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Phase diagram of the $Z(4)$ model†

V L Baltar, G M Carneiro, M E Pol and N Zagury

Departamento de Física, Pontifícia Universidade Católica Cx P 38071, Rio de Janeiro, RJ, Brasil

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Abstract. Systems with $Z(4)$ global symmetry defined on a square lattice are studied, in the whole parameter space, both by Monte Carlo simulations and by the Migdal–Kadanoff renormalisation group scheme. A phase diagram is obtained with quantitative predictions as to the location of the boundaries between the different phases. Four distinct phases are observed.

1. Introduction

Theories with $Z(N)$ symmetry have been intensively studied in recent years. The reason for such an interest in this subject is the fact that they are relevant to a wide class of physical problems. As we know, spin systems have long been used as models of magnetism and phase transitions. Elementary particle physicists also became interested in $Z(N)$ models, since space–time lattices turned into a popular technical device to regularise field theories. The study of $Z(N)$ gauge theories on a four-dimensional lattice is particularly relevant to elementary particle physics, as they seem to be related to confinement in SU(N) ('t Hooft 1978).

In this paper we study the phase diagram of the two-dimensional $Z(4)$ model (the symmetric Ashkin–Teller model) on a square lattice in the whole parameter space. We use Monte Carlo (MC) simulations (Binder 1979) and the Migdal–Kadanoff renormalisation group (MKRG) scheme (Migdal 1975a, b, Kadanoff 1976).

It is possible to define a generalised duality transformation, under which $Z(N)$ models are self-dual in a certain region of parameter space (Alcaraz and Köberle 1980).

In the region where generalised self-duality holds, the $Z(4)$ model has been studied by several different formalisms (Alcaraz and Köberle 1980, Carneiro *et al* 1982, Kohmoto *et al* 1981, Rujan *et al* 1981, Stavans and Domany 1983, Wu and Lin 1974). It is found that the $Z(4)$ model has at least three distinct phases in this region:

(a) a ferromagnetic phase (I)

(b) an intermediate partially ordered phase (II)

(c) a disordered phase (III).

The region where generalised self-duality holds is studied in this paper, first, by means of Monte Carlo simulations. We obtain the $Z(4)$ phase diagram with quantitative predictions as to the location of the boundaries between these three phases. No evidence for a massless phase is found.

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Next, we use Monte Carlo simulations to study the region where generalised self-duality does not hold. In this region, which is much less known than the previous one, we obtain another $Z(4)$ phase, with perpendicular order, and the boundary between it and the disordered phase is determined. A short account of these results has already been given (Carneiro *et al* 1982).

Finally, the $Z(4)$ model is analysed using the Migdal–Kadanoff renormalisation group scheme. The results previously obtained with this method in the region where generalised self-duality holds are reproduced (Rujan *et al* 1981, Creutz and Roberts 1983). Within the context of the MKRG scheme, we are able to define a transformation out of this region. Using this transformation, the existence of the $Z(4)$ phase with perpendicular order predicted by our MC simulations and by Kohmoto *et al* is confirmed. The phase boundaries obtained by the MKRG method and by MC simulations in the whole parameter space are found to be in excellent agreement.

The plan of this paper is as follows: in § 2 we define $Z(N)$ models and describe the Monte Carlo simulations used to obtain the $Z(4)$ phase diagram. In § 3 we use the Migdal–Kadanoff renormalisation group scheme to study this model.

2. Monte Carlo simulations results

Let us define a $Z(N)$ model on a square lattice. At each site, j, we consider a variable $S(j)$, that can take N different values:

$$S(j)=\exp\{\mathrm{i}\theta(j)\}=\exp\{\mathrm{i}(2\pi/N)n(j)\} \qquad n(j)=0,1,2\ldots N-1. \tag{2.1}$$

Taking into account nearest-neighbour interactions only, the most general form of the energy with $Z(N)$ global symmetry (invariance under global $(2\pi/N)n$ rotations) is

$$E=-\sum_{j,\mu}\sum_{\alpha=1}^{[N]} J_\alpha[\cos\alpha(\theta(j)-\theta(j+\mu))-1] \tag{2.2}$$

where μ represents the conventional primitive vectors of the square lattice, $[N]$ is the greatest integer less than or equal to $\frac{1}{2}N$ and $J_1, J_2 \ldots J_{[N]}$ are coupling constants. It is also convenient to introduce variables $x_\alpha=\exp(-E_\alpha/kT)$ where E_α is the energy required to rotate a spin by an angle $2\pi\alpha/N$, k is the Boltzmann constant and T is the temperature.

