, so

$$\begin{aligned}
\frac{\partial G_D}{\partial x}(x, y) &= \frac{1}{2}\left[\mathfrak{F}_D'^{-1}(x) - \frac{x}{\mathfrak{F}_D''\big(\mathfrak{F}_D'^{-1}(x)\big)}\right] - \frac{\beta}{2} y \\
&\leqslant \frac{1}{2}\,\frac{\mathfrak{F}_D'^{-1}(x)}{\mathfrak{F}_D''\big(\mathfrak{F}_D'^{-1}(x)\big)}\left[\mathfrak{F}_D''\big(\mathfrak{F}_D'^{-1}(x)\big) - \frac{\mathfrak{F}_D'\big(\mathfrak{F}_D'^{-1}(x)\big)}{\mathfrak{F}_D'^{-1}(x)}\right] \\
&< 0
\end{aligned}$$

At a stationary point m the function to be minimized in Eq. (2) equals [by Eq. (4)] $(1/n)\sum_{i=1}^{n} G_D(m_i, H_i)$, so we have only to compare the values of the latter at stationary points.

Thus, the point (iii) will be completely proved if we can show that for every stationary point m different from those indicated

$$|m_i| < m_i^{(n)}(\beta, H), \qquad \forall i = 1, \ldots, n \tag{13}$$

To this aim, take moduli in Eq. (7):

$$(A^{(n)}|m|)_i + H_i \geqslant |(A^{(n)}m)_i + H_i| = |F_D(m_i)| = F_D(|m_i|), \qquad \forall i = 1, \ldots, n \tag{14}$$

and remark that we can confine the analysis to the case in which at least one strict inequality appears in (14). Indeed, otherwise either $|m| = m^{(n)}(\beta, H)$, or $m = 0$ and $m^{(n)}(\beta, H) \neq 0$ [by the proof of (i)]. But $|m| = m^{(n)}(\beta, H)$ is absurd if $m \neq \pm m^{(n)}(\beta, H)$ since a change of sign between consecutive m_i implies at least one strict inequality in (14); if $|m| = 0$ and $m^{(n)}(\beta, H) \neq 0$, (13) is trivially satisfied.

Repeating the elimination procedure used in the proof of (i), made possible by Eq. (10), we find that Eq. (14) implies

$$|m_{i+1}| \geqslant f_i(|m_i|), \quad i = 1, \ldots, n-1 \qquad \text{and} \qquad 0 > f_n(|m_n|) \tag{15}$$

since, again by Eq. (10), a strict inequality for some i_0 propagates to all $i > i_0$. Equation (15) implies in turn $|m_n| < m_n^{(n)}(\beta, H)$, which propagates backwards to all i, by repeated application of Eqs. (10) and (15). ■

Remark 2.4. Equation (13) implies, moreover, for $H = 0$, $\beta \leqslant \beta_c^{(n)}$, the uniqueness in R^n of the trivial solution of Eq. (7).

The minimum point $m^{(n)}(\beta, H)$ defined in Proposition 2.2 is in fact the vector of the layer magnetizations in the Kac-type model [cf. Ref. 3, where it is shown to be $-(1/\beta)\mathrm{grad}_H \psi_D^{(n)}$, and a standard argument[9] based on the convexity of $\log \mathrm{Tr} \exp(-\beta \mathcal{H}_{D,\gamma,N}^{(n)})$ as a function of H]. The susceptibility matrix will be defined consequently by

$$\chi_{ij}^{(n)}(\beta, H) = \partial m_i^{(n)}(\beta, H)/\partial H_j \tag{16}$$

This definition makes sense for $(\beta, H) \in (0, \infty) \times \mathrm{Int}\, R_+^n$, where $m^{(n)}(\beta, H)$ is C^1 by the implicit function theorem, and, as seen by taking the H derivatives of Eq. (7), equals there the inverse of the matrix $X^{(n)}(\beta, H)$:

$$X_{ij}^{(n)}(\beta, H) = \delta_{ij} F_D'\big(m_i^{(n)}(\beta, H)\big) - A_{ij}^{(n)} \tag{17}$$

We shall be interested in the zero-field susceptibility $\chi^{(n)}(\beta, 0) \equiv \lim_{H \searrow 0} \chi^{(n)}(\beta, H)$. By Proposition 2.2(ii) and $F_D'' \geqslant 0$, $X^{(n)}(\beta, H) \geqslant X^{(n)}(\beta, 0) = \lim_{H \searrow 0} X^{(n)}(\beta, H)$, so the $\lim_{H \searrow 0} \chi^{(n)}$ will exist whenever $X^{(n)}(\beta, 0)$ is invertible, and will then be equal to $X^{(n)-1}(\beta, 0)$. We shall show in fact that $X^{(n)}(\beta, 0)$ is strictly positive definite for $\beta \neq \beta_c^{(n)}$. Indeed, if $m^{(n)}(\beta, 0) = 0$, we have [remembering Eqs. (8) and (6)]

$$X^{(n)}(\beta, 0) = F_D'(0) - A^{(n)} = \frac{1}{\beta} - J^{(n)} \geqslant \frac{1}{\beta} - \frac{1}{\beta_c^{(n)}} \equiv a_n(\beta) \qquad (\beta < \beta_c^{(n)}) \tag{18}$$

while if $m^{(n)}(\beta,0) \in \operatorname{Int} I^n$,

$$F_D'\left(m_i^{(n)}\right) > \frac{F_D\left(m_i^{(n)}\right)}{m_i^{(n)}} = \frac{m_{i-1}^{(n)} + m_{i+1}^{(n)}}{m_i^{(n)}} \qquad \left(m_0^{(n)} = m_{n+1}^{(n)} = 0\right)$$

as F_D is strictly convex, and, because the matrix

$$\left(\delta_{ij}\frac{m_{i-1}^{(n)} + m_{i+1}^{(n)}}{m_i^{(n)}} - A_{ij}^{(n)}\right)$$

is nonnegative (its $\binom{1\cdots i}{1\cdots i}$ minor equals $m_{i+1}^{(n)}/m_1^{(n)}$) we have the lower bound

$$X^{(n)}(\beta,0) \geqslant \min_i\left[F_D'\left(m_i^{(n)}\right) - \frac{F_D\left(m_i^{(n)}\right)}{m_i^{(n)}}\right] \equiv a_n(\beta) > 0 \qquad \left(\beta > \beta_c^{(n)}\right) \tag{19}$$

Note that $a_n(\beta) \searrow 0$ for $\beta \to \beta_c^{(n)}$.

