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CRITICALITY OF THE THREE-STATE CHIRAL CLOCK MODEL: A RENORMALISATION GROUP STUDY

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ABSTRACT

Within a real space renormalisation group approach, we study the phase diagram and the universality classes of the three-state chiral clock model in a self-dual planar hierarchical lattice. We find that the chiral field Δ is relevant at the pure Potts critical point with a crossover exponent $\phi \simeq 0.32$. The critical line which separates the ferromagnetic phase from the non-ferromagnetic ones is characterized by a multicritical (Lifshitz) point located at $(K,\Delta) \simeq (1.452, 0.382)$. The ferromagnetic phase appears to be divided into two regions by a wetting line which we also locate numerically. The various critical lines and point of the phase diagram are believed to be excellent approximations for the square lattice.

Key-words: Chiral clock model; Criticality; Renormalisation group; Lifshitz point.

1 INTRODUCTION

Since the first observations of modulated structures in ferroeletric and magnetic materials at the end of the fifties and beginning of sixties [1], a great interest has grown in studing statistical models which might exhibit such modulations. From the theoretical point of view, two models are basically studied, namely, the axial next-nearest neighbour Ising (ANNNI) model and the chiral clock model (sometimes referred to as "asymmetric clock", "chiral Potts" and "helical Potts" model). The Hamiltonians of both models contain competing interactions which give rise to spatially modulated structures. In the chiral clock model the competition is provided by chiral or helical interactions along a given lattice axis, while in the ANNNI model it is a nearest-neighbour ferromagnetic coupling competing with a next-nearest-neighbour antiferromagnetic one along one lattice direction which causes the modulations. For a survey of the present state of the art on these two models the reader is referred to the recent reviews by Yeomans [2] and by Selke [3].

The chiral clock model can serve as a prototype for the melting of a commensurate adsorbed phase [4]; its experimental realization in two dimensions is provided by dissociated hydrogen on Fe(110) [5]. No similar physical system is known to be described by this model in three dimensions. We focus in the present paper on the controversial two-dimensional, three-state chiral clock model. At $d=2$ it might show a floating incommensurate phase above the low-temperature commensurate phases [6,7,8]. However, a considerable controversy remains over whether there is a Lifshitz-type multicritical point or whether the floating phase extends down to a vanishing chiral field Δ [7,8,9,10,11]. Huse and Fisher[11] suggest a Lifshitz point which governs the transition from the ordered (ferromagnetic) phase to the disordered (paramagnetic) one for Δ such that $0 < \Delta \leq \Delta_L$. The present results give support to this possibility.

Here we study the two-dimensional, three-state chiral clock (ferromagnetic) model in a high-order Wheatstone-bridge hierarchical lattice within a real space renormalisation group(RG) framework which preserves the two-site correlation function. The central goal of this work is to investigate whether chirality introduces a new universality class (as suggested by Huse and Fisher) as well as to numerically determine various critical lines and points. The present results are exact for the hierarchical lattice, and approximate for the square lattice (the approximation being however excellent for the phase diagram).

In section 2 we present the model and the RG formalism; in section 3 the results are discussed; finally we conclude in section 4.

2 MODEL AND FORMALISM

The q-state chiral clock model is described by the Hamiltonian

$$\mathcal{H} = -K \sum_{<ij>} \cos\left[\frac{2\pi}{q}(n_i - n_j + \vec{\Delta}.\vec{R}_{ij})\right] \qquad (2.1)$$

where the sum runs over all pairs of nearest neighbouring sites of a given array, $K \equiv J/k_BT > 0$, $\vec{R}_{ij}$ is the unit vector starting from the site i to site j, and $\{n_i\}$ are spin variables which can take the values $n_i = 0,1,2,...,q-1$. The parameter $\Delta \gtrless 0$ might cause a tendency for the phase angle $2\pi n_i/q$ to have a continuous rotation as a function of the position along the $\vec{\Delta}$ direction. This competes with the restriction that the phase angle must be discrete and this competition leads to commensurate-incommensurate transitions. For q = 2 the chiral Hamiltonian is, for arbitrary Δ, equivalent to an (anisotropic) Ising model at zero field. When $\vec{\Delta} = 0$ and q = 3 the model reduces to the standard ferromagnetic three-state Potts model. From now on we will consider planar lattices and $\vec{\Delta} = \vec{\Delta}\hat{y}$ where $\hat{y}$ is the unit vector along a direction which is chosen once for ever.

