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The Antiferromagnetic Three-state Potts Model on a Triangular Lattice

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We study the phase diagram of the three-state Potts model on a triangular lattice with antiferromagnetic interactions between nearest-neighbor spins. The cell-spin analysis for the isotropic model reveals that the symmetry of the ground states is dual to the symmetry of the $n=3$ cubic model which is known to exhibit a first-order phase transition. For the anisotropic model, the chirality appears between the ground states. Monte Carlo simulations show that a first-order line merges from the KDP point and separates completely an antiferromagnetic ordered phase and a disordered phase.

The ferromagnetic three-state Potts model has been studied extensively. In two dimensions, its critical properties are known exactly which are independent of underlying lattices.[1,2] When interactions become antiferromagnetic, the critical properties vary with the structure of underlying lattices. The symmetry of the antiferromagnetic ground states is constrained by the structure of the underlying lattice. For example, the antiferromagnetic three-state Potts model on a square lattice is disordered at all temperatures, but on a triangular lattice a first-order phase transition appears at a finite temperature. By adding ferromagnetic next-nearest-neighbor interactions, the antiferromagnetic three-state Potts model on a square lattice exhibits a sequence of two Kosterlitz-Thouless(KT) transitions.[3] This model possesses a ground-state symmetry similar to the ferromagnetic six-state clock model,[4,5] In this paper we examine the phase diagram of the antiferromagnetic three-state Potts model on a triangular lattice.

The Hamiltonian of this model, H, is given as

$$-H=\sum_{\langle i,j\rangle} K_l \delta_{\sigma_i \sigma_j}, \tag{1}$$

where $\langle\cdots\rangle$ denotes nearest neighbors and $K_l(l=1, 2, 3)$ is a coupling constant along each of three lattice-vector directions. They are all antiferromagnetic ($K_l<0$). σ is the Potts spin at site i which takes the values of 0, 1, 2 and δ is the Kronecker delta function.

This model had six equivalent ground states; three up-states U_i and three down-states $D_i(i=1, 2, 3)$. The unit cells of these ground states are shown in Fig. 1. We say that the up-states have a positive helicity and the down-states a negative helicity. At zero temperature, the system becomes a periodic array of one of these unit cells. As the temperature goes higher, the system becomes a mixture of these unit cells and the domain walls between different unit cells appear.

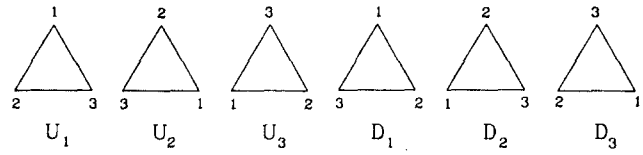

Fig. 1. Unit cells of the six ground states of the triangular-lattice model: U_i (up-state) has a positive helicity and D_i (down-state) a negative helicity.

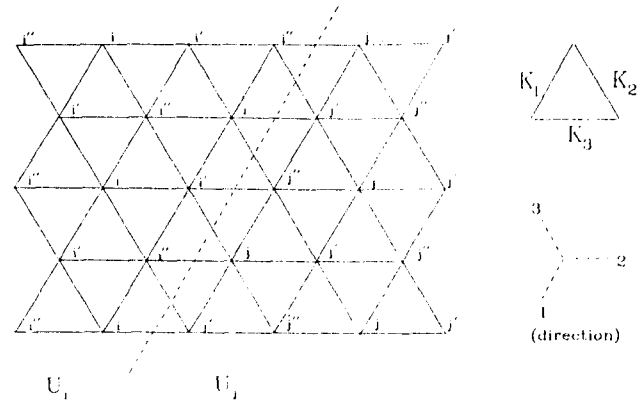

Fig. 2. The domain wall between U_i and U_j ground states in the direction 1. Here $i'=i+1$, $i''=i-1$, $j'=j+1$, $j''=i-1$.