Remark 2.5. The relation $\chi^{(n)} = X^{(n)-1}$ allows easy proofs for the positivity and monotonicity properties of $\chi^{(n)}$ as a quadratic form and of its matrix elements, in particular, for $\beta \neq \beta_c^{(n)}$,

$$0 < \chi^{(n)}(\beta,H) \leqslant \chi^{(n)}(\beta,0) \leqslant a_n(\beta)^{-1} \tag{20}$$

$$0 < \chi_{ij}^{(n)}(\beta,H) \leqslant \chi_{ij}^{(n)}(\beta,0) \qquad \forall i,j = 1,\ldots,n \tag{21}$$

The strict inequality in (21) follows, for instance, from $\chi^{(n)} = \int_0^\infty \exp(-tX^{(n)})\,dt$, valid because $X^{(n)}$ is strictly positive definite, and remarking that $[\exp(-tX^{(n)})]_{ij} > 0$, $\forall i,j$, by looking at its series expansion. (Otherwise, $X^{(n)}$ is a symmetric M matrix.[10])

Let us consider the equation

$$2x = F_D(x) \tag{22}$$

It has only the trivial solution $m_B(\beta) = 0$ if $\beta \leqslant \frac{1}{6} \equiv \beta_c$ and a unique, strictly positive solution $m_B(\beta)$ if $\beta > \beta_c$. As will be shown in Section 3, $m_B(\beta)$ is the bulk spontaneous magnetization, and, consequently, β_c^{-1} is the bulk critical temperature. Clearly, $\beta_c^{(n)} \searrow \beta_c$ when $n \to \infty$.

Because F_D is convex, we have $F_D'(0) < 2 < F_D'(m_B(\beta))$ for $\beta > \beta_c$ and, moreover, $F_D'(0) \nearrow 2$, $F_D'(m_B(\beta)) \searrow 2$ when $\beta \searrow \beta_c$.

From now on, we shall confine ourselves to the limit $H = 0$ and derive some properties of $m^{(n)}(\beta,0)$ and $\chi^{(n)}(\beta,0)$. We shall simplify the notation by omitting the arguments: $m^{(n)}(\beta,0)$, $m_B(\beta), \chi^{(n)}(\beta,0)$ will be written simply as $m^{(n)}, m_B, \chi^{(n)}$, respectively. We shall define the "distance from the boundary" by

$$d_i^{(n)} = \min(i, n+1-i) \tag{23}$$

Proposition 2.6. Let $\beta > \beta_c$ and n_0 be the smallest integer for which $\beta > \beta_c^{(n_0)}$. Then, for all $n \geqslant n_0$:

(i) $m_i^{(n)} < m_B, \quad \forall i = 1, \ldots, n.$

(ii) $m_i^{(n)} = m_{n+1-i}^{(n)}, \quad m_i^{(n)} > \frac{1}{2}(m_{i-1}^{(n)} + m_{i+1}^{(n)}), \quad \forall i = 1, \ldots, n.$

As a consequence, $m_i^{(n)}$ is a strictly increasing function of $d_i^{(n)}$.

(iii) $m_i^{(n+1)} > m_i^{(n)}, \quad \forall i = 1, \ldots, n.$

(iv) There exist constants $C, c > 0$, depending only on β (independent on n), such that

$$0 < (m_B - m_i^{(n)})/m_B < C \exp(-cd_i^{(n)}), \qquad \forall i = 1, \ldots, n$$

Proof. (i) Let i_0 be such that $m_{i_0}^{(n)}$ is maximum among $m_i^{(n)}$. Then,

$$F_D(m_{i_0}^{(n)}) = m_{i_0-1}^{(n)} + m_{i_0+1}^{(n)} \leqslant 2m_{i_0}^{(n)}$$

implying $m_{i_0}^{(n)} \leqslant m_B$. Equality is impossible because it would propagate to the first equation, giving $F_D(m_B) = m_B$, which is absurd, as $m_B > 0$ for $\beta > \beta_c$.

(ii) The symmetry of $m_i^{(n)}$ follows from that of the system for $H = 0$. The property $m_i^{(n)} \leqslant (m_{i-1}^{(n)} + m_{i+1}^{(n)})/2$ for one i gives $F_D(m_i^{(n)}) \geqslant 2m_i^{(n)}$, i.e., $m_i^{(n)} \geqslant m_B$, contradicting (i).

(iii) As already remarked, for $H = 0$, the sequence $f_i(x)$ defined in Eq. (11) is strictly decreasing, $\forall x \in \operatorname{Int} I$. Thus $m_{n+1}^{(n+1)} > m_n^{(n)}$, or by (ii), $m_1^{(n+1)} > m_1^{(n)}$. However, $f_i(m_n^{(n)}) \geqslant 0$, $\forall i = 1, \ldots, n$, and thus all f_i are strictly increasing on $[m_1^{(n)}, 1)$, implying $m_2^{(n+1)} = f_1(m_1^{(n+1)}) > f_1(m_1^{(n)}) = m_2^{(n)}$, etc.

(iv) Let

$$\omega = \sup_{x \in [m_1^{(n_0)}, m_B]} \left[\frac{m_B - x}{2x - F_D(x)} \right]$$

Then we have $\omega < \infty$, because $m_1^{(n_0)} > 0$ and $F_D'(m_B) > 2$. Now, as $m_i^{(n)} \in [m_1^{(n_0)}, m_B)$ for $n \geqslant n_0$ and all i, and $m_i^{(n)}$ increases with i for $i \leqslant n/2$, we have

$$\begin{aligned} m_B - m_i^{(n)} &\leqslant \omega\left(2m_i^{(n)} - F_D(m_i^{(n)})\right) = \omega(2m_i^{(n)} - m_{i-1}^{(n)} - m_{i+1}^{(n)}) \\ &\leqslant \omega(m_i^{(n)} - m_{i-1}^{(n)}) = \omega\left[(m_B - m_{i-1}^{(n)}) - (m_B - m_i^{(n)})\right] \end{aligned}$$

from which

$$m_B - m_i^{(n)} \leqslant \frac{\omega}{1+\omega}(m_B - m_{i-1}^{(n)})$$

which leads by iteration to the desired inequality with $c = \log(1 + 1/\omega)$, $C = 1$. For odd n and $i = (n+1)/2$, $m_B - m_i^{(n)} \leqslant 2\omega(m_i^{(n)} - m_{i-1}^{(n)})$ and (iv) extends to this case if one takes $C = 1 + 1/(2\omega + 1)$. ∎

Proposition 2.6(iv) shows that, for β far from β_c and n sufficiently large, $m_i^{(n)}$ differs significantly from m_B only near the boundary. We shall next show that the effect of replacing $m_i^{(n)}$ by m_B in the expression for $\chi^{(n)}$ is also significant only near the boundary. To this aim, let

$$\tilde{X}^{(n)} = F'_D(m_B) - A^{(n)}, \qquad \tilde{\chi}^{(n)} = \tilde{X}^{(n)-1} \tag{24}$$

In view of Proposition 2.6(i), $\tilde{X}^{(n)} > X^{(n)}$ for $\beta > \beta_c$ and $\tilde{X}^{(n)} = X^{(n)}$ for $\beta \leqslant \beta_c$, so $\tilde{X}^{(n)}$ is positive definite for all β. We have

$$\tilde{\chi}_{ij}^{(n)} = \frac{z}{1-z^2} z^{|i-j|} - \frac{z}{(1-z^2)(1-z^{2(n+1)})}\left(z^{i+j} + z^{2(n+1)-i-j} - z^{2(n+1)-i+j}\right.$$
$$\left. - z^{2(n+1)+i-j}\right) < \frac{z}{1-z^2} z^{|i-j|} \equiv \chi_{ij}^B \tag{25}$$

where z is the solution < 1 of the equation $z + 1/z = F'_D(m_B)$. [χ^B is the resolvent of the discrete Laplace operator on $l^2(Z)$ at $F'_D(m_B) - 2$; expression (25) for $\tilde{\chi}^{(n)}$ can be easily obtained in terms of χ^B by applying, for instance, the method of images, as usual for $-d^2/dx^2$.]

