Phase transition mechanisms in the Potts model on a Bethe lattice

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We solve the Q-component spin model of R. B. Potts [Proc. Camb. Phil. Soc. **48**, 106 (1952)] in an external field exactly on a Bethe lattice. We examine the critical properties of both ferromagnetic and antiferromagnetic models. Finally, we show that phase transition mechanisms are related in both cases to the asymptotic behavior of a recurrent sequence.

1. INTRODUCTION

The Potts model is widely known as a good theoretical system for studying phase transitions.[1] Though fairly simple, it possesses many nontrivial features whose study has ensured considerable progress in understanding the critical behavior of real substances. In recent years extensive research has been done using the Potts model, but many questions remain unanswered.[2]

The critical properties of the model largely depend on the sign of the coupling constant J. The situation is quite clear in the ferromagnetic case ($J>0$): there is a second order phase-transition critical point (the Curie point), and typical ferromagnetic ordering with nonzero spontaneous magnetization at lower temperatures. The behavior of the antiferromagnetic model, however, is much more complicated. Here configurations with distinct spin values at neighboring sites are energetically favored, which leads to splitting of the initial lattice into two sublattices (antiferromagnetic ordering). Already in the model with $Q=3$ there is an infinity of such configurations, which means a finite residual entropy at $T=0$ and macroscopic degeneracy of the ground state.[3]

In this paper we give the exact solution for the Q-component spin model of Potts in an external field on a Bethe lattice for both ferromagnetic and antiferromagnetic interactions. As is known, solutions that use a Bethe lattice constitute an approximation for standard lattices[4] if the boundary effects are appropriately taken into account. The effectiveness of this approach has been demonstrated on several models of statistics mechanics.[5–9] The generalization of the Bethe lattice known as the Husimi tree has been successfully used in studying models with multisite interactions.[10] Another generalization of the given approximation for describing gauge models was formulated in Ref. 11.

The plan of this paper is as follows. Section 2 formulates the model and derives the recurrence relations. The critical properties of the ferromagnetic model are discussed in Sec. 3 and the antiferromagnetic model in Sec. 4. The Conclusion is devoted to a discussion of various features of our work.

2. DEFINITION OF THE MODEL AND THE RECURRENCE RELATION

The Q-component Potts model in an external field H is specified by the Hamiltonian

$$-\beta\mathscr{H}=J\sum_{\langle ij\rangle}\delta_{\sigma_i,\sigma_j}+H\sum_i\delta_{\sigma_i,1}, \tag{1}$$

where the spin variable is determined at the lattice sites and the values it takes on are $\sigma_i=1,\ldots,Q$, δ is the Kronecker delta, the first sum is over all lattice edges, and the second is over all lattice sites.

We define the partition function as the sum over all spin configurations:

$$Z=\sum_{\{\sigma\}}\exp\left(-\frac{\mathscr{H}}{kT}\right)$$

$$=\sum_{\{\sigma\}}\exp\left\{K\sum_{\langle ij\rangle}\delta_{\sigma_i,\sigma_j}+h\sum_i\delta_{\sigma_i,1}\right\}, \tag{2}$$

where we have introduced the notation

$$K=\frac{J}{kT},\quad h=\frac{H}{kT}.$$

The free energy per lattice site is obtained from the definition

$$f=-\frac{kT}{N}\ln Z. \tag{3}$$

The magnetization of a single site is defined as the mean value

$$m=\langle\delta_{\sigma_i,1}\rangle$$

$$=Z^{-1}N^{-1}\sum_{\{\sigma\}}\delta_{\sigma_i,1}\exp\left(-\frac{\mathscr{H}}{kT}\right). \tag{4}$$

It is related to the free energy by

$$m=-\frac{\partial f}{\partial H}. \tag{5}$$

A Bethe lattice (Fig. 1) is an infinitely branching tree whose sites (vertices) all have the same coordination number $\gamma+1$. It is convenient to think of this lattice as consisting of shells:[12] the zeroth shell is the central site, its nearest neighbors constitute the first shell, etc. At the same time, a Bethe lattice can be partitioned into $\gamma+1$ separate branches with only one common central site. Then on a lattice consisting of n shells, the partition function can be written as