The Monte Carlo simulation of the thermodynamical behaviour of these systems is done as usual (Binder 1979, Carneiro *et al* 1982). Our calculations for the $Z(4)$ model are performed on square lattices of different sizes (mainly 20×20) subject to periodic boundary conditions. We take data after each run over the entire lattice (one MC step) and the number of Monte Carlo steps used to determine each point of the phase diagram varies from 1000, very far from the phase transition, up to 15000 near the transition, discarding from 30% to 50% of the initial steps, enough to 'thermalise'.

For $N=4$, we have two coupling constants J_1 and J_2 and

$$\begin{aligned} x_1&=\exp\{-(J_1+2J_2)/kT\}\\ x_2&=\exp\{-2J_1/kT\}. \end{aligned} \tag{2.3}$$

A study of the partition function $\mathcal{Z}$ reveals that it is invariant under a change of J_1 into $-J_1$, and that it obeys generalised self-duality relations in the region

$$0<x_1<\tfrac{1}{2}(1+x_2) \qquad 0<x_2<1 \tag{2.4}$$

that is, $\mathcal{Z}(x_1, x_2) = A\mathcal{Z}(x_1^*, x_2^*)$, where A is a constant and

$$x_1^* = (1 - x_2)/(1 + 2x_1 + x_2) \qquad x_2^* = (1 - 2x_1 + x_2)/(1 + 2x_1 + x_2). \tag{2.5}$$

In the region where generalised self-duality holds, previous theoretical results predicted the existence of at least three phases (Alcaraz and Köberle 1980, Kohmoto *et al* 1981, Rujan *et al* 1981):

(a) Phase I, the usual ferromagnetic phase with $\langle S \rangle \neq 0$ (and, of course, $\langle S^2 \rangle \neq 0$ also), occurring at low temperatures,

(b) Phase II, an intermediate temperature phase with $\langle S \rangle = 0$ and $\langle S^2 \rangle \neq 0$,

(c) Phase III, the disordered phase with $\langle S \rangle = \langle S^2 \rangle = 0$.

The region where generalised self-duality does not hold has been studied much less frequently (Kohmoto *et al* 1981). By simple energy considerations we can easily verify that at zero temperature and for $J_1 > 0$ the ground state is ferromagnetic if $J_2/J_1 > -0.5$. If $J_2/J_1 < -0.5$ the ground state is such that the spins on nearest-neighbour sites are perpendicular. The order in this state may be characterised as follows: first, divide the two-dimensional square lattice into two sub-lattices, A and B, defined in such a way that the nearest-neighbour sites to sub-lattice A lie on sub-lattice B, and *vice versa*. Second, define the sub-lattice order parameters $\langle S_A \rangle$, $\langle S_B \rangle$, $\langle S_A^2 \rangle$ and $\langle S_B^2 \rangle$. Then the ground state for $J_2/J_1 < -0.5$ is such that $\langle S_A \rangle = \langle S_B \rangle = 0$ and $\langle S_A^2 \rangle = -\langle S_B^2 \rangle \neq 0$.

The points on the boundaries of our phase diagram are obtained by measuring the order parameters and locating the point where they equal one half of their value in the ordered phase. These points correspond approximately to a maximum of the specific heat, as happens in the $Z(2)$ case (Landau 1976). Figures 1, 2 and 4 are typical examples of the variation of order parameters and specific heat as kT/J_1 changes, while the ratio of the coupling constants J_2 and J_1 is kept fixed.

