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Phase separation in the spherical model

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Abstract. The spherical model in an inhomogeneous external field is investigated. It is shown that whenever there is a phase transition, the phases do not separate. This, together with decoupling effects in the magnetisation profile as well as in the transverse correlation functions, suggests abnormally large fluctuations and strong field dependence. These are confirmed by the study of symmetry-breaking fields acting on portions of the boundary.

1. Introduction||

The spherical model is the only exactly soluble model of magnetism exhibiting a phase transition in three and higher dimensions ($\nu \geq 3$) (Berlin and Kac 1952). Considering this, it is surprising that, compared for example to the two-dimensional Ising model (Abraham and Reed 1974, 1976), little is known about phase separation in the spherical model. The purpose of this article is to investigate this problem in detail by studying the magnetisation profile, the transverse correlations and the effects of symmetry-breaking fields acting on portions of the boundary.

There are several arguments indicating that dimensionality should play a decisive role in the problem of phase separation in lattice or fluid systems. As first noted in the Ising case (Burton *et al* 1951), the spin layers next to the interface, which are decoupled at $T = 0$, fluctuate strongly as T approaches the value $T_c^{(\nu-1)}$, and this leads to a roughening transition in three dimensions.

It was noted next, using spin wave arguments (H Kunz, private communication), that the energy required to deform the surface by an excitation of wavelength L is proportional to $L^{\nu-3}$. Stanley's limit (Stanley 1968) connecting the spherical model to d-dimensional vectorial-spin models, together with Berlin and Kac (1952), then supports the conjecture that a phase separation should occur in the spherical model only in four or higher dimensions.

Lastly, Onsager's and Temperley's model for lattice gas interfaces (Temperley 1952, Abraham and Heilmann 1976) and the simple drumhead model of a fluid interface also exhibit a similar dimensional effect (Widom 1972).

Nevertheless, we have found that in fact dimensionality plays no role in phase separation in the spherical model. It turns out that phases do not separate in any finite

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|| A preliminary account of some of these results was given in Abraham and Robert (1979).

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number of dimensions. As we will demonstrate, this surprising result is due to the presence of abnormally large fluctuations.

However, the spherical model does exhibit physically interesting decoupling effects in the magnetisation profile and in the two-point transverse correlation function. As far as we know, these have not been observed previously in an exactly soluble model.

2. Solution of the model

Let there be $\mathcal{N}$ d-dimensional continuous spins s_i on a finite subset $\Lambda \subset \mathbb{Z}^\nu$. The interaction energy V of a spin configuration $S_\Lambda \in (\mathbb{R}^d)^\Lambda$ on Λ is taken to be

$$V(S_\Lambda) = -\sum_{\substack{i,j \in \Lambda \\ i \neq j}} \mathcal{J}(i-j) s_i s_j - \sum_{i \in \Lambda} h_i s_i,$$

where $h_i \in \mathbb{R}$ is the exterior field acting on the spin s_i. The probability of a spin configuration S_Λ on Λ is given canonically by

$$P_\Lambda(S_\Lambda) = Z_\Lambda^{-1} \exp[-\beta V(S_\Lambda)], \tag{1}$$

where

$$Z_\Lambda = \int \left(\prod_{i \in \Lambda} \mathrm{d}s_i\right) \exp(-\beta V_\Lambda)$$

is the corresponding partition function and $\beta = 1/k_B T$, with T the absolute temperature and k_B Boltzmann's constant.

In the spherical model, originally introduced as a continuous approximation to the Ising model (Berlin and Kac 1952), $d = 1$ and the local restriction that $s_i^2 = 1$, $s_i \in \mathbb{Z}$, $\forall i$, is relaxed to the global spherical one

$$\sum_{i \in \Lambda} s_i^2 = \mathcal{N} \tag{2}$$

where each spin variable s_i can now assume any real value compatible with (2).

Defining for any subset A of Λ

$$s_A = \prod_{i \in A \subset \Lambda} s_i, \tag{3}$$

the s_i being elementary spins, we will be interested in the expectation value of s_A with respect to (1) i.e. the function

$$\langle s_A \rangle = \int_{-\infty}^{+\infty} \mathrm{d}s_{\mathcal{N}} \ldots \int_{-\infty}^{+\infty} \mathrm{d}s_1\, \delta\Big(\sum_{i \in \Lambda} s_i^2 - \mathcal{N}\Big)\Big(\prod_{i \in A \subset \Lambda} s_i\Big) P_\Lambda(S_\Lambda). \tag{4}$$

The spherical condition is most conveniently imposed, following Berlin and Kac (1952), by means of an integral representation of the 'delta function'. Equation (4) then becomes

$$\langle s_A \rangle = \int_{-\infty}^{+\infty} \mathrm{d}s_{\mathcal{N}} \ldots \int_{-\infty}^{+\infty} \mathrm{d}s_1 \frac{1}{2\pi \mathrm{i}} \int_{a-\mathrm{i}\infty}^{a+\mathrm{i}\infty} \mathrm{d}z \exp\Big[z\Big(\mathcal{N} - \sum_{i \in A} s_i^2\Big)\Big]\Big(\prod_{i \in A \subset \Lambda} s_i\Big) P_\Lambda(S_\Lambda) \tag{5}$$

$$= \left(\int_{a-\mathrm{i}\infty}^{a+\mathrm{i}\infty} \mathrm{d}z \exp(z\mathcal{N}) F_A(z)\right)\left(\int_{a-\mathrm{i}\infty}^{a+\mathrm{i}\infty} \mathrm{d}z \exp(z\mathcal{N}) F_\phi(z)\right)^{-1}, \tag{6}$$

where

$$F_A(z)=\int_{-\infty}^{+\infty}\mathrm{d}s_{\mathcal{N}}\dots\int_{-\infty}^{+\infty}\mathrm{d}s_1\exp(-\boldsymbol{s}^{\mathrm{T}}\mathbf{B}\boldsymbol{s}+\boldsymbol{h}^{\mathrm{T}}\boldsymbol{s})\prod_{i\in A\subset\Lambda}s_i, \tag{7}$$

with

$$\begin{aligned}&\boldsymbol{s}=(s_1,\dots,s_{\mathcal{N}}) \qquad \boldsymbol{h}=(h_1,\dots,h_{\mathcal{N}})\\ &B_{ij}=-\tfrac{1}{2}\beta\mathcal{J}_{i-j}+z\delta_{ij}=-\tfrac{1}{2}KA_{i-j}+z\delta_{ij}\end{aligned} \tag{8}$$

for $K=\beta\mathcal{J}$ and $\mathbf{A}=\mathbf{J}/\mathcal{J}$.