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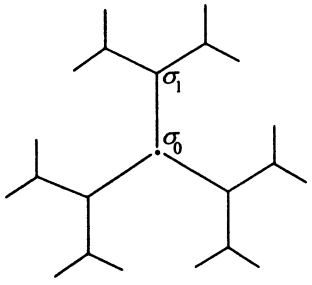

FIG. 1. A Bethe lattice with coordination number $\gamma+1=3$ and three shells.

$$Z=\sum_{\sigma_0} \exp(h\delta_{\sigma_0,1})[g_n(\sigma_0)]^{\gamma+1}, \tag{6}$$

where σ_0 is the spin of the central site, and $g_n(\sigma_0)$ is the contribution of each separate branch. The latter can be naturally expressed in terms of $g_{n-1}(\sigma_1)$, the contribution of the same branch that contains the $(n-1)$st shell and starting at a site belonging to the first shell:

$$g_n(\sigma_0)=\sum_{\sigma_1} \exp\{K\delta_{\sigma_i,\sigma_j}+h\delta_{\sigma_1,1}\}[g_{n-1}(\sigma_1)]^{\gamma}. \tag{7}$$

We assume that application of only one magnetic field "directed" along $\sigma=1$ does not break the symmetry between other spin values, $\sigma=2,...,Q$. This makes it possible to introduce the notation

$$x_n=\frac{g_n(\sigma\neq 1)}{g_n(\sigma=1)}. \tag{8}$$

Substituting g_n from Eq. (7) and summing over all values of σ_1 yields the recurrence relation for x_n:

$$x_n=\varphi(x_{n-1}), \quad \varphi(x,K,h)=\frac{e^h+(e^K+Q-2)x^{\gamma}}{e^{K+h}+(Q-1)x^{\gamma}}. \tag{9}$$

The quantity x_n has some intermediate nonphysical value. However, the thermodynamic parameters of the model can be expressed in terms of that value. For instance, if we allow for Eq. (4), we obtain an expression for the magnetization,

$$m_n=\frac{e^h}{e^h+(Q-1)x_n^{\gamma+1}}. \tag{10}$$

The free energy can be found by integrating Eq. (5). If the integration constant is determined appropriately, the result is

$$\frac{f}{kT}=\frac{K}{2}(\gamma+1)-h$$
$$-\frac{\gamma+1}{2}\ln[e^K+Q-2-(Q-1)e^{-K}]$$
$$+\frac{\gamma+1}{2}\ln[(Q-1)(e^Kx^2-2x)+e^K+Q-2]$$
$$+\ln\left(\frac{e^K+Q-2}{Q-1}-x\right). \tag{11}$$

Thus, x_n can be assumed to determine the system's state for given T and H, which means that the critical properties of the model depend on the behavior of the recurrent sequence $\{x_n\}$ as $n\to\infty$ (the thermodynamic limit). Below we will see that this behavior changes markedly as the coupling constant K is varied. Here we merely note that since by definition (7) the x_n are positive, the limit x^* of the recurrent sequence $\{x_n\}$ must obey the inequalities

$$e^{-K}<x^*<\frac{e^K+Q-2}{Q-1}$$

for the ferromagnetic model and

$$\frac{e^K+Q-2}{Q-1}<x^*<e^{-K}$$

for the antiferromagnetic.

3. CRITICAL PROPERTIES OF THE FERROMAGNETIC MODEL

In the ferromagnetic model ($K>0$) the iterated function $\varphi(x)$ increases for all values of H and T. Here the sequence $\{x_n\}$ converges to stable solutions ($\varphi'(x,K,h)<1$ is the stability condition) of the equation

$$\varphi(x,K,h)=x, \tag{12}$$

which can therefore be considered the equation of state. This equation can also be written as

$$h(x)=\gamma\ln x+\ln[e^K+Q-2-(Q-1)x]-\ln(e^Kx-1). \tag{13}$$

The solution of the equation of state (12) for different values of K and h and the shape of the function $h(x)$ at the same temperatures are depicted in Figs. 2–5 (note that each point in the figures represents a solution of the equation of state, and vice versa). The following typical cases can be identified:

1. At high temperatures ($T>T^*$), Eq. (12) has only one solution for all values of the magnetic field h (Fig. 2b). This solution is stable and determines the disordered phase of the system. Accordingly, the function $h(x)$ is a monotone decreasing one-to-one function (Fig. 2a). Critical behavior is absent in this range.

