Abstract

We use the cluster variation method (CVM) to investigate the phase structure of the 3d gonihedric Ising actions defined by Savvidy and Wegner. The geometrical spin cluster boundaries in these systems serve as models for the string worldsheets of the gonihedric string embedded in $\mathbb{Z}^3$. The models are interesting from the statistical mechanical point of view because they have a vanishing bare surface tension. As a result the action depends only on the angles of the discrete surface and not on the area, which is the antithesis of the standard 3d Ising model.

The results obtained with the CVM are in good agreement with Monte Carlo simulations for the critical temperatures and the order of the transition as the self-avoidance coupling $\kappa$ is varied. The value of the magnetization critical exponent $\beta = 0.062 \pm 0.003$, calculated with the cluster variation–Padè approximant method, is also close to the simulation results.
1 The Model

In this paper we discuss the use of the cluster variation method (CVM) in mapping out the phase diagram of the gonihedric 3d Ising model. The gonihedric 3d Ising model is a generalization of the usual 3d Ising model where planar Peierls boundaries between + and − spins can be created at zero energy cost. It has been introduced in [1] in relations with string theory. The CVM method in other contexts has shown itself to be an accurate and economical way of describing the phase diagram both for first order and continuous transitions. As both the model and the method may be unfamiliar, we outline both in turn before going on to describe our results.

The genesis of the model is in a novel discretized random surface theory, the so-called gonihedric string [4],

\[ S = \frac{1}{2} \sum_{\langle ij \rangle} |\vec{X}_i - \vec{X}_j| \theta(\alpha_{ij}), \tag{1} \]

where the sum is over the edges of some triangulated surface, \( \theta(\alpha_{ij}) = |\pi - \alpha_{ij}| \zeta \), \( \zeta \) is some exponent, and \( \alpha_{ij} \) 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, as originally defined by Steiner [2].

In eq. (1) the surface itself is discretized, rather than the space in which it is embedded. An alternative approach to discretizing the linear size would be to restrict the allowed surfaces to the plaquettes of a (hyper)cubic lattice, which corresponds to also discretizing the target space. Savvidy and Wegner [3, 4, 5, 6] did this and rewrote the resulting model as an equivalent generalized Ising model using the geometrical spin cluster boundaries to define the surfaces. The energy of a surface on a cubic lattice is then 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, \( n_4 \) is the number of links where four plaquettes meet at right angles, and \( \kappa \) is a free parameter which determines the relative weight of a self-intersection of the surface. In the limit \( \kappa \to \infty \) the surfaces are strongly self-avoiding, whereas the opposite limit \( \kappa \to 0 \) is that of "phantom" surfaces that pass through themselves without any energy penalty. It is worth emphasizing that the energy is very different from that of the standard 3d Ising model with nearest neighbour interactions where the surfaces are weighted entirely by their areas and not at all by their embeddings.

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

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

Such generalized Ising actions and their equivalent surface formulations have quite complicated phase structures for generic choices of the couplings [4, 5, 6]. The particular ratio of couplings in eq. (2), however, is special and introduces a novel symmetry into the model, related to a zero-temperature high degeneracy point where it is possible to flip any plane of spins at zero energy cost.
Various approaches have been used to investigate these models, including a zero-temperature analysis, mean-field theory and Monte Carlo simulations. We briefly outline the results thus obtained for comparison with our CVM calculation in this paper.

In an analysis of the zero temperature ground states of the model we write the full lattice Hamiltonian as a sum over individual cube Hamiltonians $h_c$ and observe that if the lattice can be tiled by a cube configuration minimizing the individual $h_c$ then the ground state energy density is $\epsilon_0 = \min h_c$. This approach confirms that a layered ground state with parallel layers of flipped spins perpendicular to one of the lattice axes and arbitrary interlayer spacing is degenerate with the ferromagnetic ground state for all $\kappa$. In addition, at $\kappa = 0$ extra ground states appear where all the spins of one of the 2 sublattices of the cubic lattice are flipped.

In the mean field approximation the spins are replaced by average site magnetizations. The calculation of the mean field free energy can be performed by considering independent magnetizations for the 8 sites of an elementary cube. Therefore, as in the zero temperature approach, the energy can be still decomposed into a sum of individual cube terms. Numerical iteration of the resulting eight coupled mean-field equations shows a single transition from a paramagnetic high temperature state to a layered, or the equivalent ferromagnetic, low temperature state. The inverse critical temperature $\beta_c$ determined in this fashion decreases quite sharply with $\kappa$.