The interchange of limits in going from (5) to (6) is allowed provided that all eigenvalues of $\mathbf{B}$ are positive when $z=a$; clearly a real a can be chosen such that this is true.

The matrix $\mathbf{A}$ is real-symmetric and can therefore be reduced to a diagonal form Λ by an orthogonal transformation $\mathbf{V}$, i.e.

$$\boldsymbol{s}^{\mathrm{T}}\mathbf{A}\boldsymbol{s}=\boldsymbol{s}'^{\mathrm{T}}\Lambda\boldsymbol{s}',$$

where $\boldsymbol{s}=\mathbf{V}\boldsymbol{s}'$ with real $\mathbf{V}$ satisfying $\mathbf{V}^{\mathrm{T}}\mathbf{V}=\mathbf{I}$. Thus (7) becomes

$$F_A(z)=\int_{-\infty}^{+\infty}\mathrm{d}s'_{\mathcal{N}}\dots\int_{-\infty}^{+\infty}\mathrm{d}s'_1\exp\Big(\sum_{j=1}^{\mathcal{N}}[-(z-\tfrac{1}{2}K\lambda_j)s_j'^2+\gamma_js'_j]\Big)\prod_{i\in A}\Big(\sum_{j=1}^{\mathcal{N}}V_{ij}s'_j\Big) \tag{9}$$

with the transformed fields

$$\gamma_j=\sum_i V_{ij}h_i. \tag{10}$$

Finally the change of variables

$$s''_j=\Big(s'_j-\frac{\gamma_j}{2(z-\frac{1}{2}K\lambda_j)}\Big)(z-\tfrac{1}{2}K\lambda_j)^{1/2}$$

reduces (9) to the standard form

$$\begin{aligned}F_A(z)=F_\phi(z)\pi^{-\mathcal{N}/2}&\int_{-\infty}^{+\infty}\mathrm{d}s''_{\mathcal{N}}\dots\int_{-\infty}^{+\infty}\mathrm{d}s''_1\exp\Big(-\sum_{j=1}^{\mathcal{N}}s_j''^2\Big)\\ &\times\prod_{i\in A}\Big[\sum_{j=1}^{\mathcal{N}}V_{ij}\Big(\frac{\gamma_j}{2z-K\lambda_j}+\frac{s''_j}{z-\frac{1}{2}K\lambda_j}\Big)\Big],\end{aligned}$$

with

$$F_\phi(z)=\pi^{\mathcal{N}/2}\exp\Big[\sum_{j=1}^{\mathcal{N}}\Big(\frac{\gamma_j^2}{2z-K\lambda_j}-\tfrac{1}{2}\ln(z-\tfrac{1}{2}K\lambda_j)\Big)\Big].$$

Consider two simple examples.

(i) Take $A=p\in\Lambda$; then

$$F_p(z)=F_\phi(z)\sum_j\frac{V_{pj}\gamma_j}{2z-K\lambda_j}. \tag{11}$$

(ii) Take $A=(p,q)\in\Lambda\times\Lambda$; then

$$F_{(p,q)}(z)=\frac{F_p(z)F_q(z)}{F_\phi(z)}+\sum_j\frac{V_{pj}V_{qj}}{2z-K\lambda_j}. \tag{12}$$

These expressions are quite general for the spherical model with arbitrary one- and two-body potentials.

It remains now to find the matrix $\mathbf{V}$ which is appropriate for the problem, i.e. we must define boundary conditions for Λ as well as an exterior field $\boldsymbol{h}$ which are suitable candidates to induce phase separation. To simplify matters, we shall turn our problem into a one-dimensional one by choosing Λ to be periodic in $\nu-1$ dimensions, leaving the top and bottom sides free in the last direction; correspondingly the exterior field will be chosen to act equally on all spins of each $(\nu-1)$-dimensional toroidal layer, being positive in the upper half Λ^+ of Λ and negative in the lower half Λ^-. Note that this global field $\boldsymbol{h}$ plays the role of the gravitational field in the liquid–vapour separation. On the middle layer, for simplicity, the field will be taken to be zero.

Equally well, phase separation could be induced by means of a boundary field acting only on the boundary spins of Λ. Λ would then be a hypercube instead of a hypercylinder. For technical reasons, only the latter case has been studied in some detail for the Ising ferromagnet using rigorous methods; but it can be shown, using duplication arguments, that as $\boldsymbol{h}\to\mathbf{0}$ the phase separation phenomena should be the same (Abraham and Issigoni 1979). There is no good reason, however, to assume the same for the spherical model, as should become apparent in the next sections.

In our case we thus obtain figure 1. In this case, the matrix $\mathbf{V}$ which brings $\mathbf{A}$ into diagonal form factorises into:

$$\mathbf{V}=\mathbf{V}^{\parallel}\otimes\left(\bigotimes_{i=1}^{\nu-1}\mathbf{V}^{\perp}_{(i)}\right),$$

where $\mathbf{V}^{\perp}_{(i)}$ and $\mathbf{V}^{\parallel}$ are the matrices which diagonalise a one-dimensional cyclic and open chain respectively. Correspondingly, the eigenvalues in the periodic hyperplane add up. Diagonalisation in the latter leaves us with a non-cyclic Töplitz matrix which is easily diagonalised in the case of nearest neighbour vertical couplings.

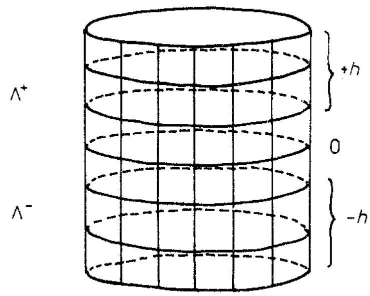

Figure 1. The boundary conditions for Λ and the global inhomogeneous symmetry-breaking field $\boldsymbol{h}$.