2. At low temperatures ($T<T^*$), there is a range of values of h within which Eq. (12) has more than one stable solution. Then $h(x)$ acquires a rising section (Fig. 3), and the following special cases can be identified:

2.1. When h is high ($h>h_{s1}$) or low ($h<h_{s2}$), Eq. (12) still has only one stable solution (Fig. 4a and e).

2.2. Two new solutions of Eq. (12), x_{s1} and x_{s2}, emerge at $h=h_{s1}$ and $h=h_{s2}$. Their characteristic feature is that $\varphi'_x(x_s,K,h_s)=1$ (Figs. 4b and d), and they correspond to extrema of $h(x)$. The solutions x_{s1} and x_{s2} are stable and physically correspond to the spinodal points of the model.

2.3. When $h_{s1}<h<h_{s2}$, Eq. (12) has three solutions (Fig. 4c). The middle solution is unstable and no physical state of the model corresponds to it. Such solutions wind up

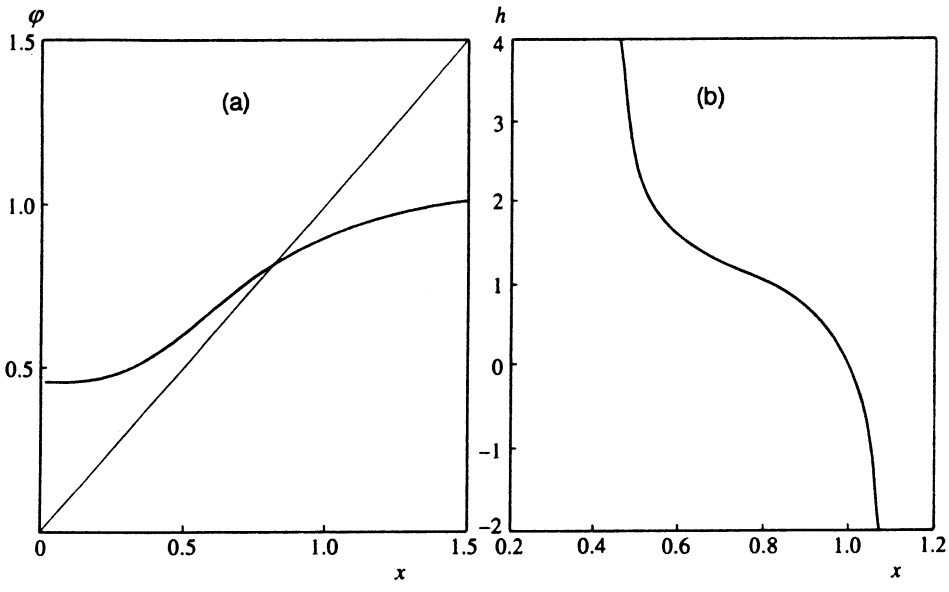

FIG. 2. The shape of the iterated function $\varphi(x)$ in the ferromagnetic case for $T>T^*$: (a) the intersection with the straight line $\varphi(x)=x$ gives the solution of Eq. (12), and (b) $h(x)$ at the same temperature $T>T^*$.

on the rising $h(x)$ section, and are of course forbidden by thermodynamic considerations. The remaining two solutions are stable, one describing the ordered phase of the system and the other the disordered. Thus, this is the region of phase coexistence, with the critical properties determined by a first order phase transition. The transition occurs at the point where the free energies of the two phases are equal:

$$f(x_{\rm I},K,h)=f(x_{\rm II},K,h). \tag{14}$$

3. At $T=T^*$ and a certain value of h^*, a second order phase transition occurs in the ferromagnetic model. The critical transition point is the endpoint of the first order phase-transition curve and the spinodal curves. At this point $\varphi'_x(x^*,K^*,h^*)=1$ (Fig. 5a), and this is the point of inflection of $h(x)$ (Fig. 5b).