Proposition 2.7. Let $\beta > \beta_c$ and n_0 be chosen as in Proposition 2.6. There exist constants C_1, $c_1 > 0$ such that, for all $n \geqslant n_0$,

$$0 < \chi_{ij}^{(n)} - \tilde{\chi}_{ij}^{(n)} \leqslant C_1 \exp\left[-c_1\left(d_i^{(n)} + d_j^{(n)}\right)\right], \qquad 1 \leqslant i, \; j \leqslant n$$

Proof. Let $V^{(n)} = \tilde{\chi}^{(n)} - X^{(n)}$. Now, $V^{(n)}$ is diagonal and, by Proposition 2.6(iv),

$$0 < V_{ii}^{(n)} = F'_D(m_B) - F'_D\left(m_i^{(n)}\right) \leqslant C' \exp\left(-c d_i^{(n)}\right) \qquad \left(C' = C \sup_{(0,m_B)} F''_D\right)$$

Thus, using Eq. (19) and

$$a_n(\beta) \geqslant \inf_{(m_1^{(n)}, m_B)} \left[F'_D(x) - \frac{F_D(x)}{x}\right] \equiv a'_n(\beta) \geqslant a'_{n_0}(\beta) \equiv a > 0$$

[by Proposition 2.6(ii), (iii)], we have, because $\tilde{X}^{(n)} \geqslant a + V^{(n)}$,

$$0 < V^{(n)1/2} \tilde{\chi}^{(n)} V^{(n)1/2} \leqslant \left(1 + a V^{(n)-1}\right)^{-1} \leqslant C'/(a + C')$$

Then $\|(1 - V^{(n)1/2} \tilde{\chi}^{(n)} V^{(n)1/2})^{-1}\| \leqslant (a + C')/a$, so

$$\chi^{(n)} - \tilde{\chi}^{(n)} = \tilde{\chi}^{(n)} V^{(n)1/2} \left(1 - V^{(n)1/2} \tilde{\chi}^{(n)} V^{(n)1/2}\right)^{-1} V^{(n)1/2} \tilde{\chi}^{(n)}$$

But, using the bound in Eq. (25), we have

$$\sum_{j=1}^{n} \tilde{\chi}_{ij}^{(n)} V_{jj}^{(n)1/2} \leqslant C'' \exp\left(-c_1 d_i^{(n)}\right)$$

with $c_1 = \frac{1}{2}\min[c, \log(1/z)]$, from which the assertion follows.

3. THE SEMI-INFINITE LIMIT

In this section we shall be concerned with the $n \to \infty$ limit of the local and global quantities characterizing the n-layer system. Specifically, we shall be interested in limits like $\lim_{n\to\infty} m_i^{(n)}$ at fixed i and $\lim_{n\to\infty}(1/n)\sum_{i=1}^n m_i^{(n)}$, which should be taken as the local and global magnetization of the semi-infinite system, respectively. Physically, it is to be expected that local quantities will approach the corresponding global quantities exponentially rapidly with distance from the boundary, as long as β is kept away from β_c.

Proposition 3.1. Let $H = 0$. Then we have the following:

(i) The sequence $f_i \in \mathcal{C}$ defined by Eq. (11) converges monotonically to a function $f \in \mathcal{C}$, which is the (unique) solution of the functional equation

$$f(x) + f^{-1}(x) = F_D(x), \qquad x \in I \tag{26}$$

(ii) $\lim_{n\to\infty} m_i^{(n)} \equiv m_i$ exists; $m_i = 0$ for $\beta \leqslant \beta_c$, while for $\beta > \beta_c$

$$m_i = (f^{-1})^{\circ i}(0), \qquad i = 1, 2, \ldots \tag{27}$$

where $(f^{-1})^{\circ i}$ means $f^{-1}\circ \cdots \circ f^{-1}$ (i times). For $\beta > \beta_c$, m_i as a function of i is strictly increasing and concave and there exist constants $C, c > 0$ such that

$$0 < (m_B - m_i)/m_B < Ce^{-ci}, \qquad \forall i = 1, 2, \ldots \tag{28}$$

(iii) $\lim_{n\to\infty} 1/n \sum_{i=1}^n m_i^{(n)} = m_B$

Proof. At $H = 0$, $f_i(x)$ is decreasing with i and bounded below by $F_D(x) - 1$, so the limit $f(x)$ exists, is convex, $f(0) < 0$ [because $f_n(0) < 0$ for all n such that $\beta_c^{(n-1)} < \beta$], and $\lim_{x\to 1} f(x) = \infty$. Equation (26) follows by taking the limit in the recurrence relation (11). Equation (26) implies in turn that f is strictly convex (because F_D itself is) and C^∞ on Int I. [As this latter fact will not be used in the following, we refrain from producing a formal proof and only remark that it follows, along with the uniqueness of the solution of Eq. (26), from general arguments, as indicated in Section 5.] So, $f \in \mathcal{C}$. Equation (27) follows from this, using the construction of $m_i^{(n)}$ in the proof of Proposition 2.2(i). The properties of m_i are consequences of Proposition 2.6. ■

Remark 3.2. (i) Because $F_D(0) = 0$, we have $f(0) = -m_1 < 0$ for $\beta > \beta_c$, which implies, via the convexity of f, that $f'(m_1) > 1$, i.e.,

$$0 < \frac{f^{-1}(y) - f^{-1}(x)}{y - x} < f^{-1\prime}(0) < 1, \qquad 0 \leqslant x < y < 1, \quad \beta > \beta_c \tag{29}$$

Moreover, the equation $f(x) = x$ has the unique solution $x = m_B$:

$$f(m_B) = f^{-1}(m_B) = m_B \tag{30}$$

This allows us to calculate all derivatives of $f(x)$ and $f^{-1}(x)$ at $x = m_B$ in terms of the derivatives of F_D; e.g., $f^{-1'}(m_B) = 1/f'(m_B) = z$, where $z < 1$ satisfies the equation $z + 1/z = F_D'(m_B)$ [see also Eq. (25)].