The matrices $\mathbf{V}^{\perp}_{x_{(i)}q^{\perp}_{(i)}}$ are the usual Fourier transforms, given in normalised real form by

$$\mathbf{V}^{\perp}_{x_{(i)}q^{\perp}_{(i)}}=\left(\frac{2}{M}\right)^{1/2}\begin{cases}\cos q^{\perp}_{(i)}x_{(i)}\\ \sin q^{\perp}_{(i)}x_{(i)}\end{cases}\tag{13}$$

where

$$q^{\perp}_{(i)}=n_{(i)}(2\pi/M)$$

with

$$n_{(i)} = 1, \ldots, M, \qquad i = 1, \ldots, \nu - 1.$$

The normalised matrices $\mathbf{V}^{\parallel}_{zk}$ are found to be (see appendix A)

$$\mathbf{V}^{\parallel}_{zk} = [2/(N+1)]^{1/2} \sin \omega z, \tag{14}$$

where

$$\omega = k\pi/(N+1), \qquad k = 1, \ldots, N.$$

In the case of isotropic nearest-neighbour couplings, the eigenvalues of $\mathbf{V}_{q^{\perp},j}$ and the parallel component of the transformed fields γ_j are respectively given by (see appendix A)

$$\lambda_{q^{\perp},j} = \sum_{j=1}^{\nu-1} \cos q^{\perp}_{(j)} + \cos \omega$$

$$\gamma_j = \begin{cases} h[2/(N+1)]^{1/2} \cot(\omega/2) & j \text{ odd} \\ 0 & j \text{ even.} \end{cases} \tag{15}$$

Following Berlin, the integrals in (6) are carried out using the method of steepest descent. The saddle point equation reads

$$W^{(\nu)}_{\mathcal{N}}(\mathfrak{z}) + H^{(\nu)}_{N}(\mathfrak{z}) = 2K \tag{16}$$

where

$$W^{(\nu)}_{\mathcal{N}}(\mathfrak{z}) = \frac{1}{\mathcal{N}} \sum_{q} \left(\mathfrak{z} - \sum_{j=1}^{\nu} \cos q_j\right)^{-1}$$

and

$$H^{(\nu)}_{N}(\mathfrak{z}) = 4 \frac{h^2}{(N+1)^2} \sum_{\substack{\omega = \pi j/(N+1) \\ j \text{ odd}}} \left(\frac{\cot(\omega/2)}{\mathfrak{z} - (\nu - 1) - \cos \omega}\right)^2 \tag{17}$$

with $\mathfrak{z} = z/K$.

We note that in the absence of an exterior field, $H^{(\nu)}_{N}(\mathfrak{z}) = 0$, and (16) just turns back into the usual saddle point equation (Berlin and Kac 1952, appendix C).

We first discuss the behaviour of equation (16) as we take the thermodynamic limit $N, M \to \infty$ with $\mathrm{Re}\, \mathfrak{z} > \nu$ and $h > 0$.

The sum $W^{(\nu)}_{\mathcal{N}}(\mathfrak{z})$ in (17) then turns into the ubiquitous Watson function

$$W^{(\nu)}(\mathfrak{z}) = \left(\frac{1}{2\pi}\right)^{\nu} \int_0^{2\pi} \mathrm{d}q_\nu \ldots \int_0^{2\pi} \mathrm{d}q_1 \frac{1}{\mathfrak{z} - \sum_{j=1}^{\nu} \cos q_j}, \tag{18}$$

whereas the field term becomes (see appendix B)

$$H^{(\nu)}(\mathfrak{z}) = 8h^2/(\mathfrak{z} - \nu)^2. \tag{19}$$

The close relationship (18) bears to the recurrence problem in the random walk is well known (Joyce 1972). For $\mathfrak{z} > \nu$, the Watson functions are monotone decreasing in $\mathfrak{z}$; a small angle analysis readily shows that whereas for $\nu = 1, 2$, $W^{(\nu)}(\mathfrak{z} = \nu)$ diverges, for $\nu \geq 3$, $W^{(\nu)}(\mathfrak{z} = \nu)$ remains finite. (The case $\nu = 3$ has been performed analytically by Watson (1939).) It then follows from (16) that for $h = 0$ the spherical model has a phase transition in three dimensions or more, the critical temperature being given by

$2K_c^{(\nu)} = W^{(\nu)}(\mathfrak{z} = \nu)$. If h were 0, then we would have the usual 'sticking' of the saddle point at $\mathfrak{z} = \nu$ for any $K \geq \frac{1}{2}W^{(\nu)}(\mathfrak{z} = \nu)$, i.e. for any $T \leq T_c$. But for $h \neq 0$, equation (16) shows that $\mathfrak{z}$ never reaches the value ν so that a normal saddle point always exists at any temperature and there is no phase transition.

Now for $K < K_c^{(\nu)}$ and letting $h \to 0$ the normal saddle point of the homogeneous phase is obtained, but if $K \geq K_c^{(\nu)}$ the saddle point equation (16), together with (19), reads

$$\mathfrak{z} - \nu = \frac{2h}{(K - K_c^{(\nu)})^{1/2}}, \tag{20}$$

showing that $\mathfrak{z}$ sticks again at ν as $h \to 0$, as it should.

3. Results (global fields)

3.1. The magnetisation profile

Together with (11) and (15), the expression for the magnetisation density of the pth layer, $-N' \leq p \leq N'(N' = (N-1)/2$, see figure 1) is obtained by letting p go to $p + (N+1)/2$, and reads (see appendix A, § A.2)

$$\langle s_{x^\perp,p}\rangle_N = \langle s_p\rangle_N = 2\frac{h}{K}\frac{1}{N+1}\sum_{\substack{\omega \\ \omega = j\pi/(N+1) \\ j \equiv 2[4]}}^{N-3} \frac{\sin p\omega}{\mathfrak{z} - (\nu - 1) - \cos\omega}\cot\left(\frac{\omega}{2}\right). \tag{21}$$

We assume 4 divides $N-1$, so $N - 3 \equiv 2$ [4].

As $N \to \infty$, this gives the following profile:

$$\langle s_p\rangle = (\operatorname{sgn} p)m(h, \beta)(1 - e^{-\nu_0|p|}), \tag{22}$$

where

$$m(h, \beta) = \frac{1}{2K}\frac{h}{\mathfrak{z} - \nu}$$

and using (17)

$$\sin h\left(\frac{\nu_0}{2}\right) = \left(\frac{\mathfrak{z} - \nu}{2}\right)^{1/2} = \frac{h^{1/2}}{(K - K_c^{(\nu)})^{1/4}}.$$

The derivation uses contour integrations and is given in appendix B.