The flip symmetry of the model poses something of a problem when carrying out Monte Carlo simulations. A simple ferromagnetic order parameter such as the magnetization

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

will be zero in general, because of the layered nature of the ground state. Staggered magnetizations also fail as order parameters because the interlayer spacing can be arbitrary. In boundary conditions have been suitably chosen in order to pick out the ferromagnetic ground state allowing the use of standard (unstaggered) magnetization to extract magnetic critical exponents. Monte Carlo simulations with such boundary conditions for different $\kappa$ values on lattices of various sizes allowed a finite size scaling analysis to be carried out in order to extract estimates for some of the critical exponents. For $\kappa = 1$ this gave $\nu = 1.2(1)$ from the ratios of slopes of Binder’s magnetization cumulants, $\gamma/\nu = 1.79(4)$ from the FSS of the susceptibility $\chi$, and $(\alpha - 1)/\nu = -1.3(2)$ from the FSS of the energy with two different sorts of fixed boundary conditions. All these exponents, rather remarkably given that the model is defined in three dimensions, are close to the Onsager values of the two-dimensional Ising model with nearest neighbour interactions, as was the critical temperature $\beta_c = 0.44$.

Simulations of other $\kappa \geq 1$ values gave very similar results. However, the $\kappa = 0$ model

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

appeared to be a special case, displaying a first order transition. The transition stayed first order at $\kappa = 0.1$ but softened rapidly as $\kappa$ increased, so the crossover to the second order behaviour seen at $\kappa = 1$ was quite sharp.
2 The Cluster Variation Method

The cluster variation method, or CVM for short, is based on a truncation of the cluster (cumulant) expansion of the free energy density functional on which the variational formulation of statistical mechanics is based \[12, 13\]. Unlike mean field theory it generally locates rather accurately the boundaries between different phases in complex phase diagrams and, using the recently proposed cluster variation–Padè approximant method \[14, 15, 16\] one can extract non-classical, precise estimates of the critical exponents.

For a generic Ising-like model described by a Hamiltonian \(H\) on a lattice \(\Lambda\) the exact free energy can in principle be obtained by minimizing the functional

\[ F[\rho_\Lambda] = \text{Tr} \left( \rho_\Lambda H + \frac{1}{\beta} \rho_\Lambda \ln \rho_\Lambda \right), \tag{5} \]

of the trial density matrix \(\rho_\Lambda\), subject to \(\text{Tr}(\rho_\Lambda) = 1\).

Assuming that the Hamiltonian can be written as a sum of cluster contributions

\[ H = \sum_{\alpha \in \Gamma} h_\alpha, \tag{6} \]

where \(\Gamma\) is a collection of clusters that suffices to enumerate the interactions, an approximate free energy functional can be written in the form \[13\]

\[ F = \sum_{\alpha \in \Gamma} \text{Tr} (\rho_\alpha h_\alpha) + \frac{1}{\beta} \sum_{\alpha \in P} a_\alpha \text{Tr}(\rho_\alpha \ln \rho_\alpha) \tag{7} \]

where \(P\) is a suitable set of clusters (which must contain \(\Gamma\) as a subset), the largest of which (called maximal clusters) have to reflect in some way the symmetry of the lattice, and the \(a_\alpha\) are numerical coefficients determined by

\[ \sum_{\alpha \subseteq \beta \in P} a_\beta = 1, \quad \forall \alpha \in P. \tag{8} \]

The constraints are now

\[ \text{Tr}(\rho_\alpha) = 1, \quad \alpha \in P \]
\[ \rho_\alpha = \text{Tr}_{\beta \setminus \alpha}(\rho_\beta), \quad \alpha \subseteq \beta \tag{9} \]

and the latter can actually be used as a definition of the density matrices of the subclusters of the maximal clusters.

An important feature of the CVM is that the local minima of the approximate free energy can be easily found by means of a simple iterative procedure called natural iteration method \[17, 18\], which has the property that, for any given initial set of density matrices, the iteration always converges to a local minimum of the free energy.

In the present work, we have used the cube approximation of the CVM, that is the maximal clusters of the set \(P\) are the elementary cubic cells of our simple cubic lattice; for this approximation the free energy density functional has the form (see \[12\] for an
application to the simple nearest neighbour Ising model)

\[ f[\rho_8] = \text{Tr}(\rho_8 H_8) + \frac{1}{\beta} \left[ \text{Tr} L(\rho_8) - \frac{1}{2} \sum_{\text{plaquettes}} \text{Tr} L(\rho_{4,\text{plaquette}}) \right. \\
+ \left. \frac{1}{4} \sum_{\text{edges}} \text{Tr} L(\rho_{2,\text{edge}}) - \frac{1}{8} \sum_{\text{sites}} \text{Tr} L(\rho_{1,\text{site}}) \right], \tag{10} \]

where \( H_8 \) is the contribution of a single cube to the hamiltonian (when splitting the total hamiltonian \( H \) into single cube contributions one has to keep in mind that nearest neighbour interactions are shared by four cubes and then will get a coefficient \( 1/4 \) in \( H_8 \), and similarly next-nearest neighbour and plaquette interactions will get a coefficient \( 1/2 \)), \( L(x) = x \ln x, \rho_{\alpha} \) with \( \alpha = 8 (4, 2, 1) \) denotes the cube (respectively plaquette, edge, site) density matrix, and the sums in the entropy part are over all plaquettes (edges, sites) of a single cube. Notice that we have not assumed any \textit{a priori} symmetry property for our density matrices.

