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# Universal critical behavior of aperiodic ferromagnetic models

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We investigate the effects of geometric fluctuations, associated with aperiodic exchange interactions, on the critical behavior of $q$-state ferromagnetic Potts models on generalized diamond hierarchical lattices. For layered exchange interactions according to some two-letter substitutional sequences, and irrelevant geometric fluctuations, the exact recursion relations in parameter space display a non-trivial diagonal fixed point that governs the universal critical behavior. For relevant fluctuations, this fixed point becomes fully unstable, and we show the apperance of a two-cycle which is associated with a novel critical behavior. We use scaling arguments to calculate the critical exponent $\alpha$ of the specific heat, which turns out to be different from the value for the uniform case. We check the scaling predictions by a direct numerical analysis of the singularity of the thermodynamic free-energy. The agreement between scaling and direct calculations is excellent for stronger singularities (large values of $q$). The critical exponents do not depend on the strengths of the exchange interactions.

Quenched disorder may change the critical behavior of ferromagnetic spin systems [1]. Although disorder provides the more usual examples, there are alternative ways to break translational invariance. For instance, the interest in the study of quasicrystals [2] inspired a number of proposals of deterministic schemes to build spatially aperiodic structures. In analogy with the Harris criterion to account for the effects of quenched disorder, Luck [3] developed a heuristic reasoning to gauge the relevance of geometric fluctuations (associated with aperiodic interactions) on the critical behavior of ferromagnetic models on Bravais lattices. In a recent publication [4], Luck's criterion has been exactly derived for a $q$-state ferromagnetic Potts model on a diamond-type hierarchical lattice. Now we revisit this problem to show the existence of an attractor that gives rise to a novel class of critical behavior.

Many investigations of aperiodic classical [5] and quantum [6] Ising chains, and two-dimensional Ising models with aperiodic layered interactions [7], use the formalism of substitution rules on alphabets for the construction of infinite aperiodic sequences of elements, which are then associated with coupling constants along a direction of the lattice. We have taken advantage of the structure of hierarchical lattices [8] to build layered aperiodic models [9] which are then amenable to simple (and exact) renormalization-group calculations. In parameter space, there is always a "diagonal", non-trivial, fixed point of the renormalization-group recursion relations. For relevant geometric fluctuations, this diagonal fixed point, associated with the critical behavior of the uniform (equal couplings) model, becomes fully unstable, and therefore cannot be reached from any nonuniform initial conditions in parameter space [4]. The critical behavior of the aperiodically perturbed system, in case of a phase transition, should then be governed by another attractor in parameter space.

Relevant aperiodicity is believed to drastically weaken, or eventually suppress, the critical singularities [6]. Recently, convincing Monte Carlo evidence [10] has been presented to indicate that relevant layered aperiodicity in the 8-state Potts model on the square lattice drives the phase transition from first to second-order (with critical exponents independent of the strength of the couplings). In the present work, we also detect a weakening of the critical singularities for relevant geometric fluctuations. Besides being numerically exact, our results can be regarded as equivalent to a Migdal-Kadanoff approximation for the analogous problems on Bravais lattices, and may thus be put in perspective with the Monte Carlo findings [10].

The $q$-state Potts ferromagnet is defined by the Hamiltonian

$$\mathcal{H} = -q \sum_{(i,j)} J_{i,j} \delta_{\sigma_i,\sigma_j}, \tag{1}$$

where $\sigma_i = 1, 2, \ldots, q$ for all sites of a lattice, $J_{i,j} > 0$, and the sum over $(i, j)$ refers to nearest-neighbor pairs of sites. We assume that the couplings can take only two values, $J_A$ and $J_B$, associated with the sequence of letters $A$ and $B$ of an aperiodic substitutional word. To generate this sequence, we can use, for example, the successive iterations of a period-doubling rule, given by $(A, B) \to (AB, AA)$. In Fig.1, we show a simple diamond hierarchical lattice with aperiodic interactions according to this sequence (the letters, and the corresponding coupling constants, are chosen to mimic a layered structure). In general, we may consider basic "diamonds" with $m$ branches and $b$ bonds along each branch, and generate hierarchical lattices with intrinsic, or fractal, dimension, $D = \ln(mb)/\ln(b)$. In each one of these structures, aperiodicity may be implemented by a substitution rule of the form $(A, B) \to (A^{n_1}B^{b-n_1}, A^{n_2}B^{b-n_2})$, with $0 \le n_1, n_2 < b$. These sequences are characterized by a substitution matrix with eigenvalues $\lambda_1 = b$ and $\lambda_2 = n_1 - n_2$. The asymptotic form of the fluctuations