Note that as $|p| \to \infty$ one recovers from (22) the magnetisation densities of the pure phases. For $h \neq 0$ ($T > T_c$) the profile has a reasonable exponential behaviour; however as $h \to 0$ ($T \leq T_c$) the inhomogeneous effects disappear completely, leaving $\langle s_p\rangle = 0$ for any finite p, however small the temperature: the interface is always diffuse, and a roughening transition is not observed at any temperature.

We also find a decoupling effect in the profile: the expression for the upper (lower) wing $\langle s_p\rangle$, $p > 0$ ($p < 0$), is exactly the same as the one we find for $\langle s_p\rangle$ in the case where p denotes the distance of the layer from the free side of Λ, and when Λ is submitted to a homogeneous global field $\boldsymbol{h} = h(1, \ldots, 1)$ ($\boldsymbol{h} = -h(1, \ldots, 1)$). This is readily checked by computing the corresponding expression for γ (see appendix A, § A.2). (This surface effect had been studied as such by Watson (1972) in his review article.) Note that a correction term, which vanishes exponentially with p, is added if the inhomogeneous field has no zero mid-component.

It must be said that such a decoupling effect in the profile is not typical, even in the absence of a sharp interface. For instance, in the case of the two-dimensional Ising model it can be proven rigorously both that the interface is diffuse (Abraham and Reed 1974, 1976) and that the profile does not decouple (Watson 1968).

3.2. *The moments of the profile*

The moments of the profile are defined by

$$M_{2k}=\left(\frac{L_{2k}}{L_0}\right)^{1/2k}$$

where

$$L_{2k}=\sum_{p=1}^{\infty} p^{2k}(m(h,\beta)-\langle s_p\rangle).$$

In our case we get, using result (21),

$$L_{2k}=\frac{h}{2K(\mathfrak{z}-\nu)}\sum_{p=1}^{\infty} p^{2k}\,\mathrm{e}^{-p\nu_0}.$$

As $h\to 0$, we have found that

$$\frac{h}{\mathfrak{z}-\nu}=\tfrac{1}{2}(K-K_{\mathrm{c}}^{(\nu)})^{1/2},$$

so

$$L_{2k}=\nu_0^{-2k-1}\frac{(K-K_{\mathrm{c}}^{(\nu)})^{1/2}}{4K}\int_0^{\infty}\mathrm{d}x\,\mathrm{e}^{-x}x^{2k},$$

and the $2k$th moment becomes

$$M_{2k}=\left(\frac{L_{2k}}{L_0}\right)^{1/2k}=\nu_0^{-1}\left(\frac{\Gamma(2k+1)}{\Gamma(1)}\right)^{1/2k}, \qquad (\Gamma(1)=1)$$

$$=(\Gamma(2k+1))^{1/2k}\left(\frac{4h}{(K-K_{\mathrm{c}}^{(\nu)})^{1/2}}\right)^{-1/2}. \tag{23}$$

Thus each moment diverges like $h^{-1/2}$ as $h\to 0$. This is an unexpected result in three dimensions, if one recalls that the same qualitative behaviour is also exhibited in the one-dimensional linearised string model of a two-dimensional interface (Widom 1972, p 79), and is probably also obtained for the Onsager–Temperley string model of a lattice gas interface (Temperley 1952). Both of these models aim to describe phase separation in two dimensions, for which the interface should be rough for any $T>0$, as proved for the Ising model (Abraham and Reed 1974, 1976). The $h^{-1/2}$ ($g^{-1/2}$, where g is the gravitational field) result may be symptomatic of the case where roughening occurs at $T=0$.

It should also be noted that both the profile and its moments have a homogeneous form which is compatible with scaling theory (Widom 1972), with ν_0 as inverse correlation length: ν_0 is a homogeneous function of h and $t=|(T-T_{\mathrm{c}})/T_{\mathrm{c}}|$.

3.3. The pair correlation function

Together with (12), the expression for the two-point correlation function between two spins located at sites x and y takes the form

$$\langle s_x s_y \rangle = \langle s_x \rangle \langle s_y \rangle + f_2(|\boldsymbol{x} - \boldsymbol{y}|)$$

where

$$f_2(r) = \int_0^{2\pi} \mathrm{d}q_\nu \ldots \int_0^{2\pi} \mathrm{d}q_1 \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{q}.\boldsymbol{r}}}{\check{z} - \sum_{j=1}^{\nu} \cos q_j}.$$

But $f_2(r)$ is just the truncated correlation in a pure phase. So for two points $x = (\boldsymbol{x}, p)$, $y = (\boldsymbol{y}, p)$ belonging to the same layer p we have, taking $\boldsymbol{x} = \boldsymbol{0}$ by translational invariance,

$$\langle s_{p\boldsymbol{0}} s_{p\boldsymbol{y}} \rangle = \langle s_p \rangle^2 + f_2(|\boldsymbol{y}|); \tag{24}$$

i.e. a slab of matter at height p behaves as though it were taken from a homogeneous phase of magnetisation $\langle s_p \rangle$ lying between the extreme values. Although not expected to hold rigorously (as suggested by Davis and Scriven (1978) for fluids close to the one-phase region), such a decoupling effect has, however, frequently been used as a procedure by numerous workers in approximate theories (e.g. Brown and March 1976). To our knowledge, it is the first time it comes out of an exactly solvable model.

4. Local symmetry-breaking fields

The absence of phase separation at low temperatures indicates the presence of strong correlations besides the usual ones, which, together with the continuous nature of the spins, lead to abnormally large fluctuations of the ordered clusters. As remarked in Lieb and Thompson (1969), these extra correlations are induced by the spherical constraint (2).

The decoupling effects in the magnetisation profile and in the transverse correlation functions suggest that the global field, which splits Λ into two non-interacting parts Λ^+ and Λ^-, is too strong, and motivates the study of the effects of weaker symmetry-breaking fields, acting for instance only on the top and bottom free edges of Λ (see figure 2).

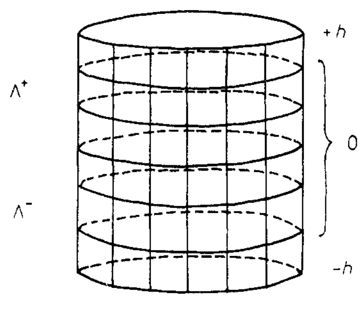

Figure 2. The local inhomogeneous symmetry-breaking field $\boldsymbol{h}$. The boundary conditions are as in figure 1.