(ii) The bound (28) follows also directly from Eq. (27) and $f^{-1}(x) \geqslant m_1 + [(m_B - m_1)/m_B]x$ on $[m_1, m_B]$, providing $C = 1$, $c = -\log(1 - m_1/m_B)$. Similarly,

$$f^{-1}(x) \leqslant m_B - \left[1/f'(m_B)\right](m_B - x) \equiv m_B - z(m_B - x)$$

provides the lower bound:

$$(m_B - m_i)/m_B \geqslant e^{-c'i} \qquad \left[c' = -\log(1 - z)m_B\right] \tag{28'}$$

(iii) Remembering that the free energy per spin is given by

$$\beta\psi_D^{(n)}(\beta; \{0\}) = \frac{1}{n}\sum_{i=1}^{n} G_D(m_i^{(n)}, 0)$$

we have, as a consequence of Proposition 3.1(ii), that the following limits exist:

$$\beta\psi_D^B(\beta) = \lim_{n\to\infty} \beta\psi_D^{(n)}(\beta; \{0\}) = G_D(m_B, 0) \tag{31}$$

$$\beta\psi_D^S(\beta) = \lim_{n\to\infty} \beta n\left[\psi_D^{(n)}(\beta; \{0\}) - \psi_D^B(\beta)\right]$$

$$= \sum_{i=1}^{\infty}\left[G_D(m_i, 0) - G_D(m_B, 0)\right] \tag{31'}$$

Equation (31′) defines the "surface free-energy." $\psi_D^S(\beta)$ vanishes for $\beta \leqslant \beta_c$.

We shall consider next the susceptibility for the semi-infinite system. Along with $\chi_{ij}^{(n)}$, which is the response of the magnetization of the layer i to a magnetic field applied at layer j, we shall be interested in $\sum_{j=1}^{n}\chi_{ij}^{(n)}$, representing the response of $m_i^{(n)}$ to a uniform magnetic field, and also in $(1/n)\sum_{i,j=1}^{n}\chi_{ij}^{(n)}$, representing the response of the mean magnetization to a uniform magnetic field.

We shall denote as usual by l^2 the Hilbert space of complex sequences $\xi = \{\xi_i, i = 1, 2, \ldots\}$ with scalar product $(\xi, \eta) = \sum_{i=1}^{\infty}\xi_i\bar{\eta}_i$. The orthogonal projection onto the first n components will be denoted P_n. The operators $X^{(n)} \oplus (1 - P_n)$ and $\chi^{(n)} \oplus (1 - P_n)$ on l^2 will be denoted for simplicity again by $X^{(n)}$ and $\chi^{(n)}$, respectively. We have chosen this way of transporting them from C^n to l^2 in order to preserve the relation $\chi^{(n)} = X^{(n)-1}$. Finally, let X and $\tilde{X}$ be the bounded self-adjoint operators on l^2 defined by the matrices $X_{ij} = F_D'(m_i)\delta_{ij} - \delta_{i,j+1} - \delta_{i+1,j}$ and $\tilde{X}_{ij} = F_D'(m_B)\delta_{ij} - \delta_{i,j+1} - \delta_{i+1,j}$, $i, j = 1, 2, \ldots,$ respectively.

Proposition 3.3. For every $\beta \neq \beta_c$ there exists $a > 0$ such that $X \geqslant a$. Let $\chi = X^{-1}$. Then

(i) $\lim_{n\to\infty}\chi_{ij}^{(n)} = \chi_{ij}, \qquad \forall i, j = 1, 2, \ldots$

(ii) $\lim_{n\to\infty}\sum_{j=1}^{n}\chi_{ij}^{(n)} = \sum_{j=1}^{\infty}\chi_{ij}, \qquad \forall i = 1,2,\ldots$
(iii) $\lim_{n\to\infty}1/n\sum_{i,j=1}^{n}\chi_{ij}^{(n)} = \lim_{i\to\infty}\sum_{j=1}^{\infty}\chi_{ij} = \sum_{j=-\infty}^{\infty}\chi_{0j}^{B}$

with χ^{B} defined in Eq. (25).

Proof. $X^{(n)} \to X$ strongly. Indeed

$$\|(X^{(n)} - X)\xi\| \leqslant \|(X^{(n)} - X)P_k\xi\| + \|X^{(n)} - X\|\,\|(1 - P_k)\xi\|$$

and the second term can be made arbitrarily small, as the $X^{(n)}$ are equally bounded, while for fixed k the first term goes to zero by Proposition 3.1(ii).

On the other hand, $X^{(n)} \geqslant a(\beta) > 0$ for $\beta \neq \beta_c$, with $a(\beta)$ independent of n [by Eqs. (18) and (19) and the proof of Proposition 2.7]. Thus $X \geqslant a$, and $X^{(n)-1} - X^{-1} = X^{(n)-1}(X - X^{(n)})X^{-1}$ converges strongly to zero. This proves, in particular, (i).

The convergence in (ii) follows from (i) and from the uniform bound: $0 < \chi_{ij}^{(n)} \leqslant \chi_{ij}^{B} + C_1 e^{-c_1(i+j)}$, resulting from Eq. (25) and Proposition 2.7 for $\beta > \beta_c$ or $\chi^{(n)} = \tilde{\chi}^{(n)}$ for $\beta < \beta_c$ and n sufficiently large.

To prove (iii), let us first remark that, again by Proposition 2.7, for all $\beta \neq \beta_c$

$$\lim_{n\to\infty}\frac{1}{n}\sum_{i,j=1}^{n}\chi_{ij}^{(n)} = \lim_{n\to\infty}\frac{1}{n}\sum_{i,j=1}^{n}\tilde{\chi}_{ij}^{(n)}$$

From the explicit form of $\tilde{\chi}^{(n)}$, Eq. (25), we see that

$$\lim_{n\to\infty}\chi_{ij}^{(n)} = \tilde{\chi}_{ij} \equiv \tilde{X}_{ij}^{(-1)} = \frac{z}{1-z^2}\left(z^{|i-j|} - z^{i+j}\right) \tag{32}$$

and that $|\tilde{\chi}_{ij}^{(n)} - \tilde{\chi}_{ij}| \leqslant C_i' \exp[-c_1'(d_i^{(n)} + d_j^{(n)})]$, which implies

$$\lim_{n\to\infty}\frac{1}{n}\sum_{i,j=1}^{n}\tilde{\chi}_{ij}^{(n)} = \lim_{n\to\infty}\frac{1}{n}\sum_{i,j=1}^{n}\tilde{\chi}_{ij} = \lim_{i\to\infty}\sum_{j=1}^{\infty}\tilde{\chi}_{ij} = \sum_{j=-\infty}^{\infty}\chi_{0j}^{B}$$

by explicit calculation. This finishes the proof for $\beta \leqslant \beta_c$. For $\beta > \beta_c$,

$$\lim_{i\to\infty}\sum_{j=1}^{\infty}\chi_{ij} = \lim_{i\to\infty}\sum_{j=1}^{\infty}\tilde{\chi}_{ij}$$

because, by Proposition 2.7,

$$0 < \chi_{ij} - \tilde{\chi}_{ij} \leqslant C_1 e^{-c_1(i+j)} \qquad \blacksquare$$

4. THE CRITICAL BEHAVIOR OF THE SEMI-INFINITE SYSTEM

This section is devoted to a detailed analysis of the critical behavior of the (layer and bulk) magnetizations and susceptibilities defined in the preceding section.