The ground-state of the q=3 model is ferromagnetic ($n_i = n_j$ for all sites) when $|\Delta| < 1/2$. For $1/2 < \Delta < 3/2$ the ground state presents a ferromagnetic configuration along the x-axis and right-handed chiral configuration along the y direction. To be more precise the spins form, along the y-axis, the pattern...01201201.... This ground state is commensurate with the lattice and the spatially modulated order has a period of p = 3 lattice constants. $\Delta = 1/2$ is a multiphase point [12] where the ferromagnetic state and any possible right-handed chiral sequence share the same energies. The ground state is then infinitely degenerated.

At $\Delta = 0$ the Hamiltonian (2.1) has a symmetry S_3, i.e, it is invariant under any permutation of the labellings of the three spin states. For $\Delta \neq 0$ the model has a lower symmetry, namely, Z_3, being invariant only under cyclic permutations of the spin labels. On the other hand, the partition function is invariant under the following transformations:

1) $\Delta \rightarrow -\Delta$ (2.2)

if one makes the identifications

$n_i \rightarrow -n_i \pmod 3$, (2.3)

that is, if we change the right-handed for a left-handed chiral ordering;

2) $\Delta \rightarrow \Delta + m$ (2.4)

where m is an arbitrary integer, since one transforms each spin n_i to

$n_i \rightarrow (n_i + y_i m) \bmod 3$ (2.5)

where y_i is the coordinate of the site i along the y-axis.

Combining these two symmetry operations with $m=1$ the partition function is invariant under the transformation

$$\Delta \rightarrow 1 - \Delta \qquad (2.6)$$

$$n_i \rightarrow (-n_i + y_i) \bmod 3 \qquad (2.7)$$

Then the phase boundaries are invariant under reflexion about the line $\Delta = 1/2$ and we only need to analyse the range $0 \leq \Delta \leq 1/2$. However, the phases themselves must be identified differently within the regimes $0 \leq \Delta < 1/2$ and $1/2 < \Delta \leq 1$. Indeed, from (2.7) we have to take into account the correspondence between ferromagnetic ($\Delta < 1/2$) and chiral ($\Delta > 1/2$) ground states.

We shall now address the chiral Hamiltonian (2.1) on the hierarchical lattice generated by the cell shown in figure 1.a. The choice of this cell has been done in order to simulate the square lattice. To do so two features seem essential: the self-duality of the square lattice, and the preservation, under renormalisation, of the ground states of the system. The cell we have selected is the *smallest* Wheatstone-bridge-type cluster with these properties. The renormalisation transformation between the cell of figure 1.a and the simple bond shown in figure 1.b is defined by imposing the equality

$$\exp\left[-\mathcal{H}'(K',\Delta')+c\right] = \sum_{n_3,\ldots,n_{14}} \exp\left[-\mathcal{H}(K,\Delta)\right] \tag{2.8}$$

After some algebraic work one obtains the following recursion relations

$$c = \frac{1}{3}\,\ell n(\phi_o\phi_1\phi_2), \tag{2.9}$$

$$K' = \frac{1}{3}\left\{\left[2\ell n\phi_o - \ell n(\phi_1\phi_2)\right]^2 + 3\left[\ell n(\phi_2/\phi_1)\right]^2\right\}^{1/2}, \tag{2.10}$$

$$\Delta' = \frac{3}{2\pi}\,\mathrm{arctg}\left[\frac{\sqrt{3}\,\ell n(\phi_2/\phi_1)}{2\ell n\phi_o - \ell n(\phi_1\phi_2)}\right]; \tag{2.11}$$

Where ϕ_o, ϕ_1 and ϕ_2 are the analytical expressions for the sums in the right-hand side of equation (2.8), with the terminal spins fixed in $(n_1,n_2) = (0,0),(1,0)$ and $(2,0)$ respectively.

Each one of such expressions involves the counting of 3^{12} configurations which were summed up through an algebraic PL1 computer program. The RG flows (determined by eqs. (2.10) and (2.11) in the (K,Δ) space will provide the phase diagram and the thermal critical exponents of the system.