The excitation energies per unit length for these domain walls, when they are straight and do not meander, depend on their directions and also on the chirality. Consider the domain wall between two up-states U_1 and U_2 in the direction 1 (Fig. 2.). When U_1 is left to the domain wall and U_2 is right to the domain wall, the excitation energy per unit length of this domain wall is $-K_3$. If the ground states are interchanged, the domain wall energy becomes $-K_2$. So when $K_2 \neq K_3$, there is a chirality in the domain wall energies. In general, one can find that the domain wall energy between two up-states U_i

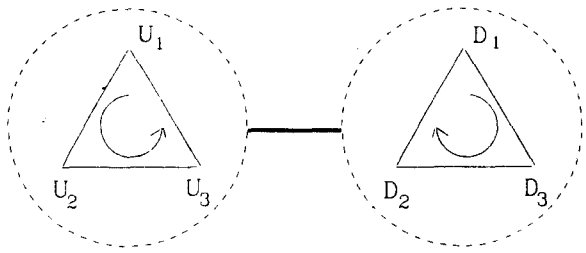

Fig. 3. Ground-state symmetry of the triangular-lattice model.

and U_j in the direction 1 is $E_1 = -K_2\delta_{i-1,j} - K_3\delta_{i+1,j}$. When $i=j-1(j+1)$, we call that the domain wall has a positive (negative) chirality. Similarly, the domain wall energies for the other directions can be obtained easily and the result is

$$E_i^{\pm}(UU) = -K_{i\mp 1}, \tag{2}$$

where the subscript i denotes the direction of the domain wall, the superscript $\pm$ the chirality, and UU in the parenthesis represents the domain wall energy between up-states. Repeating the same analysis on the domain walls between down-states and also between up- and down-states, we find

$$E_i^{\pm}(DD) = -K_{i\pm 1},$$
$$E_i^{\pm}(UD) = -\frac{1}{3}(K_{i+1}+K_{i-1}). \tag{3}$$

Notice that the domain wall energies between up- and down-states do not depend on the chirality.

The symmetry structure of the six ground states is drawn in Fig. 3. There is a ferromagnetic chiral (or helical) three-state Potts model symmetry[6] in each triangle. And these triangles are linked by the symmetry of a ferromagnetic nonchiral Ising model. when $K_1=K_2=K_3=K$ (isotropic case), the chirality disappears on the top and the bottom. Even though the number of ground states is the same as in the square-lattice model with antiferomagnetic nearest-neighbor interactions and ferromagnetic next-nearest-neighbor interactions, the symmetry between the ground states is complety different from each other.

For the isotropic model, there is no chirality. Assign two types of cell spins, t and s ($t=1, 2, 3$ and $s=1, 2$), for each unit cell. The $s=1$ state represents the up-states and the $s=2$ state the down-states. Each of three states inside the up- or down-states is represented by the spin t. Then the cell-spin Hamiltonian can be written as

$$-H = \sum_{\langle i,j\rangle}\left[-K\delta_{s_is_j}\delta_{t_it_j} + \frac{K}{3}\delta_{s_is_j} + \frac{2}{3}K\right], \tag{4}$$

which is exactly the same as the Hamiltonian of the so-called (q_s, q_t) model[7] with $q_s=2$ and $q_t=3$. For $q_t=2$ it is known as the cubic model.[8] Nature of phase transitions does not depend on the underlying lattice structure for ferromagnetic models like the above cell-spin model ($-K>0$). So we study the above model on a square lattice which has been investigated in details. The duality relation between the (q_s, q_t) model and the (q_4, q_s) model is known on a square lattice.[7] After dropping the constant term in Eq. (4), one can find the dual Hamiltonian

$$-H_D = \sum_{\langle i,j\rangle}[D\delta_{t_it_j}\delta_{s_is_j} + J\delta_{t_it_j}], \tag{5}$$

where

$$\exp(D) = 1 + \frac{6}{\exp(-2K/3)+2\exp(K/3)-3},$$
$$\exp(J) = 1 + \frac{3[\exp(K/3)-1]}{\exp(K/3)[\exp(-K)-1]}. \tag{6}$$

This is the $n=3$ cubic model Hamiltonian which is known to exhibit a first order phase transition for $J+D/2>0$ and continuous phase transition otherwise.[8] For our model, we can prove from eq. (6) that $D>0$ and $J+D/2>0$ for any value of K. Therefore the cell-spin analysis for the antiferromagnetic isotropic three-state Potts model on a triangular lattice shows that there must be a first-order transition rather than a continuous tranisition and the symmetry of the ground states is dual to the symmetry of the $n=3$ cubic model. The isotropic model has been studied previously by the real-space renormalization[9] and Monte Carlo simulations.[10] It has been shown to exhibit a strong first-order transition. Our result is consistent with the Monte Carlo results.

