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LETTER TO THE EDITOR

Monte Carlo study of the three-state square Potts antiferromagnet

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Abstract. The role of a new type of vortices introduced in the three-state square Potts antiferromagnet for decay of correlations is considered. Fluctuations of the vortex charge in a region are measured using the Monte Carlo method. Data suggest an exponential decay of correlations. At zero temperature, an equivalent surface model is considered. A Monte Carlo experiment indicates roughening, thus suggesting an algebraical decay of the zero temperature Potts antiferromagnet.

The three-state Potts antiferromagnet on a square lattice is defined by the Hamiltonian

$$H = \sum_{\langle ij \rangle} \delta(\sigma_i, \sigma_j)$$

where the sum is over nearest neighbours on a lattice Λ, $\sigma_i = 1, 2, 3$ for $i \in \Lambda$ and δ is the Kronecker delta.

Grest and Banavar (1981) in their Monte Carlo (MC) study a detected rapid change of a global ordering parameter—'sublattice magnetisation'—near $T = 0.4$ which could suggest long-range order below this temperature. However, it was not clear whether this phenomenon is an effect of finite lattice size.

Fucito (1983) studied the influence of boundary conditions on the inside magnetisation. Though the same ordering occurs, the behaviour of the susceptibility (fluctuation of magnetisation) indicates that this is due to an excess of correlation length over lattice volume.

The MC renormalisation group analysis (Jayaprakash and Tobochnik 1982) leads to a conclusion that there is no critical point at $T > 0$.

Recent theoretical considerations (Nijs *et al*, 1982, Nightingale and Schick 1982) also imply that the model exhibits phase transition only at $T = 0$.

The model at zero temperature possesses non-vanishing residual entropy which may be rigorously calculated (Lieb 1967a, b). The entropy per lattice site turns to equal $\frac{3}{2} \ln \frac{4}{3}$. Moreover, the fact that zero temperature is a critical point of the model may be shown by considering it as a special case of a three-colour model (Baxter 1970) or an extension to continuous q (Baxter 1982) within their respective critical regions. The existence of unique phase at zero temperature is also indicated using a correspondence that allows us to interpret entropical restrictions on configurations in terms of energetical excitations of a corresponding ferromagnetic model at a non-zero temperature (Kotecký 1984).

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The model at non-zero temperature may be studied in analogy with the square XY model (plane rotator). Namely, a certain type of topological excitations—vortices—play an important role in the behaviour of this model. They were introduced by Nijs *et al* (1982) using the equivalent 27-vertex model. Their description in terms of Potts model configurations amounts to the assignment of topological charge to each excitation (a pair of nearest neighbours occupied by the same spin value). An isolated excitation may have positive, negative or vanishing charge (figure 1(a)–(c)). There are also configurations of a spin wave type (figure 1(d)).

To clarify the nature of vortices and spin waves let us define three types of contours, as shown in figure 1. They may intersect only in vortex type excitation; plus and minus vortices are distinguished by the order of contours around them. The chargeless excitation only disconnects a contour.

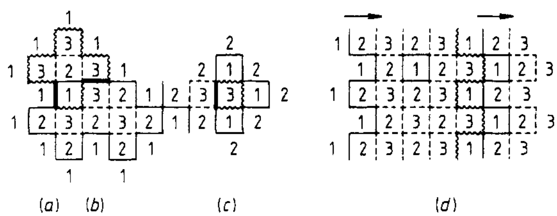

Figure 1. (a) + vortex, (b) – vortex, (c) chargeless excitation, (d) spin wave. Full, broken and wavy lines denote (1/2), (2/3) and (3/1) borders.

To be more precise we define the charge enclosed in an anticlockwise oriented loop $\gamma \subset \Lambda$ not intersecting any excited bond by

$$\tfrac{1}{6} \sum_{i \in \gamma} m(\sigma_{i+1} - \sigma_i) \tag{1}$$

where $|m(k)| = 1$ and $m(k) \equiv k \pmod 3$. It can be easily shown that this charge is an integer.