On the basis of the foregoing we can now give the exact analytic expressions describing the critical properties of the model. For instance, the second order phase-transition critical point can be found from the conditions

$$\frac{\partial h}{\partial x}=0, \quad \frac{\partial^2 h}{\partial x^2}=0, \tag{15}$$

which lead to

$$K^*=\ln\left[2-Q+\frac{1}{\gamma-1}\sqrt{Q^2(\gamma+1)^2-4\gamma(Q-2)^2}\right]-\ln 2,$$

$$h^*=\ln(Q-1)+(\gamma+1)\times\ln\frac{2(\gamma+1)}{(2-Q)(\gamma+1)-\sqrt{Q^2(\gamma+1)^2-4\gamma(Q-2)^2}}, \tag{16}$$

$$x^*=\frac{\gamma+1}{\gamma}e^{K^*}.$$

The first order phase-transition curve, the coexistence curve, can be found by solving (14) simultaneously with the equation

$$h(x_{\rm I},K)=h(x_{\rm II},K). \tag{17}$$

The result is

$$K_{\rm cr}(h)=\ln(Q-2)-\ln[(Q-1)^{(\gamma-1)/(\gamma+1)}e^{2h/(\gamma+1)}-1]. \tag{18}$$

The spinodal curves $h(x_{s1},K)$ and $h(x_{s2},K)$ can be found by setting $dh/dx=0$, with x_{s1} and x_{s2} the two roots of the quadratic equation

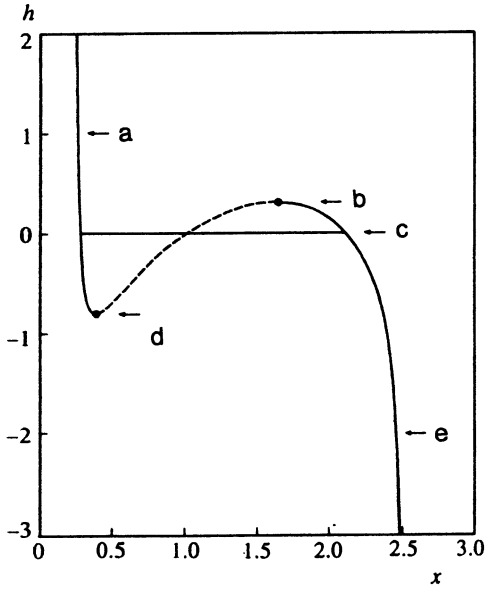

FIG. 3. $h(x)$ at some temperature $T<T^*$. The dot–dash curve corresponds to the unstable solutions of Eq. (12). Also shown are the spinodal points and first order phase transition. The arrows point to the values of h for which the diagrams of Fig. 4 have been constructed.