For such an exterior field, the transformed fields $\gamma_j = \Sigma_i V_{ij} h_i$ become

$$\gamma_j = h(\sin N\omega - \sin \omega)$$
$$= \begin{cases} 0 & j \text{ odd} \\ -2h \sin \omega & j \text{ even,} \end{cases} \qquad \left(\omega = j\frac{\pi}{N+1}\right),$$

and since for j even (appendix A, § A.2):

$$V_{jp} \simeq \begin{cases} -\sin p\omega & j \equiv 2[4] \\ \sin p\omega & j \equiv 0[4], \end{cases}$$

we get

$$\langle s_p \rangle_N \simeq \frac{2h}{N+1}\Bigg(\sum_{\substack{\omega \\ \omega = j\pi/(N+1) \\ j \equiv 2[4]}} \frac{\sin \omega \,.\, \sin p\omega}{z - (\nu - 1) - \cos \omega} - \sum_{\substack{\omega \\ j \equiv 0[4]}} \frac{\sin \omega \,.\, \sin p\omega}{z - (\nu - 1) - \cos \omega} \Bigg). \tag{25}$$

For $T > T_c$, contrary to (21), $\langle s_p \rangle$ tends to zero as $N \to \infty$, for any finite p. This is because each sum is separately integrable for $z > \nu$ and tends to the same integral as $N \to \infty$. For $T \leq T_c$, z sticks to ν and we shall see that the speed of approach of z to ν is high enough to permit the exchange of limits $N \to \infty$ and $z \to \nu$. However, for $z = \nu$, the divergence in ω^2 in the denominator is balanced by that in $p\omega^2$ in the numerator, so that both sums are again integrable, yielding $\langle s_p \rangle = 0$ for p finite as $N \to \infty$ for any temperature.

This result, together with (21), confirms and generalises the special case of a cosine field considered by Langer (1965) and Kac (unpublished). We may also note, bearing in mind more recent results on Ornstein–Zernicke systems (Stell 1969 and Theumann 1970) that the absence of phase separation in the spherical model does not appear to be linked to the lack of analytic continuation (or susceptibility divergence), the latter being a dimensional effect. This is contrary to Langer (1965).

In order to see what is going on here, we shall examine finally the effect generated by a symmetry-breaking side-field. In other words, we shall consider a local inhomogeneous field acting only on the spins of one of the free layers (see figure 3).

Taking the field $+h$ to act on the first layer ($p = 1$), the expression for the magnetisation density $\langle s_p \rangle_N$ of the pth layer now simply reads

$$\langle s_p \rangle_N \simeq \frac{h}{N+1} \sum_{\substack{\omega \\ \omega = j\pi/(N+1) \\ \text{all } j}} \frac{\sin \omega \,.\, \sin p\omega}{z - (\nu - 1) - \cos \omega}. \tag{26}$$

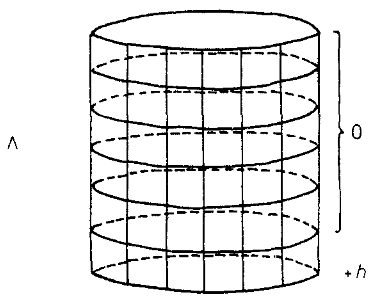

Figure 3. The local symmetry-breaking side-field h. The boundary conditions are as in figure 1.

(i) For $T > T_c$, i.e. for $\mathfrak{z}-(\nu-1)>1$, the sum is integrable, so that

$$\begin{aligned}\langle s_p\rangle &= \lim_{N\to\infty}\langle s_p\rangle_N\\ &\simeq \frac{h}{\pi}\int_0^\pi \frac{\sin\omega\,.\,\sin p\omega}{\mathfrak{z}-(\nu-1)-\cos\omega}\,\mathrm{d}\omega\\ &= \frac{h}{\pi}\,.\,\pi[\![\mathfrak{z}-(\nu-1)+\{[\mathfrak{z}-(\nu-1)]^2-1\}^{1/2}]\!]^{-p}, \qquad p>0\\ &= h\exp(-\alpha p),\end{aligned} \tag{27}$$

where

$$\alpha = \ln[\![\mathfrak{z}-(\nu-1)+\{[\mathfrak{z}-(\nu-1)]^2-1\}^{1/2}]\!]>0.$$

This is a typical surface effect. It may be compared with the corresponding pure Ornstein–Zernicke fluid model of the one-dimensional hard cores, for which the density profile is known explicitly exhibiting, moreover, oscillations which are not seen here on the lattice.

(ii) For $T \leqslant T_c$, however, $\mathfrak{z}-(\nu-1)=1$ for any T, and some care is required in taking the limit $N\to\infty$ in (27). For this, let us consider the saddle-point equation for the various local fields. The field part $H_N^{(\nu)}(\mathfrak{z})$ reads in all cases, up to a constant C,

$$H_N^{(\nu)}(\mathfrak{z}) = C\frac{h^2}{(N+1)^2}\sum_{\substack{\omega\\ \omega=j\pi/(N+1)\\ j=1,\dots,N}} \frac{\sin^2\omega}{[\mathfrak{z}-(\nu-1)-\cos\omega]^2}. \tag{28}$$

It is easy to see that, contrary to the corresponding expression for global fields (17), this sum tends to a constant as $N\to\infty$, so that the branch cut $\mathfrak{z}=\nu$ is reached for $h\neq 0$: the presence of nonzero local fields does not prevent the system from undergoing a phase transition, which is physically reasonable.

The sum in (28) may be evaluated by contour integration (appendix B, § B.2) to be for large N the sum of the terms

$$C(\mathrm{e}^{2\mathrm{i}z_\pm^0(N+1)})(\mathrm{e}^{2\mathrm{i}z_\pm^0(N+1)}-1)^{-2}$$

with $z_\pm^0=\pm\mathrm{i}[2(\mathfrak{z}-\nu)]^{1/2}$ the roots of the equation $\mathfrak{z}-(\nu-1)-\cos\omega=0$ for large N.