In the MC experiment we first studied the interaction of vortices with spin waves imposed on the lattice by appropriate boundary conditions in the limit of zero temperature. During the MC procedure vortices move in the direction perpendicular to the spin wave, i.e. in the direction of the 'contour flux'. Vortices of opposite charges move in opposite directions. Since any vortex is a source of flux, a pair of vortices will interact and it turned out that opposite charges attract each other. Recalling the contour description we can see that opposite vortices are connected by contours making rigid the non-zero entropy vacuum between vortices. The attraction can be explained as a tendency to shorten these contours.

Then a striking similarity with the XY model or Coulomb gas appears. These two models are proved to exhibit the Kosterlitz–Thouless transition at a finite non-zero temperature T_c (Fröhlich and Spencer 1981): below T_c vortices or particles condense to dipoles (or multipoles) and power decay of correlations takes place, while above T_c the Debye screening of charge density leads to an exponential decay. While in the rotator or Coulomb gas the probability of long dipole configuration decreases rapidly at low temperatures, in the Potts model the interaction is not expected to depend strongly on temperature; only bare activity of vortices will decrease like $\exp(-\beta)$.

An experiment which distinguishes whether vortices condense to dipoles or not, may be the following one, inspired by the ideas of the renormalisation group Consider some finite region A included in an infinite lattice. Denote by $\delta Q(A)=\langle Q(A)^2\rangle^{1/2}$ the fluctuation of charge enclosed in A. In the dipole phase only dipoles intersecting boundary ∂A contribute to $\delta Q(A)$ and thus $\delta Q(A)\sim|\partial A|^{1/2}$ for $A\to\infty$. In the exponential decay phase vortices are separated and an additional term of order $>|\partial A|^{1/2}$ will contribute to $\delta Q(A)$.

In our experiment a lattice $\Lambda=L\times L$ with the periodic boundary condition has been divided into square blocks $a\times a$, for several a, and the fluctuation has been measured over all blocks during the MC procedure. (Actually the lattice has been divided into blocks in two ways differing by an $a/2$-shift in both directions.) The charge of the cluster of excitations has been measured using (1) along the smallest loop surrounding the cluster and a barycentre has been considered to be the charge source. The charge in a block was simply the sum of these point-like charges.

Results (figure 2) show that vortices do not condense to short dipoles at any temperature. A probable explanation of the data is that vortices do not condense at all and charges screen. Then the contour flux connecting the vortices penetrates thickly all the volume disconnecting chargeless regions and causes exponential decay of spin–spin correlations.

We should note that if we renormalise at any temperature the a-axis by a factor 2 and the $\delta Q(a^2)$-axis by an appropriate factor depending on the vortex activity, we obtain a picture similar to the original one at a higher temperature. It is in agreement with the conclusions of Jayaprakash and Tobochnik (1982).

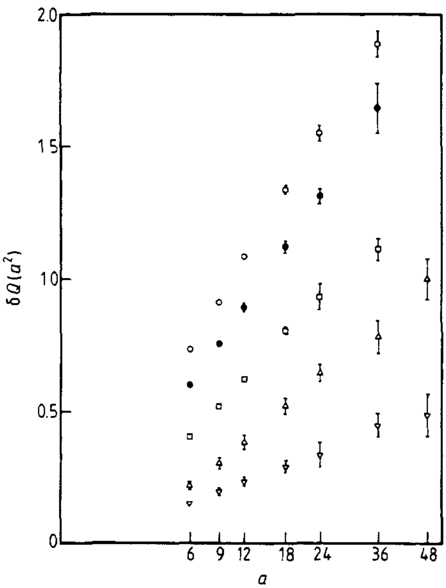

Figure 2. Charge fluctuation $\delta Q(a^2)$ in square blocks $a\times a$ on a lattice 72×72 (○, $T=0.6$; ●, $T=0.5$; □, $T=0.4$) and on a lattice 144×144 (△, $T=0.3$ hot start; ▽, $T=0.3$ cold start). The a axis has a square root scale.