When the interactions are anisotropic, the chirality between the ground states appear. There has been some interests in the role of the chirality in the ordinary ferromagnetic Potts models.[6,11] Even though the chiral operator is relevant for the three-state Potts model, it does not introduce a new independent exponent, i.e. $\chi_{CH}=\chi_T+1$ where χ_{CH} and χ_T are the chiral and temperature scaling dimension respectively.[12] So it is believed that the scaling behavior does not change in the presence of the chirality for the three-state Potts model. This has been shown analytically for the hard hexagon model[13] and numerically for the chiral three-state Potts model[6] and the triangular Ising lattice gas.[14] The ground-state structure of our anisotropic model is much more complicated than that of the chiral three state models. It has two chiral three-state model symmetries linked by the Ising symmetry. So it may be interesting to find out what kind of role the chirality plays in this model. For simplicity, we study the phase diagram only when $K_1=K_2$.

When the interactions along two lattice-vector directions are infinitely strong ($u=\exp(K_1)=0$), this model can be mapped into a six-vertex model.[5] From the exact solution of the six-vertex model,[15] we find a first-order (KDP) transition from an ordered phase into a critical phase at $v=\exp(K_3)=1/2$. The stability analysis[3,5] shows that the critical phase does not persist for finite

Table 1. Numerical values of the coupling constant u_t, the order-parameter jump Δm_{AF}, and the energy-density jump Δe at the first-order transitions. Numbers in parentheses represent the errors in the last digits

	$u=v$	$u^2=v$	$u=v^2$	$u^3=v$
u_t	0.205(1)	0.263(2)	0.120(2)	0.278(3)
Δm_{AF}	0.70 (3)	0.81 (3)	0.78 (2)	0.88 (2)
Δe	0.17 (2)	0.20 (2)	0.21 (1)	0.24 (1)

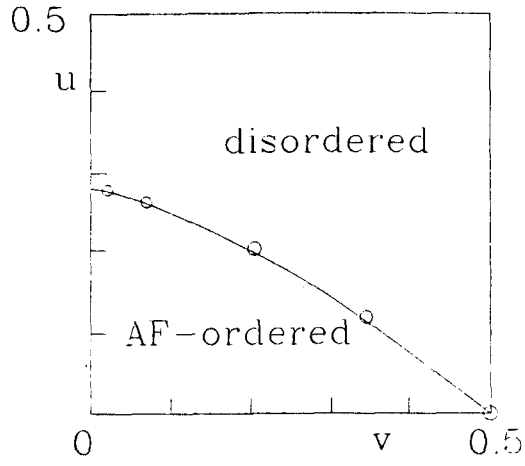

Fig. 4. Phase diagram of the antiferromagnetic three-state Potts model on a triangular lattice.

value of u.

When $u\neq 0$, we use Monte Carlo simulations to investigate the phase diagram. We run conventional heat-bath Monte Carlo simulations on a 60×60 triangular lattice along the $u=v$, $u^2=v$, $u=v^2$, and $u^3=v$ lines. Typically a few 10^4 Monte Carlo steps per spin (MCS) are performed for a given value of u and v. We measure the antiferromagnetic order parameter m_{AF}[10] and the energy density e. The order parameter m_{AF} is defined as

$$m_{AF}=\left[\frac{3}{2}\sum_{\alpha\neq\beta\neq\gamma}\left(\frac{N_\alpha^A+N_\beta^B+N_\gamma^C}{N_t}-\frac{1}{3}\right)^2\right]^{\frac{1}{2}}, \tag{7}$$

where N_α^X is the number of spins of state α in the sublattice X and N_t is the total number of spins. Unfortunately, along all four lines, we find a very strong first-order phase transition from an antiferromagnetically ordered phase into a disordered phase. In Tabel I, we list the values of the coupling constant u at the first-order transitions and the jump of the order parameter and the energy density. The five first-order transition points (including the KDP point) can be connected by a smooth line which apparently starts from the KDP point $(u, v)=(0, 1/2)$ and ends at the point (0.28, 0) (Fig. 4). As the anisotropy increases, the magnitude of the order-parameter jump becomes bigger. Our results imply that the strong first-order transition due to the cubic nature of this model preempts all possible continuous transitions in the whole antiferromagnetic region.

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