in the number of letters depends on the wandering exponent,

$$\omega = \frac{\log|\lambda_2|}{\log\lambda_1}. \tag{2}$$

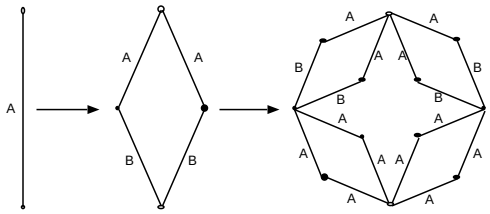


FIG. 1. Three successive generations of the simple diamond lattice ($b = m = 2$).

Now we decimate the internal degrees of freedom of the diamonds to write exact recursion relations for the reduced couplings. There is always a non-trivial fixed point on the diagonal of parameter space, which is associated with the critical behavior of the uniform model. This fixed point becomes fully unstable for [4,9]

$$\omega > 1 - \frac{D}{2-\alpha_u}, \tag{3}$$

where the critical exponent $\alpha_u$, associated with the specific heat of the underlying uniform model, depends on $q$, $m$ and $b$ (note that the transition is always continuous for the ferromagnetic Potts model on these hierarchical lattices [11]). Therefore, Eq. (3) is an (exact) alternative statement of Luck's original heuristic criterion of relevance of the geometric fluctuations. Irrelevancy of the fluctuations corresponds to accessibility of the non-trivial symmetric fixed-point, whatever the initial conditions. In the irrelevant cases, the critical behavior of the aperiodic systems remains unchanged with respect to the corresponding uniform models.

The problem now consists in the characterization of the new critical behavior under relevant geometrical fluctuations. Andrade [12] has recently used a mapping for the succession of partition functions of aperiodic Ising models ($q = 2$) on hierarchical lattices to investigate this question. For irrelevant geometric fluctuations, the critical behavior seems to remain unchanged with respect to the uniform system. Although the results are not conclusive, the critical behavior does seem to change for an Ising model on a diamond-type lattice with $m = b = 3$, and layered aperiodic exchange interactions according to the rule $(A, B) \to (ABB, AAA)$. To go beyond this work, we analyzed some families of aperiodic $q$-state Potts ferromagnets on diamond-like lattices to show that they do present a novel critical behavior (different from the uniform case, but universal) under relevant geometric fluctuations. This novel critical behavior can be exactly traced to new features in parameter space, exclusively related to the relevant geometric fluctuations.

Consider the Potts model on a lattice with $b = 2$ bonds per branch, and interactions according to the period-doubling rule. From Eq.(3), for $m = 2$, fluctuations are relevant if $q > 4 + 2\sqrt{2}$ (for $m = 3$, the threshold value of $q$ turns out to be somewhat lower, and so on). The recursion relations are given by

$$x'_A = \left(\frac{x_A x_B + q - 1}{x_A + x_B + q - 2}\right)^m, \tag{4a}$$

and

$$x'_B = \left(\frac{x_A^2 + q - 1}{2x_A + q - 2}\right)^m, \tag{4b}$$

where $x_{A,B} = \exp(q\beta J_{A,B})$, with $\beta = 1/k_B T$. Besides the uniform (diagonal) fixed-point, we have found a cycle of period two in the relevant regime (that is, the two-cycle is present when the non-trivial diagonal fixed point is fully unstable). Moreover, the two-cycle appears clearly as a bifurcation, its points running away from the symmetric fixed point as $q$ increases. In terms of the second iterate of the recursion relations (of which each point of the two-cycle is a fixed point), it displays a saddle-point character, with stable and unstable manifolds. Supposing that this two-cycle is associated with a novel critical behavior, we use standard scaling arguments to predict the critical exponent $\alpha$ of the specific heat. Let us call $x$ the single relevant variable describing the parameter space in the neighborhood of the two-cycle. In the thermodynamic limit, we write the reduced free energy per bond in the scaling form [13],