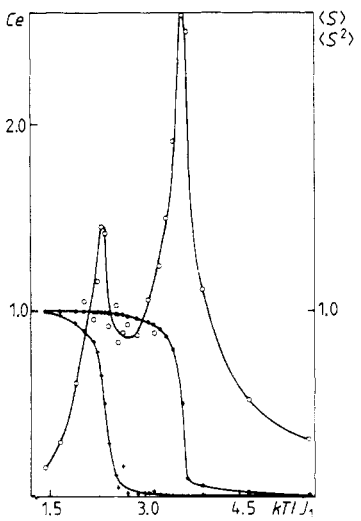

Figure 1. Specific heat per spin and order parameters variation for the thermodynamical path $J_2/J_1 = 1.50$. 15000 MC steps were used on a square 20×20 lattice. The full curves are guides to the eye. + denotes $\langle S \rangle$, ● denotes $\langle S^2 \rangle$ and ○ denotes *Ce*.

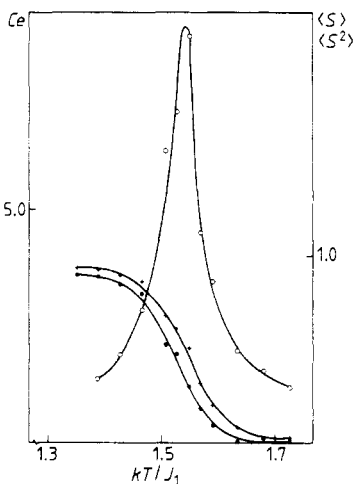

Figure 2. Specific heat per spin and order parameters variation for the thermodynamical path $J_2/J_1 = 0.27$. 15000 MC steps were used on a square 20×20 lattice. The full curves are guides to the eye. + denotes $\langle S \rangle$, ● denotes $\langle S^2 \rangle$ and ○ denotes *Ce*.

Elitzur *et al* (1979) argued that a massless intermediate phase between the ferromagnetic and disordered phases should appear in $Z(N)$ self-dual models for $N > N_c$. They estimate the value of $N_c > 4$. Recently Stavans and Domany (1983), using MC simulations, looked for indications of this phase in $Z(4)$ models in the neighbourhood of the point ($x_1 = 0.5$, $x_2 = 0.0$). Although they found two peaks in the specific heat, one very steep and narrow and another one much smaller and broader, they conclude that no strong evidence exists for a massless phase.

We also investigate the region where this phase could appear ($-0.5 < J_2/J_1 < 0$), and the results we obtain are similar to those of Stavans and Domany. Only very close to $J_2/J_1 = -0.5$ do we find two peaks. Figure 3 shows a plot of the specific heat and the magnetisation for $J_2/J_1 = -0.45$. We find a steep and narrow peak, at the temperature where the magnetisation changes rapidly, while the second peak, located at a higher temperature, is very wide and much shorter than the first one. The first peak is close to the self dual line, where the transition should be, in case we had only the usual ordered and disordered phases in this region. We also observe that the second peak is outside the region where generalised self duality holds. If an intermediate massless phase did exist, its boundaries should be related by the duality transformation, which means that, if the observed peaks correspond to the boundaries of such an intermediate phase, both should be located inside this region.

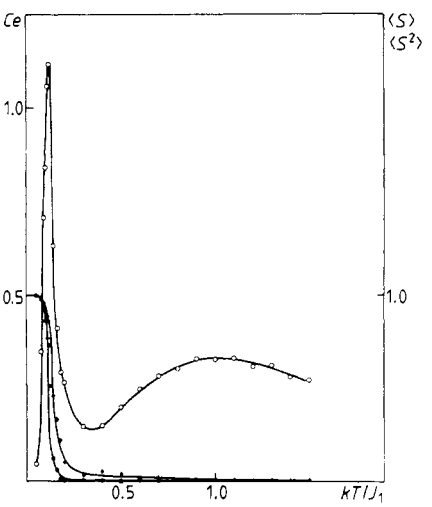

Figure 3. Specific heat per spin and order parameters variation for the thermodynamical path $J_2/J_1 = -0.45$. 15000 MC steps were used on a square lattice; the full curves are guides to the eye. + denotes $\langle S \rangle$, ● denotes $\langle S^2 \rangle$ and ○ denotes Ce.