The cluster variation method can be viewed as a generalized mean field theory, and hence it is clear that it can give only classical predictions for the critical exponents. In order to overcome this difficulty, one can use the recently proposed cluster variation–Padè approximant method (CVPAM) [14, 15, 16], which has proven to be a rather accurate technique, although not very demanding in terms of computer time. The basic idea of the CVPAM is that, since the CVM gives, for Ising-like models, very accurate results at low and high temperatures (i.e. far enough from the critical point), one can try to extrapolate this results in order to study the critical behaviour. In order to determine the critical exponent of the order parameter \( m \), for example, one calculates \( m(\beta) \) with the CVM up to a temperature at which the error can be estimated to be very small (typically of order \( 10^{-5} \)), and then constructs, by a simple interpolation, Padè approximants for the logarithmic derivative of \( m(\beta) \): the pole and the corresponding residue of each Padè approximant are then estimates for the critical temperature and for the critical exponent respectively.

## 3 The Results

In this section we describe our results for the phase diagram of the model (2) at different values of the parameter \( \kappa \). When the temperature is lowered, the model (2) undergoes a phase transition towards a low temperature ordered phase: this transition has been investigated by means of the CVM in the cube approximation described in the preceding section.

First of all we describe our results at \( \kappa = 1 \). We have solved numerically our approximate variational principle for \( \beta \) ranging in the interval \( 0 \leq \beta \leq 0.5 \) and we have calculated the values \( f_P(\beta), f_F(\beta) \) and \( f_L(\beta) \) of the local minima of the free energy corresponding respectively to the paramagnetic, ferromagnetic and layered phases. The three functions \( f_P(\beta), f_F(\beta) \) and \( f_L(\beta) \) are plotted in Fig. 3.

When \( \beta < 0.404 \) the unique local minimum is that corresponding to the paramagnetic phase; in the interval \( 0.404 \leq \beta < 0.427 \) we find both the paramagnetic and layered minima of the free energy and \( f_P(\beta) < f_L(\beta) \) in the whole interval. At low temperature
when $\beta \geq 0.427$ the ferromagnetic local minimum appears and it happens to be the global minimum of the free energy. Therefore the CVM predicts that the zero temperature degeneracy between phases with all possible sequences of “+” and “−” planes is broken at finite temperature.

The transition at $\beta_c = 0.427$ from the paramagnetic to the low temperature ferromagnetic phase is critical. Indeed, when the inverse temperature $\beta$ is lowered below $\beta_c$, the ferromagnetic local minimum of the free energy disappears.

We have studied the model (2) for other values of the parameter $\kappa$ ranging in the interval $0 \leq \kappa \leq 10$. For each $\kappa > 0$ we have found that at low temperature the model is in the ferromagnetic phase and we have calculated the inverse transition temperature $\beta_c$; in Fig. 2 we have plotted $\beta_c$ as a function of $\kappa$.

At sufficiently low values of $\kappa$, that is $\kappa < \kappa_{tr} = 0.87 \pm 0.01$, the nature of the transition changes over to a first order behaviour which is strengthened as $\kappa$ is lowered.

In Table 1 our results for $\beta_c$ are compared with Monte Carlo and mean field approximation results obtained in [10]; Monte Carlo and CVM predictions are in good agreement.

### Table 1

| $\kappa$ | 0   | 0.25 | 0.5  | 1   | 2   | 5   | 10  |
|----------|-----|------|------|-----|-----|-----|-----|
| $\beta_c$ CVM | 0.550 | 0.464 | 0.443 | 0.427 | 0.421 | 0.420 | 0.420 |
| $\beta_c$ MC [10, 11] | 0.505 | -    | 0.44 | 0.44 | 0.44 | 0.44 | 0.44 |
| $\beta_c$ MF [10] | 0.325 | 0.31 | 0.278 | 0.167 | 0.09 | 0.0335 | 0.02 |

Table 1: Our results for the inverse transition temperature $\beta_c$ at different values of the parameter $\kappa$ are listed. These CVM results are compared with Mean Field and Monte Carlo previous results.