The asymptotic behavior of m_B can be calculated from Eq. (22) using the definitions (3) and (5):

$$\lim_{\beta\searrow\beta_c}\left(\frac{\beta-\beta_c}{\beta_c}\right)^{-1/2} m_B = \lim_{\beta\searrow\beta_c}\left[\frac{\beta}{6}F_D(0)\right]^{-1/2} = \left(1+\frac{2}{D}\right)^{1/2} \tag{33}$$

The first result, showing the difference in critical behavior of the layer and the bulk magnetizations, is that the ratio

$$\mu_k = m_k/m_B \tag{34}$$

converges to zero like $(\beta-\beta_c)^{1/2}$ as $\beta\searrow\beta_c$.

We shall take as a small parameter m_B, instead of $(\beta-\beta_c)/\beta_c$, and henceforth denote m_B by t, for notational convenience. With this convention, we have, more precisely, the following proposition.

Proposition 4.1. For every $D = 1,2,\ldots$ (and $D=\infty$):

$$\lim_{t\searrow 0} t^{-1}\mu_k = k3^{1/2}(1+2/D)^{-1/2}, \qquad k=1,2,\ldots$$

Proof. It will be convenient to make a scale transformation of the functions F_D and f in Proposition 3.1(i) (omitting at the same time the D dependence). So, let F_t, f_t be defined on [0, 1] by

$$F_t(x) = t^{-1}F_D(tx), \qquad f_t(x) = t^{-1}f(tx) \tag{35}$$

Clearly, denoting as before by f_t^{-1} the inverse of the positive part of f_t, $f_t^{-1}(x) = t^{-1}f^{-1}(tx)$, f_t satisfies the functional equation

$$f_t(x) + f_t^{-1}(x) = F_t(x), \qquad x\in[0,1] \tag{36}$$

and $\mu_k = (f_t^{-1})^{\circ k}(0)$. We shall need the following lemma.

Lemma 4.2. For every $0<t<1$ and $0\leqslant x<y\leqslant 1$

$$z_t \equiv (f_t^{-1})'(1) < \frac{f_t^{-1}(y) - f_t^{-1}(x)}{y-x} < (f_t^{-1})'(0) < 1 \tag{37}$$

In particular, $t\to f_t^{-1}$ is a family of (nonlinear) contractions of [0, 1] into itself. Moreover, uniformly for $x\in[0,1]$

$$\lim_{t\to 0}\frac{f_t^{-1}(x)-x}{t} = 3^{1/2}\left(1+\frac{2}{D}\right)^{-1/2}(1-x^2) \equiv A(x) \tag{38}$$

Now, the proposition follows for $k=1$, by applying Eq. (38) at $x=0$, while for $k>1$, by induction, using

$$t^{-1}(f_t^{-1})^{\circ k}(0) = \frac{f_t^{-1}\circ(f_t^{-1})^{\circ(k-1)}(0) - f_t^{-1}(0)}{(f_t^{-1})^{\circ(k-1)}(0)}\,\frac{(f^{-1})^{\circ(k-1)}(0)}{t} + \frac{f_t^{-1}(0)}{t}$$

and Eq. (37), where $z_t\to 1$ for $t\to 0$.

Proof of Lemma 4.2. Equation (37) is the transcription of Eq. (29) in scaled form. To prove Eq. (38), we need the following information on the $t \searrow 0$ asymptotics of F_t, which can be obtained by calculation: uniformly for $x \in [0, 1]$

$$\lim_{t \searrow 0} \frac{2x - F_t(x)}{t^2} = \beta_c^{-1}\left(1 + \frac{2}{D}\right)^{-1} x(1 - x^2) \tag{39}$$

Let us denote $h_t(x) = t^{-1}[f_t^{-1}(x) - x]$, $g_t(x) = t^{-1}[x - f_t(x)]$. Both h_t and g_t are positive and concave, and, by Eq. (36) and by $f_t \circ f_t^{-1}(x) = x$, satisfy the relations

$$g_t(x) - h_t(x) = t^{-1}\left[2x - F_t(x)\right] \geqslant 0 \tag{40}$$

$$h_t(x) = g_t(x + th_t(x)) \tag{41}$$

As g_t is concave, we have, substituting Eq. (41) into Eq. (40),

$$-h_t(x)\, g_t'(x + th_t(x)) \geqslant \frac{2x - F_t(x)}{t^2} \geqslant -h_t(x)\, g_t'(x) \tag{42}$$

Also,

$$\begin{aligned} h_t'(x) &= \left[1 + th_t'(x)\right] g_t'(x + th_t(x)) \\ &\leqslant \left[1 + th_t'(1)\right] g_t'(x + th_t(x)) \\ &= z_t g_t'(x + th_t(x)) \, (< 0) \end{aligned}$$

so the first inequality in Eq. (42) gives further

$$\frac{1}{2} h_t^2(x) \geqslant z_t \int_x^1 \frac{2x' - F_t(x')}{t^2}\, dx'$$

Analogously, by $h_t(x) \geqslant g_t(x) + tg_t'(1)h_t(x)$, we have $g_t(x)/h_t(x) \leqslant 1/z_t$, so the second inequality in Eq. (42) gives

$$\frac{1}{2} g_t^2(x) \leqslant \frac{1}{z_t} \int_x^1 \frac{2x' - F_t(x')}{t^2}\, dx'$$

As $z_t \to 1$ and in view of Eq. (39), these two inequalities imply the uniform convergences

$$\begin{aligned} \lim_{t \to 0} h_t^2(x) = \lim_{t \to 0} g_t^2(x) &= 2\beta_c^{-1}\left(1 + \frac{2}{D}\right)^{-1} \int_x^1 \xi(1 - \xi^2)\, d\xi \\ &= 3\left(1 + \frac{2}{D}\right)^{-1} (1 - x^2)^2 \end{aligned}$$

which finishes the proof. ■

Corollary 4.3. For $0 < t < 1$, let

$$\eta = 12(1 + 2/D)^{-1}t^2 \tag{43}$$

and define $q_t\colon R_+ \to R_+$ by

$$q_t(x) = \mu_k \qquad \text{for} \quad (k-1)\eta^{1/2} \leqslant x < k\eta^{1/2}, \quad k = 1, 2, \ldots \tag{44}$$