$$f(x) = g(x) + \frac{1}{b^{2D}} f(x''), \tag{5}$$

where $g(x)$ is a regular function related to the free energy of the decimated spins, $x''$ is a second iterate of the recursion relations, and $b$ is the linear rescaling factor of the renormalization-group transformation (which coincides, for diamond-like lattices, with the parameter $b$ of the basic diamonds [14]). Note the presence of the factor $b^{2D}$, related to the need of two iterations to go back to the neighborhood of the starting point in parameter space. Eq.(5) has the asymptotic solution

$$f(x) \simeq |x - x^*|^{2-\alpha} P\left(\frac{\ln|x - x^*|}{\ln \Lambda_{cic}}\right), \tag{6}$$

where $x^*$ is one of the points of the two-cycle, $\Lambda_{cic}$ is the largest eigenvalue of the linearization of the second iterate of the recursion relations about any one of the points of the cycle, $P(z)$ is an arbitrary function of period one, and the critical exponent $\alpha$, associated with the specific heat, is given by

$$\alpha = 2 - 2\frac{\ln b^D}{\ln \Lambda_{cic}} = 2 - 2\frac{\ln(mb)}{\ln \Lambda_{cic}}. \qquad (7)$$

The values of $\alpha$ predicted by Eq.(7) are unequivocally different from the values $\alpha_u$ for the specific heat exponent in the uniform cases, as can readily be seen in Table I, for the simple diamond lattice, $m = b = 2$, with layered exchange interactions according to the period-doubling sequence. As in the Monte Carlo simulations for the aperiodic 8-state Potts model on the square lattice [10], there is a clear weakening of the critical singularities due to the geometric fluctuations (a feature also present in disordered systems). Similar conclusions can be drawn for $b = 2$ diamond-type lattices with different values of $m$ and $q$, and the period-doubling substitution.

TABLE I. Results for the location of the two-cycle, eigenvalues of the second iterate of the recursion relations about the points of the two-cycle and the specific-heat critical exponent, $\alpha$, as predicted by Eq.(7), for some values of $q$, in the case of the $m = b = 2$ diamond with the period-doubling substitution. The value of the exponent in the uniform ($J_A = J_B$) case, $\alpha_u$, is also shown for comparison.

| | Location of the two-cycle | | Eigenvalues of 2nd iterate | | | |
|---|---|---|---|---|---|---|
| $q$ | $(x_A, x_B)_1$ | $(x_A, x_B)_2$ | $\Lambda_1$ | $\Lambda_2$ | $\alpha$ | $\alpha_u$ |
| 7 | (5.285...,7.642...) | (6.697...,4.750...) | 3.993... | 0.985... | -0.0022... | 0.010... |
| 25 | (6.942...,234.34...) | (39.023...,3.831...) | 4.243... | 0.343... | 0.0817... | 0.404... |
| 100 | (181.71...,5.721...) | (13.753...,5151.84...) | 4.975... | 0.074... | 0.2720... | 0.648... |

We performed the same analysis for the Potts model on the $b = 3$ generalized diamond lattice, with interactions according to the rule $(A, B) \to (ABB, AAA)$. Now, the recursion relations are given by

$$x'_A = \left( \frac{x_A x_B^2 + (q-1)x_A + 2(q-1)x_B + q(q-3) + 2}{x_B^2 + 2x_A x_B + (q-2)x_A + 2(q-2)x_B + q(q-3) + 3} \right)^m , \qquad (8a)$$

and

$$x'_B = \left( \frac{x_A^3 + 3(q-1)x_A + q(q-3) + 2}{3x_A^2 + 3(q-2)x_A + q(q-3) + 3} \right)^m . \qquad (8b)$$

For all values of $m$, the condition of relevance, given by Eq.(3), is satisfied for $q \geq 2$ (including the Ising model, $q = 2$). Again, besides the fully unstable fixed point, we have detected the presence of a two-cycle. The same sort of scaling analysis has been performed. Table II gives some results for $b = 3$ and $m = 2$. We see that the weakening of the critical singularities is again indicated by these data, the same trend being present for $m = 3$.