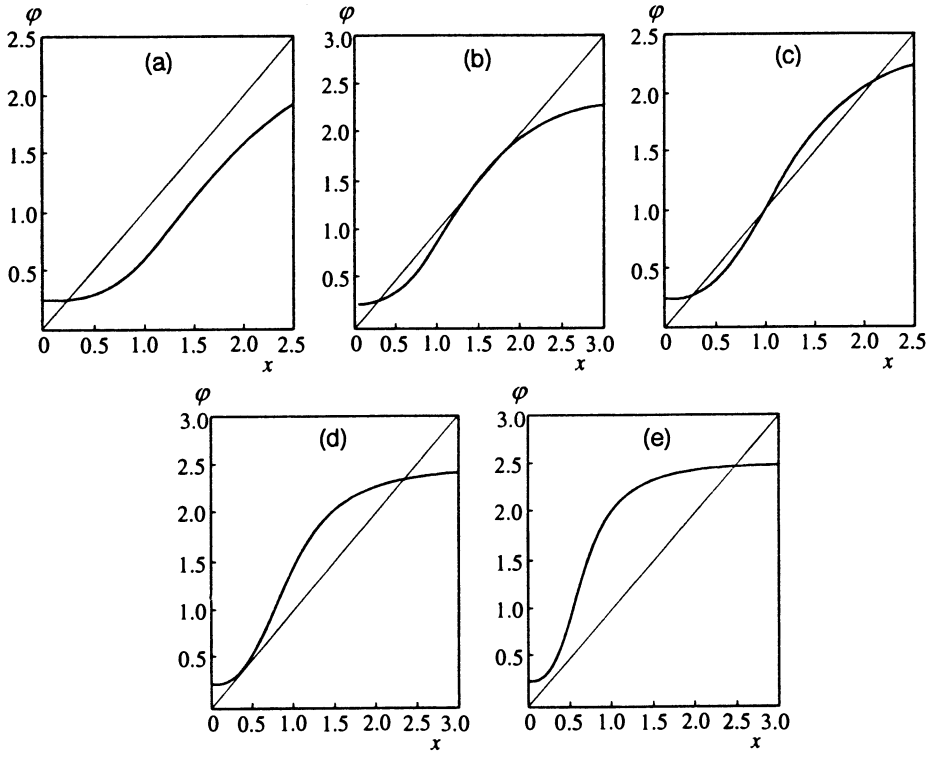

FIG. 4. The shape of the iterated function $\varphi(x)$ for values of h indicated in Fig. 3.

$$x^2-\left[\frac{\gamma+1}{\gamma}e^{-K}+\frac{\gamma-1}{\gamma}\frac{e^K+Q-2}{Q}\right]x-\frac{e^K+Q-2}{e^KQ}=0. \quad (19)$$

The above expressions simplify considerably in the Ising model ($Q=2$). All phase transitions, as expected, take place in zero magnetic field, and the critical point is determined by

$$K^*=\ln\frac{\gamma+1}{\gamma-1}. \quad (20)$$

If $Q\geqslant 3$, the second order phase-transition critical point lies in the region where $h>0$. In zero magnetic field, only a first order phase transition is possible. The two coexisting phases (disordered and ordered) are determined by two values of x,

$$x_{\rm dis}=1, \quad x_{\rm or}=\frac{1}{(Q-1)^{-2/(\gamma+1)}}, \quad (21)$$

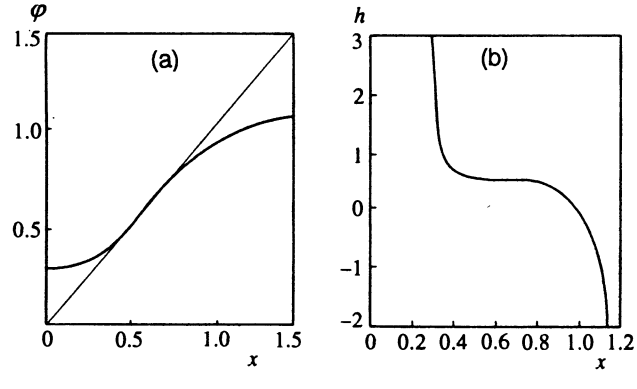

FIG. 5. Behavior of the functions a) $\varphi(x)$ and b) $h(x)$ at $T=T^*$.

i.e., by the magnetization values (10):

$$m_{\rm dis}=\frac{1}{Q}, \quad m_{\rm or}=\frac{Q-1}{Q}. \quad (22)$$

4. CRITICAL PROPERTIES OF THE ANTIFERROMAGNETIC MODEL

When the sign of K is reversed, the iterated function (7) transforms from an increasing to a decreasing function.[13] This means that Eq. (12) now has only one solution for all values of h and for $K<0$.

