Evidence for a first-order transition in a plaquette three-dimensional Ising-like action

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Abstract. We investigate a three-dimensional Ising action which corresponds to a class of models defined by Savvidy and Wegner, originally intended as discrete versions of string theories on cubic lattices. These models have vanishing bare surface tension and the couplings are tuned in such a way that the action depends only on the angles of the discrete surface, i.e. on the way the surface is embedded in $\mathbb{Z}^3$. Hence the name gonihedric by which they are known. We show that the model displays a rather clear first-order phase transition in the limit where self-avoidance is neglected and the action becomes a plaquette one. This transition persists for small values of the self avoidance coupling, but it turns to second-order when this latter parameter is further increased. These results exclude the use of this type of action as models of gonihedric random surfaces, at least in the limit where self avoidance is neglected.

In three dimensions the Ising model can be thought of as describing volumes of negative spins in a sea of positive ones, or vice versa. It is well known that the familiar Ising action weights such configurations according to the number of 'broken' links, i.e. with an action which is approximately proportional to the area of such volumes. Apart from entropy effects, the energy of a given configuration depends only on the surface, thus leading to a non-zero bare surface tension, but it is independent of the 'form' of the surface, i.e. of the precise way the surface is embedded in the lattice. A rough surface weighs exactly the same as a smooth one as long as the area is the same.

Is it possible to define an Ising-like action where precisely the opposite situation takes place? That is, is it possible to assign weights to an Ising action in such a way that smooth surfaces are preferred? The extreme case of such a situation would be one where the bare surface tension would be zero and, if at all, a renormalized surface tension would be generated by fluctuations¶.

Savvidy *et al* [3] recently answered the above question in the positive. They started by suggesting a a novel discretized random surface theory, the so-called gonihedric string, whose action is

$$S = \tfrac{1}{2} \sum_{\langle ij \rangle} |\boldsymbol{X}_i - \boldsymbol{X}_j| \theta(\alpha_{ij}) \qquad (1)$$

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¶ It should be noted that *higher-spin* models that display very low interfacial tension have been investigated by Schick and collaborators [1]. Such models are of interest for describing wetting phenomena [2].

where the sum is over the edges of some triangulated surface, $\theta(\alpha_{ij}) = |\pi - \alpha_{ij}|^\zeta$, ζ is some exponent, and α_{ij} is the dihedral angle between neighbouring triangles with common link $\langle ij \rangle$. This definition of the action was inspired by the geometrical notion of the linear size of a surface, originally defined by Steiner. Some difficulties with the model for $\zeta = 1$ were already pointed out in [4]. Possible ways to cure these difficulties are to add additional Gaussian terms [5] or simply to choose $\zeta < 1$, for which the model is believed to be satisfactory, but perhaps lacking a direct geometrical interpretation. Lattice models of random surfaces are prone to these types of difficulties and one may wonder to what extent these are caused by the discretization. Notice that in equation (1) it is the surface itself that is discretized, rather than the space in which it is embedded.

The next step consists in discretizing the embedding space itself by restricting the allowed surfaces to be the plaquettes of a cubic lattice (if we stay in three dimensions, as we will hereafter). Savvidy and Wegner [6–9] rewrote the resulting theory as a generalized Ising model by using the geometrical spin cluster boundaries to define the surfaces. This will be the model object of our interest here.

Savvidy and Wegner take the energy of a surface on a cubic lattice to be given by $E = n_2 + 4\kappa n_4$, where n_2 is the number of links where two plaquettes meet at a right angle and n_4 is the number of links where four plaquettes meet at right angles. Thus, flat surfaces are energetically favoured. κ is a free parameter which determines the relative weight of a self-intersection of the surface. In the limit $\kappa \to \infty$ the surfaces would be strongly self-avoiding, whereas the opposite limit $\kappa \to 0$ would be that of phantom surfaces that could pass through themselves without hindrance. Naively this model would seem to correspond precisely to $\zeta = 1$. The contribution of the different configurations in this model should be contrasted with the familiar three-dimensional Ising model with nearest-neighbour interactions where the surfaces contribute to the partition function according to their areas. Here we have no area term at all.