TABLE II. Same as Table I, for the lattice with $b = 3$ and $m = 2$, with the rule $(A, B) \to (ABB, AAA)$.

| | Location of the two-cycle | | Eigenvalues of 2nd iterate | | | |
|---|---|---|---|---|---|---|
| $q$ | $(x_A, x_B)_1$ | $(x_A, x_B)_2$ | $\Lambda_1$ | $\Lambda_2$ | $\alpha$ | $\alpha_u$ |
| 2 | (6.446...,135.10...) | (34.794...,5.224...) | 3.255... | 0.311... | -1.0358... | -0.902... |
| 7 | (11.469...,1649.66...) | (126.59...,8.525...) | 4.755... | 0.075... | -0.2981... | -0.185... |
| 100 | (57.223...,1121275.02...) | (3272.70...,34.683...) | 9.808... | 0.001... | 0.4304... | 0.898... |

The presence of these two-cycles seems to be associated with the alternance of two energy scales, given by $J_A$ and $J_B$. The iteration of the recursion relations leads to the alternative dominance of each one of them (as it can already be seen in the behavior of the fluctuations in the number of letters $A$ and $B$ along a substitution sequence). To check this argument, we performed some calculations for the ferromagnetic Potts model on a simple diamond lattice, $m = b = 2$, with aperiodic interactions according to the four-letter Rudin-Shapiro rule, $(A, B, C, D) \to (AC, DC, AB, DB)$, whose fluctuations are known to be relevant even in the Ising case [9]. Indeed, we have found a cycle of period four, along with fully unstable two-cycles, in regions of parameter space associated with the symmetries of the sequence.

To test the validity of the scaling arguments, and of

the role of the two-cycle as the responsible for the new critical behavior, we have performed a direct numerical analysis of the singularity of the free energy. In real-space renormalization-group calculations, it is well known that the (reduced) free energy can be expressed as an infinite series [15]. For the Potts model on the $b = 2$ diamond-type lattice, with the period-doubling rule, it takes the form

$$f(x_A, x_B) = \sum_{n=0}^{\infty} \frac{1}{(2m)^n} \left[ \frac{1}{3} \ln \left( x_A^{(n)} + x_B^{(n)} + q - 2 \right) + \frac{1}{6} \ln \left( 2x_A^{(n)} + q - 2 \right) \right], \quad (9)$$

where $x_{A,B}^{(n)}$ indicate the $n$-th iterates of the recursion relations, Eq.(4). If we assume uniform convergence, this series can be differentiated term-by-term, and then summed in a computer, to obtain the specific heat per bond. We also used direct numerical differentiation as a control of this assumption of uniform convergence. The critical temperature can be determined with high precision by making use of the existence of the trivial paramagnetic fixed point at $T = 0$, corresponding to $x_{A,B} = \infty$, which causes the apparent divergence of the series (9) if summed without the use of any regularization trick. Fixing the parameters $q$ and $m$, and also the strengths of $J_A$ and $J_B$, the critical temperature thus calculated in fact places $x_{A,B}$ in the attraction basin of the two-cycle. For irrelevant aperiodicity, as well as for the uniform model, this method yields a critical temperature that locates the system on the stable manifold of the uniform fixed point.

The singularity in the specific heat can be analyzed by a (non-linear) fitting of a function to the data over a somewhat arbitrary scaling region. For the uniform and irrelevant cases, we have always obtained very good fittings, in excellent agreement with the values of $\alpha_u$ predicted by the usual scaling theory around the uniform fixed point. As it should be anticipated, these fitted values did not present any detectable sensitivity on the values of $J_A$ and $J_B$. The particular problem of the Ising model ($q = 2$) on the simple $m = b = 2$ diamond lattice, with exchange interactions according to a period-doubling sequence, had already been studied by Andrade [12], with the same conclusions. In the relevant cases, the situation is much subtler, and demands a more refined analysis. For large values of $q$, in which cases the scaling analysis predicts positive values of $\alpha$ (although, of course, smaller than the corresponding values of $\alpha_u$), the fittings presented excellent agreement with the scaling predictions. For weaker singularities (mainly $\alpha$ negative), the fitted values were always somewhat bigger than the scaling predictions, with better agreement for increasing values of $q$. For $m = b = 2$, and the period-doubling sequence, let us give some results of the fittings of the specific heat data to a function of the form $A + B\,|t|^{-\alpha}$, where $t$ is the reduced temperature, and the parameters $A$ and $B$ must not be universal. For $q = 7$, we obtained $\alpha = -0.005(4)$, which should be compared with $\alpha = -0.0022\ldots$. For $q = 25$, we have $\alpha = 0.08(2)$, to be compared with the scaling value $\alpha = 0.0817\ldots$. For $q = 100$, we have $\alpha = 0.27(1)$, to be compared with $\alpha = 0.2720\ldots$. Even in the cases of disagreement with the scaling predictions, the fittings indicate no sensitivity on the particular values of $J_A$ and $J_B$, and thus characterize the universal nature of the critical behavior. For weak singularities, the discrepancies in the results cannot probably be explained in terms of lack of numerical precision, although it is in fact difficult to obtain a fully reliable fitting in these cases. This behavior can be probably traced to corrections to scaling that we are not considering in the direct application of the scaling ideas to the two-cycles. It should be pointed out that the free energy takes different values in each point of the two-cycle, in such a way that it may be ill-defined in terms of just a simple scaling field.