At high temperatures ($T>T^*$) this solution is stable and, as before, describes the disordered paramagnetic phase of the model. The stability condition in this case is

$$\varphi_x'(x,K,h)>-1,$$

which is violated, however, in the low-temperature range $T<T^*$. It is well known that $\varphi_x'(x,K,h)<-1$ at fixed points signifies the emergence of a so-called period-doubling bifurcation. The recurrent sequence $\{x_n\}$ converges not to a unique fixed point but to a stable 2-cycle $\{x_Ax_B\}$ (Fig. 6). (The first to notice the emergence of a 2-cycle in the antiferromagnetic Ising model on a Bethe lattice was Thompson.[14]) It is natural to identify the period doubling in the sequence $\{x_n\}$ with the emergence of a sublattice structure, with x_A and x_B describing the state of each sublattice.

Thus, Eq. (12) is no longer an equation of state. To examine the behavior of the model in this case one must consider subsequent iterations of the function $\varphi^n(x)=\varphi\{\varphi[\cdots\varphi(x)]\}$. Below we list some of the simple properties of the limit points of iterated maps:[15]

a) The fixed points of the first iterated function are fixed points of all subsequent functions:

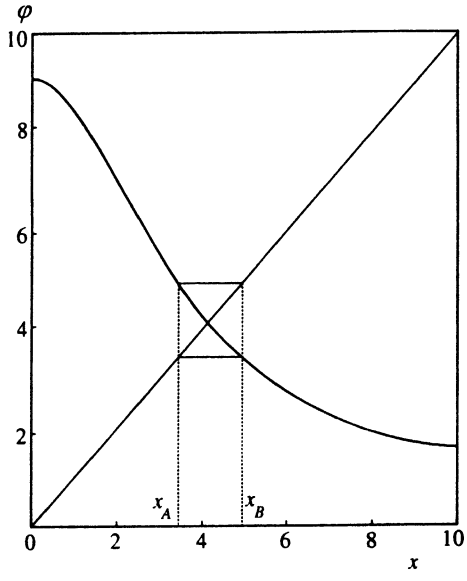

FIG. 6. Period doubling for the function $\varphi(x)$ in the antiferromagnetic case at $T<T^*$.

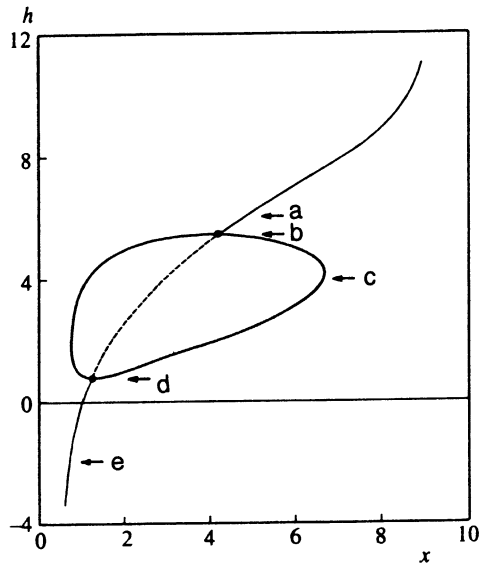

FIG. 7. $h(x)$ at temperature $T<T^*$ in the antiferromagnetic case. The dashed curve corresponds to the unstable solutions of Eq. (23). Also shown are second order phase-transition points. The arrows point to the values of h for which the diagrams of Fig. 8 have been constructed.

$$\varphi(x^*)=x^*\Rightarrow\varphi^n(x^*)=x^*.$$

b) If a fixed point of the first iterated function becomes unstable, it is unstable for all subsequent functions:

$$|\varphi(x^*)|>1\Rightarrow|\varphi^n(x^*)|>1.$$

c) The limit points x_A and x_B of a stable 2-cycle at the nth iteration are stable fixed points of the $(n+1)$st iteration:

$$\begin{cases}\varphi^n(x_A)=x_B,\\ \varphi^n(x_B)=x_A\end{cases}\Rightarrow\varphi^{n+1}(x_A)=x_A,\quad \varphi^{n+1}(x_B)=x_B.$$

There is only one period doubling in the given model; consequently, we can limit attention to the second iteration:

$$\varphi^2(x,K,h)=x. \tag{23}$$

The behavior of the function $\varphi^2(x)$ for $K<0$ somewhat resembles the behavior of $\varphi(x)$ for $K>0$.