Furthermore, as we change the lattice size from 10×10 to 20×20, these peaks do not scale, as they should, in a transition to a critical phase.

We therefore conclude that, up to this point, the MC analysis does not favour the existence of a massless phase in the $Z(4)$ model. We don't believe, however, that the subject is conclusively settled, and we plan to study it further.

It is interesting to note that for the $Z(4)$ gauge 4D model some authors (Alcaraz and Jacobs 1983, Creutz and Okawa 1982) claim to have found this intermediate massless phase.

In spite of the many similarities between $Z(N)$ 4D gauge systems and 2D spin systems, there is no guarantee that their phase diagrams must be the same. It is true that the MKRG transformation does predict identical phase diagrams for both systems (Kadanoff 1977), but this scheme is an approximation. Therefore, we do not believe that the results on the existence of a massless phase on 4D gauge systems, obtained by Alcaraz and Jacobs (1983) and by Creutz and Okawa (1982), furnish conclusive evidence for the 2D spin problem.

In figure 5 we show the phase diagram obtained through our Monte Carlo simulation. In the ferromagnetic region each point is determined starting both from an ordered and a disordered state. Some of our results on the 20×20 lattice were checked

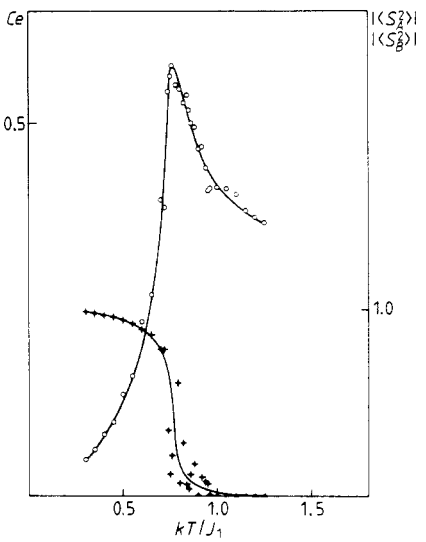

Figure 4. Specific heat per spin and order parameters variation for the thermodynamical path $J_2/J_1 = -0.60$. 15000 MC steps were used on a square lattice. The full curves are guides to the eye. + denotes $|\langle S_A^2 \rangle|$, ● denotes $|\langle S_B^2 \rangle|$ and ○ denotes *Ce*.

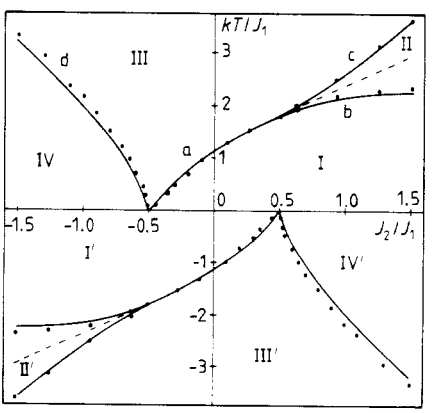

Figure 5. Phase diagram for the $Z(4)$ model. Dots correspond to Monte Carlo simulations and full curves were obtained by the MKRG scheme.

on 10×10 and 50×50 lattices, and no significant difference was found. Continuum lines a, b, c and d are the results of our MKRG calculations which are described in § 3. Line a is the self-dual line. Lines b and c are dual to each other. Boundaries for the $J_1<0$ portion of the diagram are obtained from the $J_1>0$ portion, using the fact that the partition function is invariant under the change of J_1 into $-J_1$. Phase I is ferromagnetic, phase III is disordered and II is the intermediate temperature phase. MC results are very close to boundaries a, b and c, and therefore are compatible with duality. Phase I′ is an antiferromagnetic phase with order parameters defined in the sublattices $\langle S_A\rangle=-\langle S_B\rangle\neq0$ and $\langle S_A^2\rangle=\langle S_B^2\rangle\neq0$. Phase II′ has $\langle S_A\rangle=\langle S_B\rangle=0$ and $\langle S_A^2\rangle=\langle S_B^2\rangle\neq0$. Phase III′ is disordered. Phases IV and IV′ are phases with perpendicular order and parameters $\langle S_A\rangle=\langle S_B\rangle=0$ and $\langle S_A^2\rangle=-\langle S_B^2\rangle\neq0$.