On a cubic lattice the generalized gonihedric Ising Hamiltonian which reproduces the desired energy $E = n_2 + 4\kappa n_4$ contains nearest-neighbour ($\langle i, j \rangle$), next to nearest-neighbour ($\langle\langle i, j \rangle\rangle$) and round a plaquette ($[i, j, k, l]$) terms

$$H = 2\kappa \sum_{\langle ij \rangle} \sigma_i \sigma_j - \frac{\kappa}{2} \sum_{\langle\langle i, j \rangle\rangle} \sigma_i \sigma_j + \frac{1-\kappa}{2} \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l. \tag{2}$$

Such generalized Ising actions have quite complicated phase structures for generic choices of the couplings [10–12]. The particular ratio of couplings in equation (2), however, is non-generic. In fact actions such as equation (2) have a symmetry which is not present for generic couplings—it is possible to flip any plane of spins at zero energy cost. The phase diagram displays only a single transition to a low temperature layered state that, as a consequence of the flip symmetry, is equivalent to a ferromagnetic ground state. This low temperature phase is strongly reminiscent of the floating incommensurate phase of the two-dimensional ANNNI model [12]. Simulations of the model at $\kappa = 1$ [7, 13] suggest, rather remarkably given that the model is defined in *three dimensions*, that the critical exponents and even the critical temperature are close to the Onsager values of the *two-dimensional* Ising model with nearest-neighbour interactions. In addition, the simulations of [13] indicated that this picture still held for $\kappa > 1$.

The nature of the transition for $\kappa < 1$ was rather less clear. A zero temperature analysis [13] shows that there is an increased symmetry in the ground state when $\kappa = 0$, which is already apparent from the Hamiltonian itself. In effect, for $\kappa = 0$ it is now possible to flip spins independently on the two interpenetrating sub-lattices of the cubic lattice, in addition to the plane-flip symmetry that is present for any κ.

Although not a local gauge symmetry, the flip symmetry of the model is intermediate between this and a global symmetry. This symmetry poses something of a problem when carrying out simulations, as it means that a simple ferromagnetic order parameter

$$M = \left\langle \frac{1}{L^3} \sum_i \sigma_i \right\rangle \tag{3}$$

will be zero in general, because of the layered nature of the ground state. Even staggered magnetizations would not do as the interlayer spacing can be arbitrary. On a finite lattice it is possible, however, to force the model into the ferromagnetic ground state, which is equivalent to any of the layered ground states, with a suitable choice of boundary conditions.

We have used a variety of boundary conditions to do the job. We have, for instance, used fixed boundary conditions which penalize any flipped spin planes by a boundary term. We have also considered mixed boundary conditions in which half the boundary of the box is set to a prescribed value and the other half to the opposite one. (This technique allows us to measure the renormalized surface tension, but these results merit a separate analysis [14].) Another possibility is to fix internal planes of spins in the lattice, whilst retaining the periodic boundary conditions. This has the desired effect of picking out the ferromagnetic ground state, whilst minimizing any finite size effects. With either fixed spin planes or boundaries we can therefore still employ the simple order parameter of equation (3).

For $\kappa = 0$ the Hamiltonian we simulate is thus

$$H = \tfrac{1}{2} \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l. \tag{4}$$

In a sense, this Hamiltonian represents the opposite limit to the $\kappa = 1$ case, where no plaquette term is present. In this case the nearest-neighbour and next to nearest-neighbour terms are absent. We emphasize that the spins live on the *vertices* of the cubic lattice rather than the links, so the model of equation (4) is not the three-dimensional Z_2 gauge model that is dual to the three-dimensional Ising model.

We shall now describe our simulations and the results for $\kappa = 0$ and then discuss to what extent these survive when we go to $\kappa \neq 0$. For $\kappa = 0$ we carried out the bulk of the simulations on lattices of size $L = 10^3, 12^3, 15^3, 18^3$ and 20^3 we also carried out further simulations for $L = 22^3, 25^3$. Periodic boundary conditions were imposed in the three directions and three internal perpendicular planes of spins fixed to be $+1$. The updated algorithm used was a simple Metropolis update and we carried out 4×10^4 thermalization sweeps followed by 10^5 measurement sweeps at each β value simulated. We measured the usual thermodynamic quantities for the model: the energy E, specific heat C, (standard) magnetization M, susceptibility χ and various cumulants. The zero temperature analysis shows that the large β limit of the energy is $-\frac{3}{2}$ which gives a useful check on the veracity of the results. A glance at figure 1 shows that this limit is approached satisfactorily and that there is a strong signal for a discontinuity in the energy, and hence a first-order transition, with increasing lattice size at $\beta_c \simeq 0.505$. The emergence of a discontinuity in the energy is reflected in the measurements of the specific heat which scales linearly with the volume.