When $T>T^*$, Eq. (23) has only one solution, coinciding with the solution of Eq. (12) and describing the paramagnetic phase. When $T<T^*$, there exists a range of h within which Eq. (23) has three solutions. The middle solution [which is also the solution of Eq. (12)] is unstable. The other two are stable and, as mentioned earlier, correspond to the limit points of the 2-cycle and describe the states on each sublattice.

The solutions of Eq. (23) at a fixed temperature $T<T^*$ and various values of h [these values are marked on the $h(x)$ diagram in Fig. 7 obtained from Eq. (23)] are depicted in Fig. 8. Three cases can be identified here:

a) When $h<h_{c1}(K)$ or $h>h_{c2}(K)$, the system is in the paramagnetic state.

b) When $h_{c1}<h<h_{c2}$, the system is in the ordered antiferromagnetic phase, characterized by the fact that sublattice symmetry is broken and the magnetization difference is nonvanishing:

$$m_s=m_A-m_B\neq 0,$$

where m_A and m_B are the magnetizations of separate sublattices defined by (4) as $m_{A,B}=m(x_{A,B})$.

c) For each temperature $T<T^*$ there are two points $h_{c1}(K)$ and $h_{c2}(K)$ at which the system goes from the paramagnetic phase to the antiferromagnetic. This transition is continuous, i.e., the system undergoes a second order phase transition. The points $h_{c1}(K)$ and $h_{c2}(K)$ correspond to period-doubling bifurcation points of the function $\varphi(x)$.

Below we list the analytic expressions corresponding to this picture. In the phase diagram of the model, the antiferromagnetic phase is separated from the paramagnetic by the second order phase-transition curve. The transition points can be defined as those at which the solutions of Eq. (12) and the new solutions appearing in Eq. (23) intersect. The result is the quadratic equation

$$x^2-\left[\frac{\gamma-1}{\gamma}e^{-K}+\frac{\gamma+1}{\gamma}\frac{e^K+Q-2}{Q}\right]x-\frac{e^K+Q-2}{e^KQ}=0, \tag{24}$$

from which the two branches $h_{c1}(K)$ and $h_{c2}(K)$ of the phase-transition curve are obtained by substituting the roots of this equation into the function (13). The two branches leave the h axis at the points $h_L(0)$ and $h_U(0)$,

$$\frac{h_U(0)}{J}=\begin{cases}-(\gamma+1) & \text{if } Q=2,\\ 0 & \text{if } Q>2,\end{cases}\qquad \frac{h_L(0)}{J}=\gamma+1, \tag{25}$$

and converge to the point h^* at the aforementioned temperature T^*. Thus, this temperature can be determined by requiring that the determinant of Eq. (24) vanish:

$$\frac{J}{kT^*}=\ln\left[\sqrt{(Q-2)^2-4(Q-1)\left(\frac{\gamma-1}{\gamma+1}\right)^2}-(Q-2)\right]-\ln 2, \tag{26}$$