Near the point $J_2/J_1=-0.5$ and $kT/J_1=0$, the MC results for the transition points seem to converge at $T=0$, indicating that the model with $J_2/J_1=-0.5$ and $J_1>0$ has no transition at $T\neq0$. Therefore, the four-state antiferromagnetic Potts model (Wu 1982) which corresponds to $J_2/J_1=0.5$ and $J_1<0$ should have a similar phase structure, due to the symmetry of the diagram. This result is in agreement with previous theoretical prediction (Baxter 1982).

3. Migdal–Kadanoff renormalisation group results

The diagram of the $Z(4)$ model is also investigated by using an infinitesimal MKRG scheme. These transformations have been used before in the ferromagnetic region (Rujan *et al* 1981, Creutz and Roberts 1983). In order to preserve the symmetry of the ground state for both the ferromagnetic and antiferromagnetic regions we define a MKRG finite transformation with decimation of an even number of spins only. Starting from those transformations we are able to define an infinitesimal transformation which is valid for both the ferromagnetic and antiferromagnetic region.

The details of the MKRG transformation are left to the appendix. Here we limit ourselves to describe the results and compare them with the phase diagram obtained in the previous section.

The MKRG flow is shown in figure 6 in terms of the variables x_1 and x_2 defined in equation (2.3). We consider only the region $0\leqslant x_2\leqslant1$, $x_1\geqslant0$. The portion of the diagram for $x_2\geqslant1$ can be obtained by the symmetry relation $x_2\to1/x_2$, $x_1\to x_1/x_2$ (or, equivalently, $J_1\to-J_1$).

We obtain four phases:

(a) the usual ferromagnetic phase (I) which is the region of attraction of the strong coupling fixed point L ($x_1=x_2=0$);

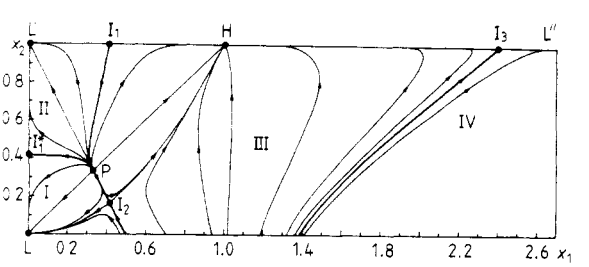

Figure 6. MKRG flow trajectories.

(b) phase II, the partially broken $Z(4)$ symmetry phase, which is the region of attraction of the fixed point L'($x_1 = 0, x_2 = 1$);

(c) the disordered phase (III), which is the region of attraction of the fixed point H ($x_1 = x_2 = 1$), and

(d) phase IV, with perpendicular order, which is the region of attraction of the fixed point L'' ($x_1 = \infty, x_2 = 1$).

The boundaries between phases I and II, and between phases II and III are, respectively, the critical surfaces which contain the Ising fixed points I_1^* ($x_1 = 0, x_2 = \sqrt{2} - 1$) and I_1 ($x_1 = \sqrt{2} - 1, x_2 = 1$). These surfaces are related to one another by the duality transformation. In the MKRG approximation, the boundary between phases I and III is the critical surface of the Ising fixed point I_2 ($x_1 = \sqrt{2} - 1$, $x_2 = (\sqrt{2} - 1)^2$), whereas it is known exactly that it should be a line of critical points (Rujan *et al* 1981). P is the four-state Potts model fixed point ($x_1 = x_2 = \frac{1}{3}$). The boundary between phases III and IV is the critical surface which contains the antiferromagnetic Ising fixed point I_3 ($x_1 = 1 + \sqrt{2}$, $x_2 = 1$); therefore we expect that the transition III–IV is in the Ising universality class (Drugovich *et al* 1982).