Relying directly on the energy, or even properties like hysteresis, to divine the order of a transition is a rather perilous business but one usually reliable indicator is the scaling of Binder's energy cumulant

$$U_E = 1 - \frac{\langle E^4 \rangle}{3 \langle E^2 \rangle^2} \tag{5}$$

which scales to $\frac{2}{3}$ at a continuous transition and a non-trivial value ($< \frac{2}{3}$) at a first-order transition. In figure 2 we show the minimum values of U_E (which occur very close to
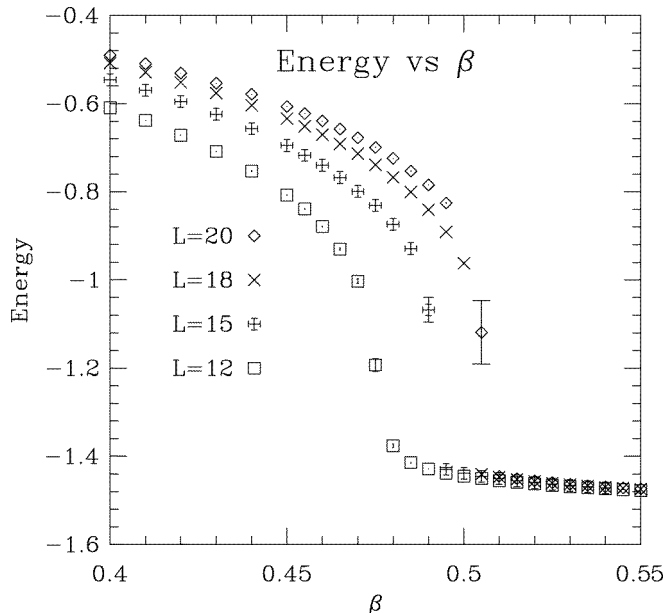
Figure 1. The energy for various lattice sizes at $\kappa = 0$.

the observed transition point) at $\kappa = 0$ for various lattice sizes. Although the error bars for the various lattice sizes are large due to both fluctuations close to the transition points and uncertainty in determining the real minimum values, there are clear indications of a non-trivial scaling (a second-order transition would be expected to approach the horizontal $U_E = \frac{2}{3}$ line smoothly with increasing lattice size). We also plot the values of U_E for $\kappa = 0.1, 0.5$ on smaller lattices, but with better statistics, discussed below.

It is not only the energy which displays a discontinuity at $\beta \simeq 0.505$. There is a very sharp change in the magnetization in this region too, as illustrated in figure 3. This is another generic feature of first order transitions and is also reflected in the very large peak that appears in the susceptibility χ with increasing lattice size which also displays trivial first-order scaling.