Then, uniformly on compacts of $[0, \infty)$

$$\lim_{t \searrow 0} q_t(x) = q_0(x) = \tanh(x/2) \tag{45}$$

Proof. By a nonlinear version of the Trotter–Chernoff formula (Ref. 11, Theorem 3.6), $(f_{x/k}^{-1})^{\circ k}(0)$ converges uniformly on compact x intervals to the (continuous) semigroup generated by A. As a consequence, whenever $\xi_k(x)$ converges uniformly to x,

$$\left(\frac{f_{\xi_k(x)}^{-1}}{k}\right)^{\circ k}(0) \to q(x)$$

uniformly on compact, where $q(x)$ is the solution of

$$q'(x) = A(q(x)), \qquad q(0) = 0 \tag{46}$$

With A given by Eq. (38), this can be integrated, giving

$$q(x) = \tanh\left[x\sqrt{3}\,(1 + 2/D)^{-1/2}\right]$$

For every fixed x, and for every t, let $k - 1$ be the integer part of $\eta^{-1/2}x$ and define $\xi_t(x) = kt$. Then $\xi_t(x)$ converges uniformly to $x/2\sqrt{3}\,(1 + 2/D)^{1/2}$ when $t \searrow 0$. Since

$$q_t(x) = \left(\frac{f_{\xi_t(x)}^{-1}}{k}\right)^{\circ k}(0)$$

the lemma follows from what has been said above. ■

Remark 4.4. The physical content of Corollary 4.3 is that it provides the limiting form (at the critical point) of the magnetization profile when the magnetization is normalized to unity in the bulk and distances are measured in units

$$\eta^{-1/2} \simeq \frac{1}{2\sqrt{3}}\left(\frac{\beta - \beta_c}{\beta_c}\right)^{-1/2}$$

times the lattice constant. This unit is of the order of the bulk correlation length. It is interesting to translate this result (going back to the original notations) as

$$m_k \approx m_B \tanh\left[\sqrt{3}\left(\frac{\beta - \beta_c}{\beta_c}\right)^{1/2} k\right] \tag{47}$$

in which the crossover from the boundary layer critical behavior (as described in Proposition 4.1) to the bulk critical behavior is clearly exhibited. Equation (47) is in fact the scaling ansatz usually made when studying the critical behavior of systems with surfaces. (See, for instance Ref. 12.)

We shall consider next the critical behavior of the susceptibility. We have to consider separately the asymptotics from the paramagnetic ($\beta < \beta_c$) and ferromagnetic ($\beta > \beta_c$) regions.

In the paramagnetic region, the susceptibility matrix is explicitly known: $\chi = \tilde{\chi} = \tilde{X}^{-1}$ [cf. Eq. (32)] and the following results are immediate consequences of $\lim_{\beta \nearrow \beta_c}(1_c - \beta/\beta_c)^{-1/2}(1-z) = \sqrt{6}$.

Proposition 4.5

(i) $\lim_{\beta \nearrow \beta_c} \chi_{ij} = \min(i, j)$

(ii) $\lim_{\beta \nearrow \beta_c}(1_c - \beta/\beta_c)^{1/2} \sum_{j=1}^{\infty} \chi_{ij} = i/\sqrt{6}$

(iii) $\lim_{\beta \nearrow \beta_c}(1_c - \beta/\beta_c) \lim_{i\to\infty} \sum_{j=1}^{\infty} \chi_{ij} = 1/6$

In the ferromagnetic region, we no longer have a simple expression for χ and we shall use the perturbation formula

$$\chi = \tilde{\chi} + \tilde{\chi} V^{1/2}(1 - V^{1/2}\tilde{\chi} V^{1/2})^{-1} V^{1/2}\tilde{\chi} \tag{48}$$

where $V = \tilde{X} - X$ is diagonal and positive (see the proof of Proposition 2.7). As the critical behavior of $\tilde{\chi}$ for $\beta \searrow \beta_c$ is again immediately available from

$$\lim_{\beta \searrow \beta_c}\left(\frac{\beta - \beta_c}{\beta_c}\right)^{-1/2}(1 - z) = 2\sqrt{3}$$

we are left with evaluating the contribution of the second term in Eq. (48). To this end, it will be convenient to transport this term as an operator in $L_2(R_+)$, taking advantage of Corollary 4.3, which shows that the scaled magnetization profile (and thus also V) interpolates a continuous function in the limit. More exactly, let

$$\begin{gathered} W_t(x) = \eta^{-1} V_{kk} = \eta^{-1}[F_t'(1) - F_t'(\mu_k)] \\ \text{for } (k-1)\eta^{1/2} \leqslant x < k\eta^{1/2}, \quad k = 1, 2, \ldots \end{gathered} \tag{49}$$

Since, together with Eq. (39), we also have uniformly on [0, 1]

$$\lim_{t\searrow 0}\frac{2-F_t'(x)}{t^2}=\beta_c^{-1}\left(1+\frac{2}{D}\right)^{-1}(1-3x^2)$$

$$\lim_{t\searrow 0}\frac{F_t''(x)}{t^2}=6\beta_c^{-1}\left(1+\frac{2}{D}\right)^{-1}x \tag{39'}$$

we can conclude from Eq. (28) [with $C=1$, $c=-\log(1-\mu_1)$, cf. Remark 3.2(ii)] and Proposition 4.1, that, with C_0, $c_0>0$ independent of t

$$W_t(x)\leqslant C_0e^{-c_0x} \tag{50}$$

and, moreover, uniformly on $[0,\infty)$

$$\lim_{t\searrow 0}W_t(x)=W_0(x)\equiv\tfrac{3}{2}\cosh^2(x/2) \tag{51}$$

Let us define the isometry U_t: $l_2\to L_2(R_+)$ by

$$(U_t\xi)(x)=\eta^{-1/4}\xi_k \qquad \text{for } (k-1)\eta^{1/2}\leqslant x<k\eta^{1/2}, \qquad k=1,2,\ldots \tag{52}$$

The adjoint U_t^*: $L_2(R_+)\to l_2$ acts as

$$(U_t^*\varphi)_k=\eta^{-1/4}\int_{(k-1)\eta^{1/2}}^{k\eta^{1/2}}\varphi(x)\,dx \tag{52'}$$

Clearly, $U_t^*U_t=1$ on l_2 and $s-\lim_{t\searrow 0}U_tU_t^*=1$ on $L_2(R_+)$.

Now, Eqs. (51) and (50) imply, on the one hand, that $\eta^{-1}U_tVU_t^*$ converges strongly when $t\searrow 0$ to the multiplication by $W_0(x)$ on $L_2(R_+)$, and, on the other hand, that the image of the vector $(\eta^{-1/4}V_{kk}^{1/2})_{k=1,2,\ldots}$ converges in norm to $W_0^{1/2}(\cdot)\in L_2(R_+)$. Further

$$\eta[U_t\tilde{\chi}U_t^*\varphi](x)=\int_0^\infty K_t(x,y)\varphi(y)\,dy\equiv(K_t\varphi)(x) \tag{53}$$

where the kernel K_t is given by

$$\begin{aligned}&K_t(x,y)=\eta^{1/2}\tilde{\chi}_{ij} \qquad \text{for } (i-1)\eta^{1/2}\leqslant x<i\eta^{1/2}\\ &(j-1)\eta^{1/2}\leqslant y<j\eta^{1/2} \qquad i,j=1,2,\ldots\end{aligned} \tag{54}$$

It can be seen from its explicit form, Eq. (32), that

$$\lim_{t\searrow 0}K_t(x,y)=\tfrac{1}{2}\left[e^{-|x-y|}-e^{-(x+y)}\right]\equiv K_0(x,y) \tag{55}$$

and K_t converges in Hilbert–Schmidt norm to the operator K_0 defined by this kernel. As expected, K_0 is the resolvent at $\lambda=-1$ of $-d^2/dx^2$ on $[0,\infty)$ with Dirichlet boundary condition.