In the region where generalised self-duality holds (equation (2.4)), our results are similar to those obtained by Rujan *et al* (1981) and Creutz and Roberts (1983). We also do not find a massless phase in this region. This, however, should not be taken as conclusive evidence against the existence of this phase, since the Migdal–Kadanoff method is not exact (Kadanoff 1976).

The phase diagram obtained by our MKRG calculation is compared with our MC simulation results in figure 5. The agreement between both of them is excellent, within the error of the simulation. The phase with perpendicular order detected by our MC simulation is therefore confirmed by our MKRG calculations. This phase structure in the antiferromagnetic region is not surprising since as $J_2/J_1 \to -\infty$, the $Z(4)$ model becomes an Ising antiferromagnet, which undergoes a phase transition when defined on a square lattice†. It should be noted that our MKRG results predict that the antiferromagnetic four-state Potts model (equivalent by symmetry to line $x_1 = 1$) has no transition.

Appendix

Here we describe in detail the MKRG method applied to the $Z(N)$ model on a square lattice.

It is convenient to rewrite the Hamiltonian equation (2.2), as

$$-\frac{E}{kT} = \sum_{j,\mu} V(\theta(j) - \theta(j+\mu)) \tag{A1}$$

where $(-V)$ is the nearest-neighbour interaction energy (in units of kT)

$$V(\{K_\alpha\}, \Delta\theta) = \sum_{\alpha=1}^{[N]} K_\alpha(\cos \alpha\Delta\theta - 1), \tag{A2}$$

$$K_\alpha = J_\alpha/kT \text{ and } |\Delta\theta| = (2\pi/N)r \qquad (r = 0, 1, \ldots, N-1).$$

† The absence of a phase transition in the antiferromagnetic Ising model on a triangular lattice suggests that the $Z(4)$ model on such a lattice does not have a phase with spin order similar to phase IV.

The variables x_r can be written as

$$x_r = \exp\{V(\{K_\alpha\}, (2\pi/N)r\}$$
$$= \exp i \sum_{\alpha=1}^{[N]} K_\alpha(\cos(2\pi r/N)\alpha - 1) \qquad (r = 0, 1, 2, \ldots, N-1). \quad \text{(A3)}$$

Note that $x_0 = 1$ and $x_{N-r} = x_r$, so that there are only $[N]$ independent x-variables.

The MKRG used here is, as usual, a combination of a bond-shifting operation followed by decimation, as shown in figure 7. After shifting n bonds, the coupling constants become (see figure 7(*b*))

$$K'_\alpha = (1+n)K_\alpha \qquad (\alpha = 1, 2, \ldots, [N]). \quad \text{(A4)}$$

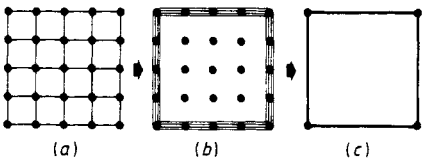

Figure 7. Schematic representation of the Migdal–Kadanoff renormalisation scheme: (*a*) original interaction, (*b*) interaction after bond shifting, (*c*) new interaction.

The corresponding transformation for the x variables is

$$x' = \exp\{V(\{K'_\alpha\}, (2\pi/N)r)\}$$
$$= x_r^{(1+n)} \qquad (r = 0, 1, \ldots, N-1). \quad \text{(A5)}$$

After decimation of n spins, the renormalised couplings (figure 7(*c*)) can be expressed in terms of the original ones:

$$K''_\alpha = R_\alpha^{(\lambda)}(\{K'_\beta\}) = R_\alpha^{(\lambda)}(\{\lambda K_\beta\}) \quad \text{(A6)}$$

where $\lambda = 1+n$ is the scale factor of the MKRG transformation. The corresponding expression for the x-variables is

$$x''_r = \exp\{V(\{K''_\alpha\}, (2\pi/N)r)\}$$
$$= F_r^{(\lambda)}(\{x'_s\}) = F_r^{(\lambda)}(\{x_s^\lambda\}). \quad \text{(A7)}$$