Let us now turn to $\kappa \neq 0$. The Hamiltonian of equation (2) was shown in [13] to display a second-order transition for $\kappa \geqslant 1$, so it is of some interest to determine the nature of the crossover to the first-order behaviour. Our simulations at $\kappa = 0.1$ were carried out on lattices up to 18^3, using both fixed and mixed boundary conditions in order to facilitate string tension measurements. They show that β_c is greater than the $\kappa \geqslant 1$ value of 0.44, but smaller than the one of $\kappa = 0$, and that the discontinuity in the energy is already quite marked. The minimum values of U_E (figure 2) provide evidence for a first-order transition at $\kappa = 0.1$. The difference with the asymptotic value expected for a second-order transition ($\frac{2}{3}$) is now much smaller than for $\kappa = 0$, but the smaller error bars due to the increased statistics (10^6 sweeps per β-value) make the evidence for scaling to a non-trivial value of equivalent statistical significance. Furthermore it is clear from figure 4 that the peak in the specific heat is scaling linearly with the volume for both sets of boundary conditions, as would be expected at a first-order transition. As for $\kappa = 0.5$ earlier simulations reported briefly in [13] suggested a second-order transition at $\beta_c = 0.44$, albeit with a slightly larger specific heat peak than at $\kappa = 1$. We have now performed further simulations at $\kappa = 0.5$ confirming
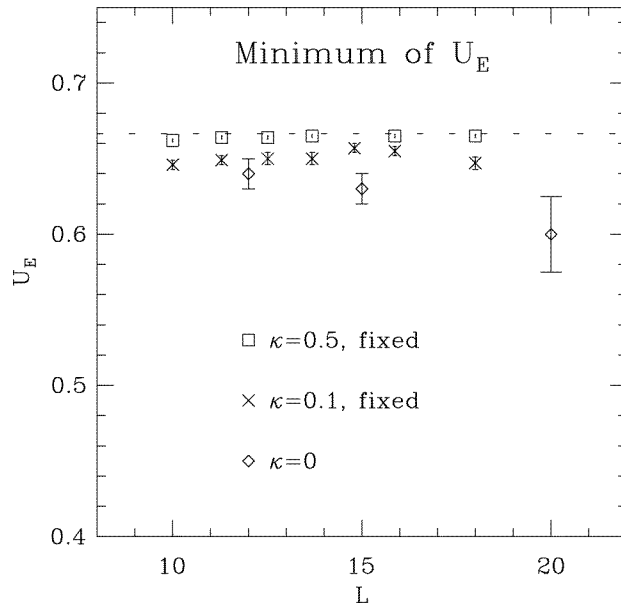
Figure 2. The minimum value of U_E for various lattice sizes. The expected value of $\frac{2}{3}$ at a second-order transition is indicated as a horizontal line.
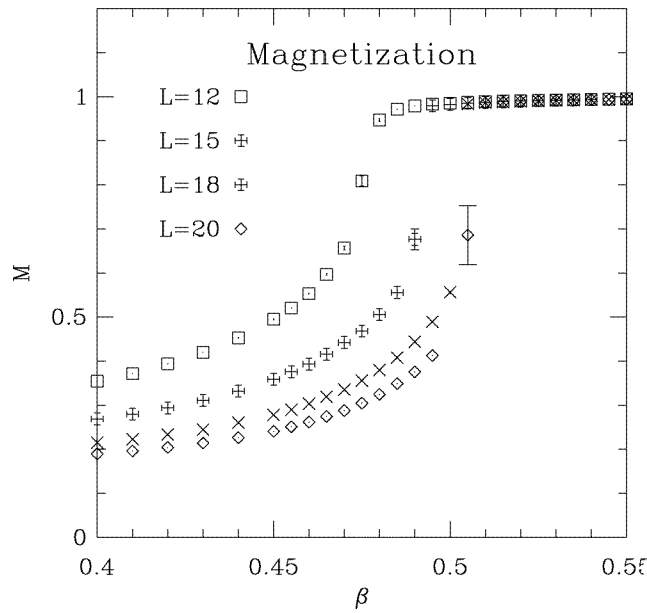

Figure 3. The magnetization for various lattice sizes at $\kappa = 0$.

that U_E clearly scales to the second-order value of $\frac{2}{3}$. This is also shown in figure 2. A non-trivial exponent for the specific heat scaling is also found. It would thus appear that the gonihedric Ising model has a sharp crossover to first-order behaviour somewhere between
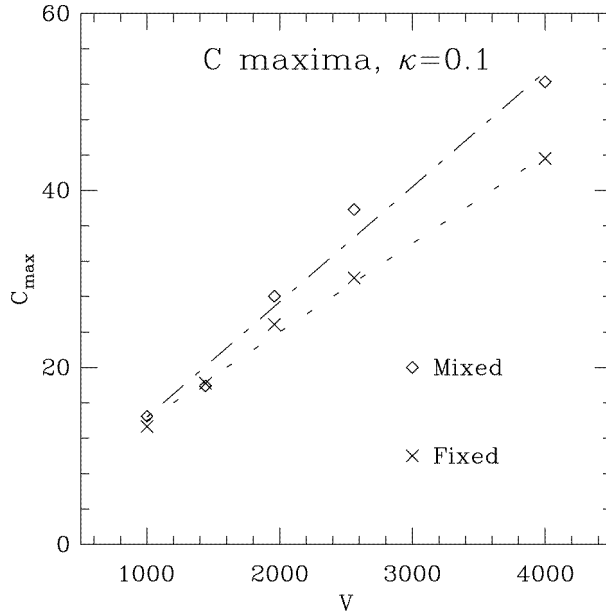
Figure 4. The scaling of the specific heat maximum for the two sorts of boundary conditions used at $\kappa = 0.1$. The best fit lines of the form $A + BV$ are shown.