This shows that the branch cut is approached at a speed of N^{-2} as $N\to\infty$:

$$\mathfrak{z}-\nu\simeq N^{-2}. \tag{29}$$

We now evaluate the sum (26) by contour integration (appendix B, § B.2) and find

$$\langle s_p\rangle_N \simeq \mathrm{e}^{\mathrm{i}pz_+^0}+\frac{\mathrm{e}^{\mathrm{i}pz_-^0}}{\mathrm{e}^{2\pi\mathrm{i}Nz_-^0}-1}.$$

Using result (29), this shows that the effect of the wall propagates undamped macroscopically throughout the system: all the layers within a finite distance (p finite) of the wall are 'frozen' to a constant value. Note that this could have also been noticed directly in using (29) to exchange the order of limits in (27), finding

$$\begin{aligned}\langle s_p\rangle &= Ch\int_0^\pi \frac{\sin\omega\,.\,\sin p\omega}{1-\cos\omega}\,\mathrm{d}\omega\\ &= Ch\pi/2, \qquad \forall p<\infty.\end{aligned} \tag{30}$$

More surprisingly, the constant value s_0 to which it tends in the bulk of the system ($p \to \infty$) is to be sure nonzero, but has nothing to do with the spontaneous magnetisation $m^*(\beta)$. This contrasts sharply with the two-dimensional Ising case, known to be more realistic (Watson 1968 pp 133–41). Finally, notice that the magnetisation in the bulk is discontinuous at the transition; contrary to the global field case, h has to be kept here nonzero, as we have already mentioned.

These abnormally large effects ($\sim N$) are to be compared to the normal ones ($\sim N^{1/2}$) exhibited in two dimensions both by the Ising model (Abraham and Reed 1974, 1976) and the Onsager–Temperley string (Abraham and Heilmann 1976).

These results show that in spite of the fact that the spherical model has proved to be a good reference model for homogeneous properties, it has to be considered with care when it comes to inhomogeneous effects. Besides, some anomalous features had already been found in other contexts (Barber and Fisher 1973, Widom 1972, p 149).

Appendix A

A.1. Diagonalisation of $\mathbf{V}^{\parallel}_{zk}$

In the open vertical direction, although cyclicity is lost, the case of nearest-neighbour vertical coupling is easy to solve: the eigenvector problem for a tridiagonal matrix of the form

$$\begin{pmatrix} a & b & & & & \\ b & a & b & & \mathbf{0} & \\ & b & \ddots & \ddots & & \\ & & \ddots & \ddots & b & \\ & \mathbf{0} & & b & a & b \\ & & & & b & a \end{pmatrix}$$

reads explicitly

$$bz_{k-1}^{(n)} + az_k^{(n)} + bz_{k+1}^{(n)} = \lambda^{(n)} z_k^{(n)}, \tag{A1}$$

where $z_k^{(n)}$ denotes the kth component of the nth eigenvector, $1 \leqslant k, n \leqslant N$.

The *ansatz*

$$z_k^{(n)} = A(z_1^{(n)})^k + B(z_2^{(n)})^k, \tag{A2}$$

together with the boundary conditions

$$z_0^{(n)} = z_{N+1}^{(n)} = 0,$$

yields

$$z_1^{(n)} z_2^{(n)} = 1$$

with

$$A(z_1^{(n)})^{N+1} + B(z_2^{(n)})^{N+1} = 0$$

and

$$A = -B.$$

The eigenvectors are, therefore,

$$z_k^{(n)}=\sin\left(nk\frac{\pi}{N+1}\right),$$

and, after e.g. Hansen (1975, No. 15.1.2, p 234), normalise to

$$\left(\frac{2}{N+1}\right)^{1/2}\sin\left(nk\frac{\pi}{N+1}\right). \tag{A3}$$

The eigenvalues follow from (A1) and (A2), which give

$$\begin{aligned}\lambda^{(n)}&=b(z_i^{(n)}+(z_i^{(n)})^{-1}) \qquad i=1 \text{ or } 2\\ &=2b\cos\left(n\frac{\pi}{N+1}\right)+a.\end{aligned} \tag{A4}$$

A.2. Expression for the transformed fields

Together with (14), (10) becomes, up to the normalisation constant,

$$\begin{aligned}\gamma_j&=h\,\mathrm{Im}\left(\sum_{j'=\frac{1}{2}(N-1)+2}^{N}\mathrm{e}^{\mathrm{i}\omega j'}-\sum_{j'=1}^{(N-1)/2}\mathrm{e}^{\mathrm{i}\omega j'}\right), \qquad \omega=j\frac{\pi}{N+1},\\ &=h\,\mathrm{Im}\left(\frac{\mathrm{e}^{\mathrm{i}\omega}}{\mathrm{e}^{\mathrm{i}\omega}-1}[\mathrm{e}^{\mathrm{i}\omega N}-\mathrm{e}^{\frac{1}{2}\mathrm{i}\omega(N+1)}-(\mathrm{e}^{\frac{1}{2}\mathrm{i}\omega(N-1)}-1)]\right).\end{aligned}$$

Making the denominator real, we get

$$\frac{1}{2-2\cos\omega}(\mathrm{e}^{\mathrm{i}\omega N}-\mathrm{e}^{\frac{1}{2}\mathrm{i}\omega(N-1)}-\mathrm{e}^{\mathrm{i}\omega(N+1)}+\mathrm{e}^{\mathrm{i}\omega[\frac{1}{2}(N+1)+1]}-\mathrm{e}^{\mathrm{i}\omega}-1).$$

We drop the term -1 in the numerator since we want finally the imaginary part of this number. Using $\omega=j\pi/(N+1)$, we get

$$\begin{aligned}&\mathrm{e}^{\mathrm{i}\omega N}=(-1)^j\,\mathrm{e}^{-\mathrm{i}\omega}; \qquad &&\mathrm{e}^{\frac{1}{2}\mathrm{i}\omega(N-1)}=\mathrm{i}^j\,\mathrm{e}^{-\mathrm{i}\omega};\\ &\mathrm{e}^{\mathrm{i}\omega(N+1)}=(-1)^j; \qquad &&\mathrm{e}^{\mathrm{i}\omega[\frac{1}{2}(N+1)+1]}=\mathrm{i}^j\,\mathrm{e}^{\mathrm{i}\omega}.\end{aligned} \tag{A5}$$

We now compute, dropping (-1),

$$\mathrm{Im}((-1)^j\,\mathrm{e}^{-\mathrm{i}\omega}-\mathrm{i}^j\,\mathrm{e}^{\mathrm{i}\omega}+\mathrm{i}^j\,\mathrm{e}^{\mathrm{i}\omega}-\mathrm{e}^{\mathrm{i}\omega})=\mathrm{Im}\{2\mathrm{i}^{j+1}\sin\omega-[\mathrm{e}^{\mathrm{i}\omega}+(-1)^{j+1}\,\mathrm{e}^{-\mathrm{i}\omega}]\}. \tag{A6}$$