We have performed the same kind of numerical check for a lattice with $b = 3$, and with the aperiodic rule $(A, B) \to (ABB, AAA)$. Now, aperiodicity is already relevant for $q = 2$ (Ising model), and the two-cycle can be found for $q \geq 2$, and all values of $m$. The situation turns out to be exactly the same as before. The numerical value of the critical temperature indeed locates the system on the attraction basin of the two-cycle. The agreement between the numerical fittings and the scaling predictions for $\alpha$ improves as the critical singularity grows stronger, which happens with increasing values of $q$. In the special case $q = 2$, and $m = b = 3$, we and Andrade [12] have calculated similar values, $\alpha = -0.90(9)$, to be compared with the scaling prediction, $\alpha = -0.9684\ldots$.

From the numerical calculations, we have observed an oscillatory behavior in the specific heat as a function of temperature above $T_c$. The period of these oscillations is roughly given by Eq.(6), with better agreement for increasing values of $q$. These oscillations have also been found by Andrade [12], and are well known phenomena related to hierarchical structures [16].

In conclusion, we have given a number of examples of ferromagnetic Potts models on diamond-type hierarchical lattices to show that irrelevant geometric fluctuations do not change the (universal) critical behavior with respect to the uniform cases. On the other hand, for two-letter substitutional sequences, relevant geometric fluctuations give rise to a novel universal critical behavior associated with a two-cycle in parameter space.

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[1] A. B. Harris, J. Phys. C **7**, 1671 (1974).
[2] D. Schechtman, I. Blech, D. Gratias and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).
[3] J. M. Luck, Europhys. Lett. **24**, 359 (1993).
[4] A. C. N. de Magalhães, S. R. Salinas and C. Tsallis, J. Phys. A **31**, L567 (1998).
[5] Y. Achiam, T. C. Lubensky and E. W. Marshall, Phys. Rev. B **33**, 6460 (1986).
[6] J. M. Luck, J. Stat. Phys. **72**, 417 (1993); F. Iglói, L. Turban and F. Szalma, Phys. Rev. B **56**, 11031 (1997); J. Hermisson, U. Grimm and M. Baake, J. Phys. A **30**, 7315 (1997).
[7] C. A. Tracy, J. Phys. A **21**, L603 (1988); F. Iglói, J. Phys. A **21**, L911 (1988); L. Turban, P. E. Berche and B. Berche, J. Phys. A **27**, 6349 (1994).
[8] A. N. Berker and S. Ostlund, J. Phys. C **12**, 4961 (1979); R. B. Griffiths and M. Kaufman, Phys. Rev. B **26**, 5022 (1982).
[9] S. T. R. Pinho, T. A. S. Haddad and S. R. Salinas, Physica A **257**, 515 (1998).
[10] P. E. Berche, Ch. Chatelain and B. Berche, Phys. Rev. Lett. **80,** 297 (1998); Ch. Chatelain, P. E. Berche and B. Berche, Eur. Phys. J. B **7**, 439 (1999).
[11] B. Hu, Phys. Rev. Lett. **55**, 21 (1986).
[12] R. F. S. Andrade, Phys. Rev. E **59**, 150 (1999).
[13] B. Derrida, J. P. Eckmann and A. Erzan, J. Phys. A **16**, 893 (1983).
[14] J. R. Melrose, J. Phys. A **16**, 3077 (1983).
[15] M. Nauenberg, J. Phys. A **8**, 925 (1975).
[16] B. Derrida, C. Itzykson and J. M. Luck, Commun. Math. Phys. **94**, 115 (1984).