3 RESULTS

The recursion relations (2.10) and (2.11) present an unstable fixed point at $\Delta = 0$ and $K=\frac{2}{3}\ \ell n(\sqrt{3}+1)$ which corresponds to the 3-state Potts ferromagnetic critical point. Its critical exponents are $\nu_T \simeq 0.975$ and $\nu_\Delta \simeq 3.052$; consequently the crossover exponent is $\phi = \nu_T/\nu_\Delta \sim 0.319$. This value is to be compared with the den Nijs's value $\phi = 1/6$ [13] and the series value [14] $\phi = 0.19 \pm 0.06$ for the square lattice. For an hierarchical lattice (with intrinsic dimensionality $d_{eff} = 2$) where the Migdal-Kadanoff renormalisation method is exact, Huse [15] obtains $\phi = 1/2$. There is a second unstable fixed point at $\Delta = 1/2$ and $K^{-1} = 0$. Also a semi-stable fixed point is present at $Z \simeq 0.113$ ($K \simeq 1.452$) and $\Delta \simeq 0.382$, where the convenient variable Z is defined as $Z \equiv \exp(-3K/2)$. For this fixed point we have the critical exponent $\nu_L \simeq 0.949$. This point is to be identified with a Lifshitz-type fixed point and our estimative for its (K,Δ) is consistent with the reference [7] which suggests $K \sim 1.053$ and $\Delta \in [0.4, 0.425]$, and with the reference [8] which suggests $(K,\Delta) \simeq (1.111, 0.4 \pm 0.03)$.

In order to complete the analysis of the fixed points and of the RG flow we have considered the asymptotic form of the recur sion relations (2.10) and (2.11) when Z goes to zero ($T \to 0$). The leading term involves the ground and first excited states of the system under the special conditions imposed by the fixed values assigned to the two terminal spins in the cell of figure 1.a. Indeed, it will appear interfacial wetting transitions [14] that divide the commensurate phase into two distinct regions, namely, $0 \leq \Delta \leq 1/4$ and $1/4 < \Delta \leq 1/2$. For $0 \leq \Delta \leq 1/4$ we have the following asymptotic recursion relations for (2.10) and (2.11)

$$Z' \sim Z^b \tag{3.1}$$

$$\Delta' \sim \Delta \tag{3.2}$$

where b is the scale factor ($b = 4$ in our case). The Jacobian of these transformations is

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.3}$$

In other words, Δ is a marginal parameter, and we have a *line of fixed points* for $Z = 0$ and $\Delta \in [0,1/4]$. This line of fixed points seems to be due to the incomplete wetting in this part of the ferromagnetic phase. For $1/4 < \Delta < 1/2$, the asymptotic recursion relations are.

$$Z' \sim Z^{b(\sqrt{3}\cos\frac{2\pi\Delta}{3} - \mathrm{sen}\frac{2\pi\Delta}{3})} \tag{3.4}$$

$$\Delta' = 1/4 \tag{3.5}$$

So the fixed point is located at $(Z,\Delta) = (0,1/4)$ and the associated Jacobian vanishes. Starting with a small Z, the line

$Z = 0$ behaves as an atractor for Δ such that $b(\sqrt{3}\cos\frac{2\pi\Delta}{3} - \mathrm{sen}\frac{2\pi\Delta}{3}) > 1$ and a repulsor otherwise. The complete renormalization group flow diagram is shown in figure 2. Figure 3 shows the critical line as well as the line corresponding to the wetting transition.

4 CONCLUSION

We have focused the criticality (phase diagram and thermal critical exponents) of the three-state chiral clock model in a suitable planar hierarchical lattice (see Fig. 1). To do this we have adopted a real space renormalisation group formalism which preserves the correlation function between two sites.

We find that the chiral parameter $\vec{\Delta}$ is relevant and therefore any point of the ferromagnetic-disordered phase boundary with $\Delta \neq 0$ is governed by a fixed point distinct from the pure Potts critical point. Therefore, we have a new "chiral" universality class. Our results support the possibility of the Lifshitz point which characterises this new universality class. Also, we calculate numerically the line of wetting transition resulting from the interface properties of the model. These novel interface features are "seen" in our method due the special conditions imposed to the two terminal spins in the cell. We believe that the various critical lines and points of the phase diagram are excellent approximations for the square lattice.

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CAPTION FOR FIGURES

Figure 1 - Cells used to construct the renormalisation group; and o respectively denote internal and terminal sites. (a) b = 4 graph; (b) b' = 1 graph.

Figure 2 - Renormalisation group flow diagram. P and L repectively denote the Potts and Lifshitz fixed points. At $\Delta = 0$ the flow is that of the three-state Potts model. We see that the fixed point L governs the ferromagnetic-disordered phase transition for $\Delta \neq 0$. Also, the fixed point at $Z = 0$ and $\Delta = 1/4$ is an atractor for a special line (the wetting line). At the line $Z = 0$ we have a segment of fixed points for $\Delta \in [0,1/4]$.