Now since we have

$$\mathrm{i}^{j+1}=\begin{cases}-1 & j\equiv 1[4]\\ +1 & j\equiv 3[4]\\ \mathrm{i} & j\equiv 0[4]\\ -\mathrm{i} & j\equiv 2[4]\end{cases}$$

and

$$(-1)^{j+1}=\begin{cases}+1 & j\equiv 1[2]\\ -1 & j\equiv 0[2],\end{cases}$$

it is easily checked that all cases yield pure real values except the case $j \equiv 2[4]$, which gives for (A6):

$$-2\mathrm{i}\sin\omega - (\mathrm{e}^{\mathrm{i}\omega} - \mathrm{e}^{-\mathrm{i}\omega}) = -4\mathrm{i}\sin\omega,$$

so that, putting things together and using $\sin\omega/(1-\cos\omega) = \cot(\omega/2)$,

$$\gamma_j = \begin{cases} -2\left(\dfrac{2}{N+1}\right)^{1/2} h\cot\left(\dfrac{\omega}{2}\right) & \text{for } \omega = j\dfrac{\pi}{N+1},\ j \equiv 2[4] \\ 0 & \text{otherwise.} \end{cases} \tag{A7}$$

The expression for $V^{\parallel}_{pj}$ when p is shifted by $(N+1)/2$ is readily found:

$$\sin p'\omega = \sin\{[\tfrac{1}{2}(N+1) \pm p]\omega\} = \sin(j\pi/2 \pm p\omega)$$

since $\omega = j\pi/(N+1)$, and developing, we get

$$\sin p'\omega = \begin{cases} \cos p\omega & j \equiv 1[4] \\ -\cos p\omega & j \equiv 3[4] \\ \mp\sin p\omega & j \equiv 2[4] \\ \pm\sin p\omega & j \equiv 0[4] \end{cases}.$$

Now γ_j contributes only for $j \equiv 2[4]$, so the product $\gamma_j V^{\parallel}_{pj}$ which appears in $\langle s_p \rangle_N$ goes like

$$-\cot(\tfrac{1}{2}\omega)(\mp\sin p\omega) = \pm\cot(\tfrac{1}{2}\omega)\sin p\omega, \qquad p \gtrless 0,$$

which is the result used in the text (21).

Finally, for a homogeneous field $\boldsymbol{h} = (h, \ldots, h)$, we have to compute using (A5)

$$\sum_{j'=1}^{N} \mathrm{e}^{\mathrm{i}\omega j'} = \mathrm{e}^{\mathrm{i}\omega}\frac{\mathrm{e}^{\mathrm{i}\omega N} - 1}{\mathrm{e}^{\mathrm{i}\omega} - 1} = \frac{(-1)^{j'}\mathrm{e}^{\mathrm{i}\omega} + (-1)^{j'+1} + \mathrm{e}^{\mathrm{i}\omega} - 1}{2 - 2\cos\omega};$$

dropping the real terms, which will not contribute, we get

$$\begin{aligned} \mathrm{Im}\left(\sum_{j'=1}^{N} \mathrm{e}^{\mathrm{i}\omega j'}\right) &= \frac{1}{2-2\cos\omega}\,\mathrm{Im}(\mathrm{e}^{\mathrm{i}\omega} + (-1)^{j'}\mathrm{e}^{-\mathrm{i}\omega}) \\ &= \begin{cases} 0 & j' \text{ odd} \\ \cot(\tfrac{1}{2}\omega) & j' \text{ even.} \end{cases} \end{aligned} \tag{A8}$$

Now in this case p is not shifted since $p = 1$ denotes the first (bottom) layer, so $V^{\parallel}_{pj} = \sin p\omega$, $1 \leqslant p \leqslant N$.

Notice the factor 2 in (A7) which is absent in (A8). However, since the sum (21) extends over only half as many terms, this factor cancels in the thermodynamic limit, yielding the exact decoupling effect mentioned in the text.

Appendix B

The method being essentially the same for all the sums involved, we shall illustrate it by working out the details for one of them in § B.1, and shall mention in § B.2 the features specific to the others.

B.1. Evaluation of $\lim_{N\to\infty} H_N^{(\nu)}(\mathfrak{z})$ *for the local fields*

In order to rewrite the sum (28) as a complex integral, we consider the integral

$$\oint \mathrm{d}z\, f_N(z) \tag{B1}$$

for

$$f_N(z) = g_N(z) f(z),$$

where

$$f(z) = \frac{\sin^2 z}{[\mathfrak{z} - (\nu - 1) - \cos z]^2}$$

and

$$g_N(z) = \frac{1}{(\mathrm{e}^{\mathrm{i}z(N+1)} - 1)(\mathrm{e}^{\mathrm{i}z(N+1)} + 1)} = \frac{1}{\mathrm{e}^{2\mathrm{i}z(N+1)} - 1}.$$

$g_N(z)$ having simple poles located at $z = z_j = \pi j/(N+1)$, $j = 1, \ldots, N$, we evaluate (B1) by the method of residues. $C_1 \supset \{z_j\}$ being the contour shown in figure 4, we find:

$$2\pi\mathrm{i} \sum_j f(z_j) = A_N \oint_{C_1 \supset \{z_j\}} \mathrm{d}z\, g_N(z) f(z)$$

$$= 2\pi\mathrm{i} \sum_j \mathrm{Res}(g_N f, z_j)$$

with $A_N = 2\mathrm{i}(N+1)$. Thus

$$H_N^{(\nu)}(\mathfrak{z}) = \frac{Ch^2}{N^2} \frac{2\mathrm{i}(N+1)}{2\pi\mathrm{i}} \oint_{C_1} f_N(z)\, \mathrm{d}z.$$

But since $f(z)$ is even, $\oint_{C_1} = \frac{1}{2} \oint_{C_1 \cup C_2}$ and by periodicity of $f_N(z)$, $\oint_{\Gamma_1 \cup \Gamma_3} = 0$ (figure 4); so provided we can find upper and lower horizontal lines Γ_2 and Γ_4 on which $N^{-1} f_N(z)$ vanishes as $N \to \infty$, we will have (figure 4)

$$\oint_{\bigcup_{i=1}^4 \Gamma_i} = \oint_{C_1 \cup C_2} - \oint_{\Gamma_5 \cup \Gamma_6} = 0,$$