In order to obtain the MKRG transformation equations we need to decimate n $Z(N)$-spins on a line, that is, we have to calculate (see figure 7(*b*))

$$e^{K''_0} e^{V[\{K''_\alpha\},(2\pi/N)(r-r')]} = e^{K''_0} x''_r = \sum_{r_1, r_2, \ldots r_n} x'_{r-r_1} x'_{r_1-r_2} \ldots x'_{r_{n-1}-r_n} x'_{r_n-r'} \quad \text{(A8)}$$

where K''_0 is chosen such that $V(\{K''_\alpha\}, 0) = 0$ (or $x''_0 = 1$). Using the identity

$$\frac{1}{N} \sum_{R=0}^{N-1} \exp\left[im\left(\frac{2\pi}{N} R\right)\right] = \delta_{m,0} \qquad (m = 0, 1, \ldots, N-1) \quad \text{(A9)}$$

we can write x_r as

$$x'_r = \frac{1}{N} \sum_{m=0}^{N-1} a_m \exp\left(-im\frac{2\pi}{N} r\right), \quad \text{(A10)}$$

with

$$a_m = \sum_{r=0}^{N-1} x'_r \exp\left(\mathrm{i}m\frac{2\pi}{N}r\right). \tag{A11}$$

Substituting (A10) in (A8) we find

$$\mathrm{e}^{K''_0}x''_r = \frac{1}{N}\sum_{m=0}^{N-1}(a_m)^\lambda \exp\left(-\mathrm{i}m\frac{2\pi}{N}r\right). \tag{A12}$$

Using (A11), (A12) becomes

$$\begin{aligned}\mathrm{e}^{K''_0}x''_s &= \mathrm{e}^{K''_0}F_s^{(\lambda)}(\{x'_r\}) \\ &= \frac{1}{N}\sum_{m=0}^{N-1}\exp\left(-\mathrm{i}s\frac{2\pi}{N}m\right)\left[\sum_{r=0}^{N-1}x'_r\exp\mathrm{i}m\frac{2\pi}{N}r\right]^\lambda.\end{aligned} \tag{A13}$$

Finally, using (A5), we obtain the following equations for the MKRG transformation with scale factor λ

$$\mathrm{e}^{K''_0}x''_s = \frac{1}{N}\sum_{m=0}^{N-1}\exp\left(-\mathrm{i}s\frac{2\pi}{N}m\right)[b_m(\lambda)]^\lambda \tag{A14}$$

where

$$b_m(\lambda) \equiv \sum_{r=0}^{N-1} x_r^\lambda \exp\left(\mathrm{i}m\frac{2\pi}{N}r\right). \tag{A15}$$

In order to preserve the symmetry of the ground state, *both* in the ferromagnetic and antiferromagnetic regions, we must choose λ to be *odd*. Since λ is odd and $b_m(\lambda)$ is real we can write

$$(b_m(\lambda))^\lambda = b_m(\lambda)|b_m(\lambda)|^{\lambda-1} = b_m(\lambda)\,\mathrm{e}^{(\lambda-1)\ln|b_m(\lambda)|}. \tag{A16}$$

We take this equation as a definition, even for infinitesimal changes $\lambda = 1+\varepsilon$. To first order in ε the RHS of (A16) becomes

$$b_m(1) + \varepsilon[b_m(1)\ln|b_m(1)| + \partial b_m/\partial\lambda|_{\lambda=1}].$$

Substituting this result in equation (A14) we obtain

$$x''_s = x_s + \varepsilon G_s(\{x_r\}) \tag{A17}$$

where G_s is given by

$$\begin{aligned}G_s(\{x_r\}) = x_s\ln x_s &+ \frac{1}{N}\sum_{m=0}^{N-1}\sum_{r=0}^{N-1}x_r\exp\left(\mathrm{i}r\frac{2\pi}{N}m\right) \\ &\times\left[1 - x_s\exp\left(\mathrm{i}s\frac{2\pi}{N}m\right)\right]\ln\left|\sum_{p=0}^{N-1}x_p\exp\left(\mathrm{i}p\frac{2\pi}{N}m\right)\right|.\end{aligned} \tag{A18}$$

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