Figure 3 - Part of the phase diagram of the three-state chiral clock model. (P) denotes the disordered, (F) the ferromagnetic and (C) the chiral phases. The ferromagnetic phase is itself divided, by the wetting line, into two regions, namely, the non-wetting (NW) and the wetting (W) ones. The boundary between paramagnetic and incommensurate or high commensurate phases (I) is indicative.

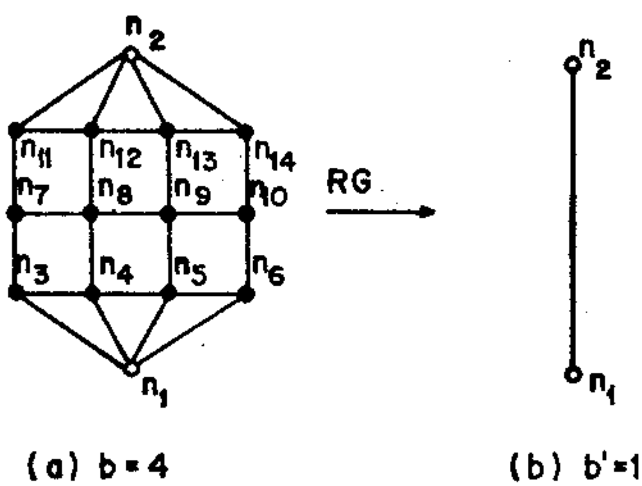

FIG.1

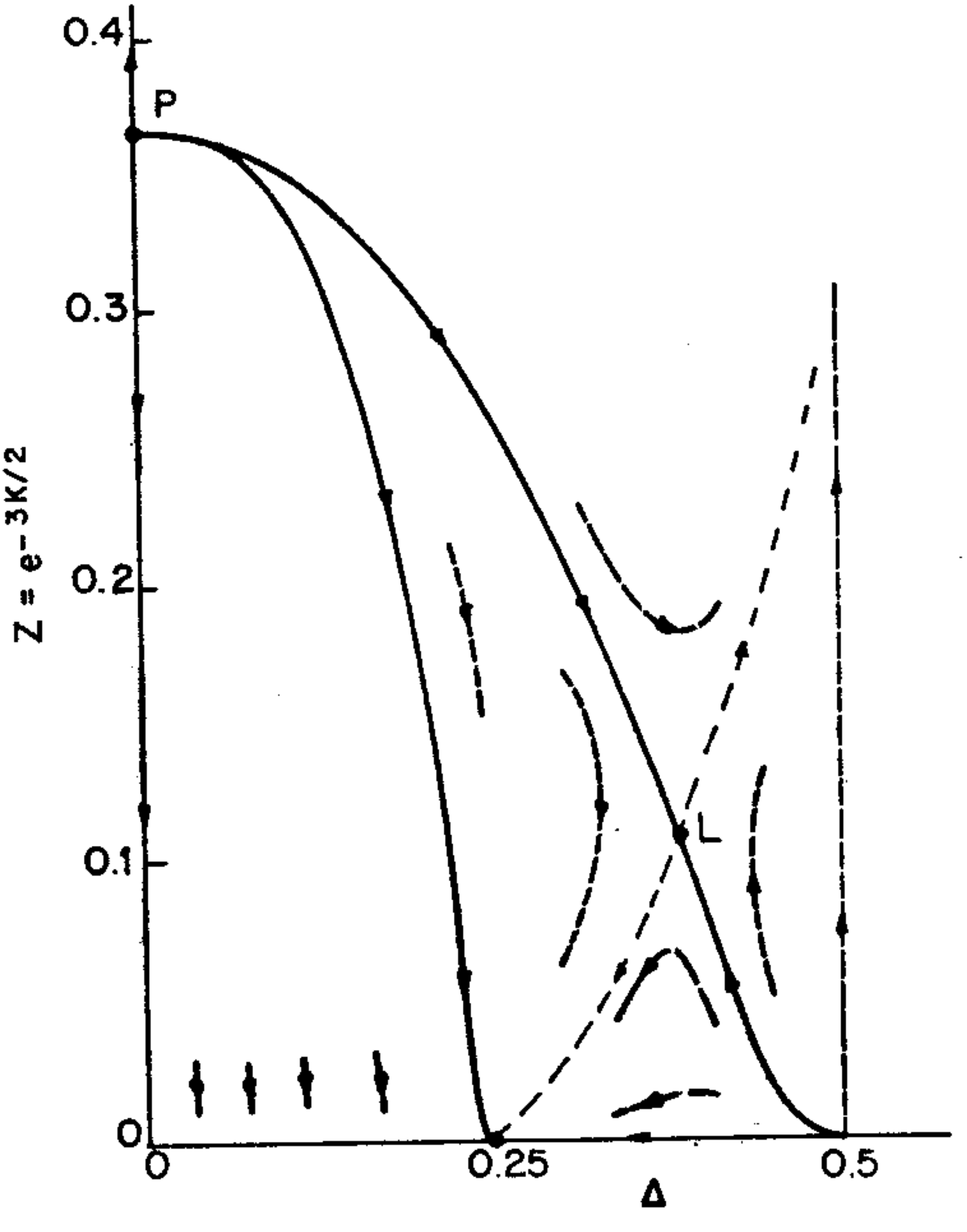

FIG.2

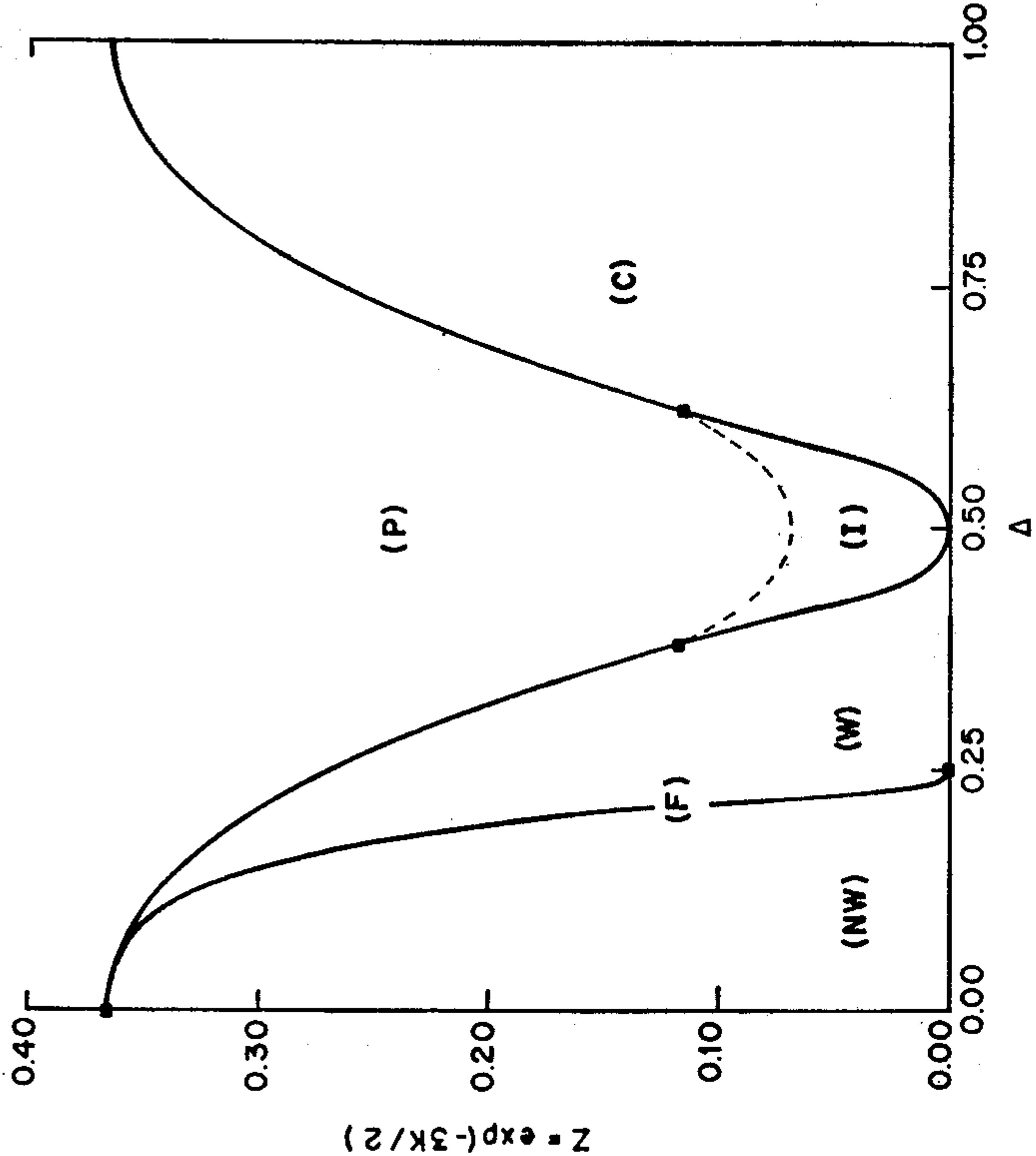

FIG. 3

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