0.1 and 0.5†.

We can get some hints as to why there is a first-order transition in the $\kappa = 0$ model by considering the dual Hamiltonian [6]. This can be written in various forms, but the most illuminating for our purposes is

$$H_{\text{dual}} = \sum_{\xi} \Lambda^{\chi}(\xi)\Lambda^{\chi}(\xi + \chi) + \Lambda^{\eta}(\xi)\Lambda^{\eta}(\xi + \eta) + \Lambda^{\zeta}(\xi)\Lambda^{\zeta}(\xi + \zeta) \qquad (6)$$

where $\Lambda^{\chi} = (1, 1, -1, -1)$, $\Lambda^{\eta} = (1, -1, 1, -1)$ and $\Lambda^{\zeta} = (1, -1, -1, 1)$ are one-dimensional irreducible representations of the fourth-order Abelian group and ξ, η, ζ are unit vectors in the dual lattice. The spins may also be considered as Ising (± 1) spins if we set $\Lambda^{\zeta} = \Lambda^{\chi} \Lambda^{\eta}$, which gives the following Hamiltonian

$$H_{\text{dual}} = \sum_{\xi} \Lambda^{\chi}(\xi)\Lambda^{\chi}(\xi + \chi) + \Lambda^{\eta}(\xi)\Lambda^{\eta}(\xi + \eta) + \Lambda^{\chi}(\xi)\Lambda^{\eta}(\xi)\Lambda^{\chi}(\xi + \zeta)\Lambda^{\eta}(\xi + \zeta).$$

$$(7)$$

This is recognizable as an anisotropically coupled Ashkin–Teller model. In particular, because all the couplings in front of the different terms are equal, it looks like the four-state Potts model limit of the Ashkin–Teller family. As isotropic $Q > 2$ state Potts models have a first-order phase transition in three dimensions and it is perhaps not so surprising that the particular anisotropic variant in equation (7), and hence its dual in equation (4) which we have simulated, show a first-order transition. The dual Hamiltonian is only valid at $\kappa = 0$ so there is no contradiction in the continuous transition that has been observed in simulations at larger non-zero values of κ.

To summarize, we have simulated the gonihedric three-dimensional Ising model suggested by Savvidy and Wegner in the context of string theory at an exceptional value

† An application of the cluster variational method to the model arrives at similar conclusions [15].

of the self-avoidance coupling, $\kappa = 0$, where the theory possesses an enhanced symmetry. We have found a first-order transition and given some arguments from the dual theory as to why this might be expected. We have also observed in further simulations at small κ values that the crossover to a continuous transition is quite sharp. The presence of some degree of self-avoidance, in the form of a non-zero value for κ, would thus appear to have an important influence on the universality properties of the Savvidy–Wegner/gonihedric models. Although the model at $\kappa = 0$ is not a candidate for constructing a continuum string theory in three dimensions because it does not possess a continuous transition, it still constitutes an interesting addition to the bestiary of Ising-like models. It is possible to construct Savvidy–Wegner models in four and higher dimensions, so extending the investigations of the current paper to four dimensions, which is more directly relevant for (Euclideanized) relativistic string theory, may be profitable.

The Savvidy–Wegner models are obviously a very special 'slice' of the extremely complicated phase diagram that Ising models with extended range and competing interactions display. It would be interesting to explore the connections between their phase diagram and that of both the ANNNI models in [12] and the interfacial models of [1]. The enhanced symmetry of the Savvidy models with respect to those with generic couplings clearly plays a major role in determining their phase structure.

Acknowledgments

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