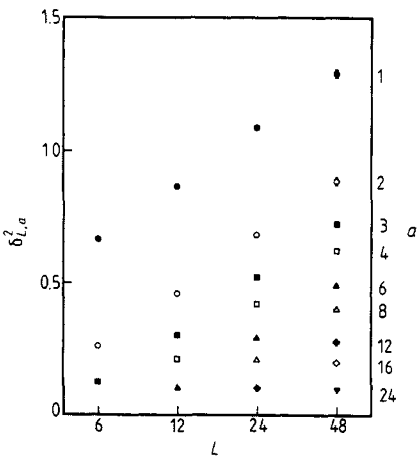

Figure 3. Height fluctuation $\delta^2_{L,a}$ in the Potts-surface model for block size a and lattice size L. For the definition of $\delta_{L,a}$ see (3) and (4).

Turning to the zero temperature, an absence of excitations implies that all the sums (1) are zero, hence (modulo an additive constant) integers s_i exist so that $s_i \equiv \sigma_i \pmod 3$ and $|s_i - s_j| = 1$ for $|i-j| = 1$. Viewing the variables s_i as the height of a surface above zero level, we can see the similarity to the solid-on-solid model or the discrete Gaussian model in two dimensions at a fixed temperature. Both models are known to exhibit a roughening transition at a finite non-zero temperature T_r (Fröhlich and Spencer 1981, Fröhlich *et al* 1982), which means that the expectation

$$\langle (s_i - s_j)^2 \rangle \sim \log |i-j| \tag{2}$$

for $T > T_r$ and

$$\langle (s_i - s_j)^2 \rangle \sim 1$$

for $T < T_r$ if $|i-j| \to \infty$. The surface is plane below T_r and logarithmically rough above T_r. It also has been suggested (Fröhlich and Spencer 1981, Gawędzki and Kupiainen 1982) that the surface in rough region in the continuous limit is described by zero mass Gaussian measure.

To decide which behaviour takes place at our Potts-surface model we measured fluctuation of surface height above mean level on a lattice $\Lambda = L \times L$ with periodic boundary conditions, i.e. values

$$\delta^2_{L,1} = \left\langle \frac{1}{|\Lambda|} \sum_{i \in \Lambda} (s_i - s)^2 \right\rangle_{\mathrm{MC}} \tag{3}$$

where

$$s = \frac{1}{|\Lambda|} \sum_{i \in \Lambda} s_i$$

and, similarly to non-zero temperature simulation, fluctuations of levels averaged in blocks $a \times a$ into which the whole lattice has been divided:

$$\delta^2_{L,a} = \left\langle \frac{a^2}{|\Lambda|} \sum_{I \in \Lambda/(a \times a)} (s_{I,a} - s)^2 \right\rangle_{\mathrm{MC}} \tag{4}$$

where

$$s_{I,a} = \frac{1}{a^2} \sum_{i \in a \times a + I} s_i$$

and shifted blocks have been included.

Data (figure 3) clearly follow (2) and we may conclude that roughening occurs in this Potts-surface model. In addition, if distribution of $s_i - s_j$ for $|i-j| \to \infty$ is discrete Gaussian, the expectation $\langle \delta(\sigma_i, \sigma_j) \rangle - \frac{1}{3}$ of the original Potts model has power law of $|i-j|$.

For the MC simulation we used the method of the heat bath. In one MC step the four spins in a square 2×2 were changed simultaneously with probability proportional to the Boltzmann factor (Creutz *et al* 1979, Obdržálek 1981). Then in one MC cycle each site on a lattice is visited four times. We performed from 212 ($T = 0.3$, $L = 144$ each start) to 2500 ($T = 0$, $L = 48$) cycles for each temperature and each different lattice.

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