Collecting this information, we have that

$$s-\lim_{t\searrow 0}U_t\left[1-V^{1/2}\tilde{\chi}V^{1/2}\right]U_t^*=1-W_0^{1/2}K_0W_0^{1/2}$$

The latter operator is strictly positive definite, because the differential operator $-d^2/dx^2 - W_0(x)$ on $[0,\infty)$ with Dirichlet boundary condition has the lowest eigenvalue equal to $-\frac{1}{4}$ (>-1). (Actually, its spectrum is exactly known; see, e.g., Ref. 13, Problem 1.14, where only the eigenvalue corresponding to antisymmetric wave functions is to be considered.) Thus, also

$$s-\lim_{t\searrow 0} U_t\left[1 - V^{1/2}\tilde{\chi}V^{1/2}\right]^{-1}U_t^* = \left[1 - W_0^{1/2}K_0W_0^{1/2}\right]^{-1} \tag{56}$$

We are now prepared to state the following proposition.

Proposition 4.6. (i) $\lim_{\beta\searrow\beta_c}\chi_{ij} = \min(i,j)$

(ii) $\lim_{\beta\searrow\beta_c}(\beta/\beta_c - 1)^{1/2}\sum_{j=1}^{\infty}\chi_{ij} = i/\sqrt{12}\ [1 + (\varphi,(1 - W_0^{1/2}K_0W_0^{1/2})^{-1}\psi)_{L_2}]$ where $\varphi(x) = (1-e^{-x})W_0^{1/2}(x)$, $\psi(x) = e^{-x}W_0^{1/2}(x)$.

(iii) $\lim_{\beta\searrow\beta_c}(\beta-\beta_c)/\beta_c \lim_{i\to\infty}\sum_{j=1}^{\infty}\chi_{ij} = 1/12$

Proof. (i) Let $\xi_k^{(i)} = \tilde{\chi}_{ik}V_{kk}^{1/2}$. As $z^{x/\sqrt{\eta}} \to e^{-x}$ when $t\searrow 0$, and, for η sufficiently small and $(k-1)\eta^{1/2} \leqslant x < k\eta^{1/2}$,

$$\eta^{-1/4}\left(U_t\xi^{(i)}\right)(x) = \frac{z(z^{-i}-z^{i})}{1-z^2}z^k\left(\eta^{-1}V_{kk}\right)^{1/2}$$

we have

$$(L_2)\lim_{t\searrow 0}\eta^{-1/4}U_t\xi^{(i)} = i\psi \tag{57}$$

Hence

$$\begin{aligned}\chi_{ij} - \tilde{\chi}_{ij} &= \left(\xi^{(i)},\left[1 - V^{1/2}\tilde{\chi}V^{1/2}\right]^{-1}\xi^{(j)}\right)_{l_2}\\ &= \eta^{1/2}\left(\eta^{-1/4}U_t\xi^{(i)},\left[1 - W_t^{1/2}K_tW_t^{1/2}\right]^{-1}\eta^{-1/4}U_t\xi^{(j)}\right)_{L_2}\\ &= O(\eta^{1/2})\end{aligned}$$

(ii) Let

$$\xi_k = \sum_{i=1}^{\infty}\xi_k^{(i)} = \frac{z(1-z^k)}{(1-z)^2}V_{kk}^{1/2}$$

Then we have

$$(L_2)\lim_{t\searrow 0}\eta^{3/4}U_t\xi = \varphi \tag{58}$$

and thus

$$\eta^{1/2} \sum_{j=1}^{\infty} (\chi_{ij} - \tilde{\chi}_{ij}) = \eta^{1/2}\left(\xi^{(i)}, \left[1 - V^{1/2}\tilde{\chi}V^{1/2}\right]^{-1}\xi\right)_{l_2}$$

$$= \left(\eta^{-1/4}U_t\xi^{(i)}, \left[1 - W_t^{1/2}K_t W_t^{1/2}\right]^{-1}\eta^{3/4}U_t\xi\right)_{L_2}$$

from which (ii) follows using Eqs. (56)–(58).

Property (iii) follows from $(l_2)\lim_{j\to\infty}\xi^{(j)} = 0$ for every $\eta > 0$, which allows us to replace χ by $\tilde{\chi}$. ■

5. CONCLUDING REMARKS

5.1. As shown in Section 2, the model layer magnetizations are the $\gamma \searrow 0$ limits of the expectations of $S^1_{\mu i}$. One would expect naturally that other combinations of correlation functions also converge in this limit and their limits are directly related to the derivatives of the model free energy. For instance, χ_{ij} is expected to be the $\gamma \searrow 0$ limit of

$$\lim_{N\to\infty} (ND)^{-1} \sum_{\alpha,\beta=1}^{D} \sum_{\mu,\nu=1}^{N} \langle S^\alpha_{\mu i} S^\beta_{\nu j} \rangle^T$$

In fact this is true at least in the cases $D = 1$ and $D = \infty$, due to the concavity of the magnetization which is known to hold for the Ising model[14] and the spherical model.[15] However, to the best of our knowledge, proving the convergence of all the correlations of the D-vector model as $\gamma \searrow 0$ (which is a necessary step in defining completely the state of the Kac model) is still an open problem.

5.2. We shall outline below an alternative, more geometric, picture of the results in Sections 2 and 3.

Let Φ: $R \times (-1, 1) \to (-1, 1) \times R$ be defined by

$$(x, y) \xrightarrow{\Phi} (y, F_D(y) - x) \tag{59}$$

The point in making this definition is that, for every m_{i-1}, m_i, m_{i+1} satisfying Eq. (7) with $H_i = 0$, i.e., $m_{i+1} = F_D(m_i) - m_{i-1}$, we have

$$\Phi(m_{i-1}, m_i) = (m_i, m_{i+1}) \tag{60}$$

Thus Φ is a kind of transfer function for the system (7).

The Φ is a diffeomorphism onto its image. The tangent map at a point (x, y) is given by the invertible matrix

$$D\Phi_{(x,y)} = \begin{pmatrix} 0 & 1 \\ -1 & F'_D(y) \end{pmatrix} \tag{61}$$

When $F'_D(y) > 2$, this matrix has eigenvalues $z \in (0, 1)$ and $z^{-1} > 1$, while

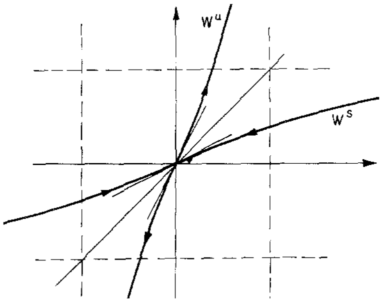

Fig. 1. Invariant manifolds of Φ for $\beta \leqslant \beta_c$.

when $F_D'(y) \leqslant 2$, its eigenvalues are on the unit circle. Clearly

$$T\Phi = \Phi^{-1}T, \qquad S\Phi = \Phi S \tag{62}$$

where $T(x, y) = (y, x)$ and $S(x, y) = (-x, -y)$. We shall be interested in the orbit structure of Φ.

Let us consider first $\beta < \beta_c$, when $F_D'(y) > 2$ everywhere. In this case, Φ has the origin as its unique fixed point, which is hyperbolic.