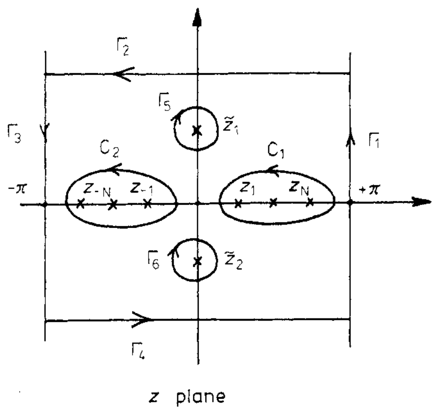

Figure 4. Poles and contours for the local fields term $H_N^{(\nu)}(\mathfrak{z})$.

so that

$$\lim_{N\to\infty} H_N^{(\nu)}(\mathfrak{z}) = \lim_{N\to\infty} \frac{1}{N} \sum_k \mathrm{Res}(f_N, \tilde{z}_k), \tag{B2}$$

where

$$\tilde{z}_k \neq z_i \qquad i = 1, \ldots, N;\ k = 1, \ldots, K$$

are the K eventual poles of $f_N(z)$ lying inside $\Gamma = \bigcup_{i=1}^4 \Gamma_i$. In this example, we have

$$|f_N(z)| < \frac{1}{4} \frac{(\mathrm{e}^{-\mathrm{Im}\, z} + \mathrm{e}^{\mathrm{Im}\, z})^2}{\{\mathrm{e}^{\mathrm{Im}\, z} - [\mathfrak{z} - (\nu - 1)]\}^2 (1 - \mathrm{e}^{-2\mathrm{Im}\, z(N+1)})},$$

so that for large Im z, $N^{-1}|f_N(z)|$ vanishes as $N \to \infty$, whereas for Im $z \to -\infty$, $|f_N(z)|$ already vanishes.

The poles $\tilde{z}_k$ of $f_N(z)$, i.e. those of $f(z)$, are given by the roots of the equation

$$\mathfrak{z} - (\nu - 1) - \cos z = 0$$

which reads, since $\mathfrak{z} - \nu \geq 0$,

$$\tfrac{1}{2}(\cos z - 1) = [\mathrm{i} \sin(z/2)]^2 = [\sinh(\mathrm{i}z/2)]^2 = \tfrac{1}{2}(\mathfrak{z} - \nu),$$

and for large N

$$\tilde{z}_{1,2} \simeq \pm \mathrm{i}[2(\mathfrak{z} - \nu)]^{1/2} = \pm \mathrm{i} z_0.$$

These poles are of order two, and the formula

$$\mathrm{Res}(f_N, \tilde{z}_k) = \frac{\mathrm{d}}{\mathrm{d}z} f_N(z)(z - \tilde{z}_k)^2 |_{z = \tilde{z}_k}$$

gives for (B2)

$$-\frac{2\mathrm{i}(N+1)\, \mathrm{e}^{2\mathrm{i}\tilde{z}_k(N+1)}}{(\mathrm{e}^{2\mathrm{i}\tilde{z}_k(N+1)} - 1)^2}.$$

The factor $N + 1$ will drop out in the $1/N$ limit.

B.2. The other sums

B.2.1. $H_N^{(\nu)}(\mathfrak{z})$ for the global field (17). Only odd j contribute, so the appropriate kernel is

$$g_N(z) = \frac{1}{\mathrm{e}^{\mathrm{i}k(N+1)} + 1}.$$

As $N \to \infty$, only the new pole $\tilde{z}_3 = 0$ contributes a residue of $-2\mathrm{i}(N+1)/(\mathfrak{z} - \nu)^2$.

B.2.2. $\langle s_p \rangle$ for the global field (21). The kernel is as in § B.2.1; we choose the contours as in figure 5. As $N \to \infty$, $g_N(z)$ vanishes on Γ_4 and on Γ_2' for $p > 0$ (on Γ_4' for $p < 0$), so that

$$\oint_C = \oint_{\bigcup_{i=1}^4 \Gamma_i} = 2\pi \mathrm{i}\, \mathrm{Res}(g_N, 0),$$

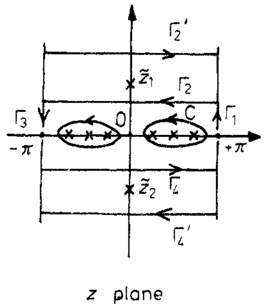

Figure 5. Poles and contours for the global fields magnetisation.

with

$$\oint_{\bigcup_{i=1}^{4}\Gamma_i} = \int_{\Gamma_2} = \int_{\Gamma_2'} = 2\pi \mathrm{i}\, \mathrm{Res}(g_N, \tilde{z}_1).$$

The residues at 0 and $\tilde{z}_1$ are respectively $1/(\mathfrak{z} - \nu)$ and $-\mathrm{e}^{\mathrm{i}p\tilde{z}_1}/(\mathfrak{z} - \nu)$.

For $p < 0$, Γ_4' replaces Γ_2', and the residues are $-1/(\mathfrak{z} - \nu)$ and $\mathrm{e}^{-\mathrm{i}p\tilde{z}_2}/(\mathfrak{z} - \nu)$, which checks with $\langle s_{-p} \rangle = -\langle s_p \rangle$ from (21).

B.2.3. $\langle s_p \rangle$ *for the side-field (27).* The appropriate kernel is $(\mathrm{e}^{2\mathrm{i}z(N+1)} - 1)^{-1}$, as in § B.1. The contours Γ_2 and Γ_4 are sent to $\pm\infty$ respectively, where $g_N(z)$ vanishes. The residues at $\tilde{z}_1$ and $\tilde{z}_2 = -\tilde{z}_1$ are respectively $\mathrm{e}^{\mathrm{i}p\tilde{z}_1}$ and $\mathrm{e}^{-\mathrm{i}p\tilde{z}_1}/(\mathrm{e}^{2\pi\mathrm{i}\tilde{z}_1 N} - 1)$.

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Note added to typescript.

We have just learned that it has recently been shown by C Pfister that the thickness of the interface in spin systems with continuous symmetry already diverges at zero temperature.

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