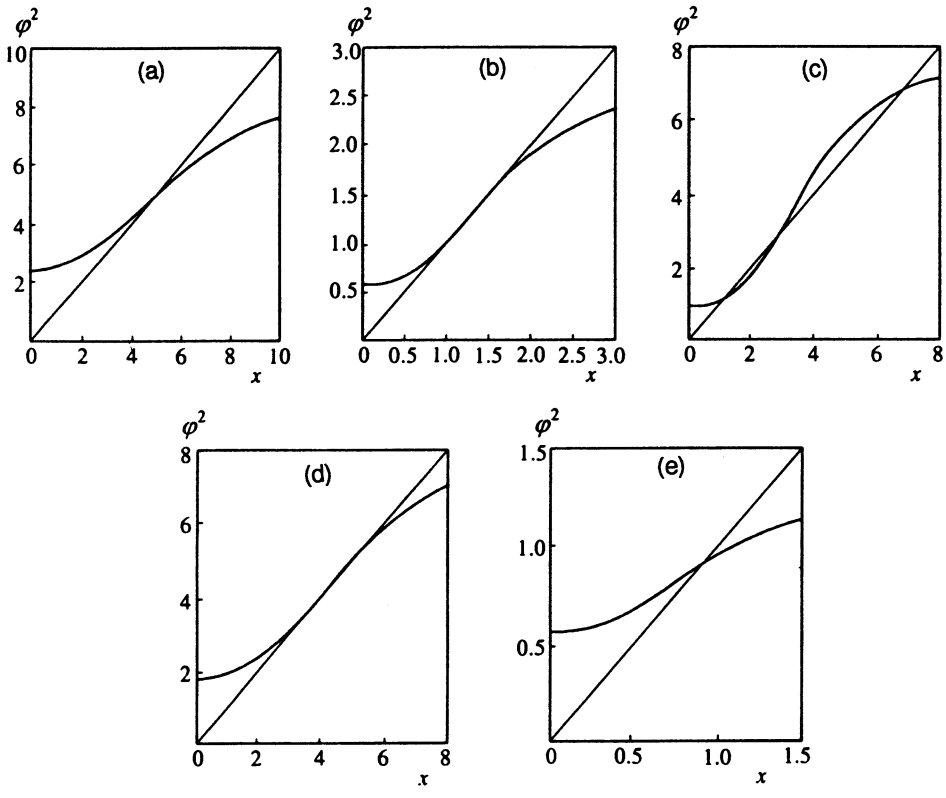

FIG. 8. The shape of the second iteration of the iterated function, $\varphi^2(x)$, at $T<T^*$ for values of h indicated in Fig. 7.

and this is the maximum temperature at which antiferromagnetic ordering is possible.

At $Q=2$ the phase diagram is symmetric about the T axis and, accordingly, $h^*=0$. When $Q\geqslant 3$, h^* shifts to positive values.

It is also interesting to examine the case of zero temperature. According to (25), in the Potts model with $Q\geqslant 3$, one branch of the critical curve starts at the point ($H=0$, $T=0$). This corresponds to the prevalent idea that in models with a macroscopically degenerate ground state in a vanishing external field, a phase transition can occur only at zero temperature. However, for $Q<\gamma+1$ the phase-transition curve crosses the T axis for the second time at the point

$$\frac{J}{kT_0}=\frac{\gamma-Q+1}{\gamma+1}. \tag{27}$$

Berker and Kadanoff[16] first suggested in 1980 that there may be a phase transition at nonzero temperature with an algebraic correlation function, but this problem is as yet unresolved.

5. CONCLUSION

The study of critical phenomena is one of the most important problems of modern physics. According to the universality hypothesis, this study can be carried out using the simplest possible models. One such model is the Potts model considered above. Unfortunately, even such models cannot be solved exactly. There are solutions of two-dimensional Ising models ($Q=2$) and Potts models at critical points, but there is not even one exact solution with dimension $d>2$ and in a nonvanishing external field. Basically, the existing approximate methods are either not accurate enough, as, e.g., the mean-field approximation, or are entirely devoid of analytic expressions (the Monte Carlo method).

From this standpoint, the Bethe lattice is a fortunate exception. Although the lattice is a topological abstraction nonexistent in nature, the exact solution of a model using this lattice is, as noted in the Introduction, an approximation for standard lattices corresponding to what is known as the Bethe–Peierls approximation. The accuracy of this approximation considerably exceeds that of the mean-field approximation.[11]

Here an indisputable advantage of the Bethe-lattice approximation is the presence of analytic expressions, which allows for a much better understanding of the qualitative behavior of the system. In particular, as we have seen, phase transition mechanisms in the Potts model on a Bethe lattice (and, hence, in a sense on standard lattices) can be linked in an extremely graphic manner to the behavior of the limit points of the recurrence relation. This is the object of study in the theory of nonlinear dynamical systems,[17] which suggests that there is a deep underlying link between these two branches of physics. It is interesting to study the caliber model based on the windows,[18] as an analogue for the Potts spin model.

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