In a neighborhood of the origin, the Hadamard–Perron–Hartmann theorem(16) provides two C^∞ manifolds W^s and W^u, tangent at the origin to the eigenspaces of $D\Phi_{(0,0)}$ (i.e., to $y = zx$ and $y = z^{-1}x$), which are stable under Φ and Φ^{-1}, respectively. In our case, these manifolds define locally two C^∞ functions, f^{-1} and f, which satisfy the functional equation (26) and, by uniqueness, can be identified with f^{-1} and f used in Section 3. The functional equation allows us to construct f and f^{-1} globally as C^∞ functions. The situation is depicted in Fig. 1. Every point outside the graph of f^{-1} is thrown away from the domain of Φ after a finite number of applications of Φ. In particular, Φ has no periodic points.

For $\beta > \beta_c$, Φ has (m_B, m_B) and $(-m_B, -m_B)$ as hyperbolic fixed points and the origin as an elliptic fixed point. The same kind of analysis can be carried out around $(\pm m_B, \pm m_B)$; also making use of the symmetry under S in Eq. (62), it will be sufficient to consider (m_B, m_B).

In contrast to the previous case, the stable manifold W^s has a much more complicated structure; in particular, it may have several connected components.[2] However, the connected component containing (m_B, m_B) has a simple structure in the half-plane $x > 0$, given by the graph of a C^∞

[2] This is due to the singular behavior of Φ^{-1} at the lines $x = \pm 1$. Indeed, since for sufficiently large β, F_D can take arbitrarily large negative values, one can easily see that $\Phi^{-1}(W^s \cap \{x \geqslant 0\})$ may intersect the line $x = -1$ twice, implying that its intersection with the domain of Φ^{-1} will not be connected; by again applying Φ^{-1}, one can see that W^s itself is not connected.

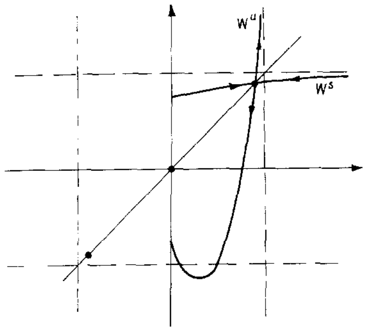

Fig. 2. Invariant manifolds of Φ for $\beta \gg \beta_c$.

function f^{-1}: $[0, \infty) \to (0, 1)$, which, again by uniqueness, can be identified with f^{-1} used earlier. The situation (for sufficiently large β) is illustrated in Fig. 2.

We now make the connection with the layer magnetizations for the finite slab and the semi-infinite system constructed in Sections 2 and 3. For finite n and $H = 0$ this is done by remarking that the distribution of layer magnetizations is given by n consecutive points in the first quadrant of an orbit of Φ: $\{\Phi^k(0, y),\ k = 1, \ldots, n\}$, such that $\Phi^n(0, y)$ is on the positive $0x$ axis. These conditions determine $y = m_1^{(n)}$. Making use of symmetry, it can be seen that $(0, m_1^{(n)})$ is a periodic point of ϕ with period $2(n + 1)$. When n goes to infinity the points $\Phi^k(0, m_1^{(n)})$, $1 \leqslant k \leqslant n/2$, approach the stable manifold W^s of Φ. In other words, the magnetization profile of the semi-infinite system is given by the orbit of $(0, f^{-1}(0))$, which is contained in W^s. This is consistent with the fact that the only point of the $0y$ axis with infinite orbit completely contained in the first quadrant is $(0, f^{-1}(0))$.

When $\beta \searrow \beta_c$, the two invariant manifolds in Fig. 1 become tangent at the origin. When $\beta \searrow \beta_c$, the three fixed points in Fig. 2 coalesce into a single point, the origin. Thus the study of the critical behavior requires consideration of the limiting case of a degenerate hyperbolic fixed point or of coalescing fixed points.

5.3. The description given in the above remark makes it possible to give a simple discussion of other boundary conditions. Leaving a more detailed exposition for a future publication, here we consider as an example the result for the semi-infinite system with two different kinds of boundary perturbations.

(a) A positive magnetic field H_1 on the first layer, i.e., the modification of the first equation as $m_2 = F_D(m_1) - H_1$. (This can be alternatively viewed, if $H_1 < 1$, as given magnetization $m_0 = H_1$ on a supplementary layer, numbered zero.) If m_1 were known, the other magnetizations could be obtained as $(m_k, m_{k+1}) = \Phi^k(H_1, m_1)$. This has to be an infinite trajectory of Φ, completely contained in the first quadrant [cf. Proposition

2.2(ii)]. The only chance is for (H_1, m_1) to be on the stable manifold of (m_B, m_B). This implies that, for $\beta > \beta_c$, m_i approaches m_B exponentially as $i \to \infty$, while for $\beta < \beta_c$, m_i approaches zero exponentially.

(b) A modified coupling constant within the first layer, i.e., the modification of the first equation as $m_2 = F_D(m_1) - 4\Delta \cdot m_1$. Since the interaction within the first layer should remain ferromagnetic, we impose $\Delta \geqslant -1$. Again, if m_1 were known, the other magnetizations could be obtained as $(m_k, m_{k+1}) = \Phi^k(4\Delta m_1, m_1)$. By the same argument, the iteration should start with the intersection of $y = 4\Delta x$ with the stable manifold.

If $\beta > \beta_c$, one has always a positive solution with $m_i \to m_B$ exponentially. For $\Delta < \frac{1}{4}$, $m_i \to m_B$ from below; the critical index of m_i is the same as for $\Delta = 0$, i.e., m_i behaves as $(\beta - \beta_c)/\beta_c$, where $\beta \searrow \beta_c$. For $\Delta > \frac{1}{4}$, $m_i \to m_B$ from above; in fact, m_1 does not approach zero when $\beta \searrow \beta_c$.

If $\beta < \beta_c$, there are nontrivial intersections with the stable manifold if and only if $4\Delta > f'(0)$. Because $f'(0)$ decreases as a function of β from $+\infty$ to 1 when β increases from 0 to β_c, we conclude the existence, for every $\Delta > \frac{1}{4}$, of a new phase transition at $\beta_{c,s}(\Delta)$ given by $4\Delta = f'(0)$: for $\beta < \beta_{c,s}(\Delta)$ the semi-infinite system has all layer magnetizations equal to zero, while for $\beta_{c,s}(\Delta) < \beta < \beta_c$, the layer magnetizations are all positive and they approach zero exponentially as $i \to \infty$. When $\beta \searrow \beta_{c,s}(\Delta)$, m_i behaves as $\{[\beta - \beta_{c,s}(\Delta)]/\beta_{c,s}(\Delta)\}^{1/2}$. See also Ref. 17, Appendix A.

NOTE ADDED IN PROOF

After submitting this paper for publication, we learned that the calculation of the magnetization profile in the "scaling limit" (see Section 4, Remark 4.4) for another exactly soluble model, the two-dimensional Ising model with n.n. interactions, has been performed by Bariev.[18]

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