At $\kappa = 0$ the first order transition is at $\beta_c = 0.550$. Moreover at low temperature the layered phases, the ferromagnetic phase and their antiferromagnetic versions obtained by flipping the site-magnetizations of one of the 2 sublattices of the cubic lattice coexist with the same free energy. In Fig. 3 the free energy of the paramagnetic phase (dash-dotted line) and of the coexisting ordered phases (solid line) are depicted.
Therefore, at $\kappa = 0$ the zero temperature symmetry of the model is not violated, and the CVM correctly respects the ferro-antiferromagnetic exact symmetry of the partition function.

Finally, for some values of $\kappa$ such that the transition is critical, that is $\kappa = 1, 2, 5, 10$, we have evaluated the magnetization critical exponent $\beta$ by means of the cluster variation-Padè approximant method [14, 15, 16], obtaining $0.059 \leq \beta \leq 0.062$ at $\kappa = 1$ and $\beta \simeq 0.065$ at $\kappa = 2, 5, 10$. These results clearly suggest that the exponent is independent of $\kappa$ and a prudent estimate is $\beta = 0.062 \pm 0.003$, which has to be compared with the conjectured Onsager value $1/8$ on one side, but also with the estimate, based on finite size scaling of Monte Carlo results [10], $\beta/\nu = 0.04(1)$: given the Monte Carlo estimate $\nu = 1.2(1)$ one can say that the $\beta$ values predicted by CVM and simulations are in rather remarkable agreement.

4 Conclusions

In this work we have applied the cube approximation of the Cluster Variation Method to find the phase diagram of the gonihedric 3$d$ Ising model defined in eq. (2). Moreover the low-temperature CVM results for the order parameter have been used to evaluate the exponent $\beta$ at $\kappa = 1, 2, 5, 10$ via the cluster variation–Padè approximant method.

We summarize here our main results. The CVM approximation gives values of the inverse critical temperature in quite good agreement with those predicted by Monte Carlo simulations. The transition remains critical for $\kappa > \kappa_{tr} = 0.87 \pm 0.01$, where it becomes of first order. Our evaluation of the critical exponent $\beta = 0.062 \pm 0.003$ of the magnetization is also close to the simulations results of [10].

The new result of this paper is that the CVM predicts at finite temperatures a violation of the symmetry of the hamiltonian (2). We find that in the ordered region of the model the ferromagnetic phase is always stable with respect to the lamellar phase. This suggests to study the model (2) in a parameter space larger than the one used in this paper. The knowledge of the global topology of the phase diagram in an enlarged parameter space [19] could be useful to answer the main question set by the Monte Carlo results and confirmed by the results of this paper about the nature of the critical transition of the model (2) at sufficiently high values of $\kappa$. 
References

[1] R.V. Ambartzumian, G.S. Sukiasian, G. K. Savvidy and K.G. Savvidy, Phys. Lett. B275 (1992) 99;
G. K. Savvidy and K.G. Savvidy, Int. J. Mod. Phys. A8 (1993) 3393;
G. K. Savvidy and K.G. Savvidy, Mod. Phys. Lett. A8 (1993) 2963.

[2] J. Steiner, Über parallel Flächen, Gesammelte Werke Band 2 (Berlin, 1882) 171.

[3] G. K. Savvidy and F.J. Wegner, Nucl. Phys. B413 (1994) 605;
G. K. Savvidy and K.G. Savvidy, Phys. Lett. B324 (1994) 72;
G. K. Savvidy, K.G. Savvidy and P.G. Savvidy, “Dual Statistical Systems and Geometric String,” [hep-th/9409031];
G. K. Savvidy and K.G. Savvidy, Phys. Lett. B337 (1994) 333;
G. K. Savvidy, K.G. Savvidy and F.J. Wegner, Nucl. Phys. B443 (1995) 565.

[4] G. K. Bathas, K. G. Floratos, G. K. Savvidy and K.G. Savvidy, “Two Dimensional and Three Dimensional Spin Systems with Gonihedric Action”, [hep-th/9504054].

[5] G. K. Savvidy and K.G. Savvidy, “Interaction Hierarchy: Gonihedric String and Quantum Gravity,”[hep-th/9506184].

[6] R. Pietig and F. Wegner, “Phase Transition in Lattice Surface System with Gonihedric Action”, Heidelberg preprint, December 95.

[7] A. Cappi, P. Colangelo, G. Gonnella and A. Maritan, Nucl. Phys. B370 (1992) 659.

[8] T. Sterling and J. Greensite, Phys. Lett. B121 (1983) 345;
M. Karowski and H. Thun, Phys. Rev. Lett. 54 (1985) 2556;
M. Karowski, J. Phys. A19 (1986) 3375.

[9] W. Selke, Phys. Rep. 170 (1988) 213;
D.P. Landau and K. Binder, Phys. Rev. B31 (1985) 5946.

[10] D.A. Johnston and R.P.K.C. Malmini, Phys. Lett. B378 (1996) 87.

[11] D. Espriu, M. Baig, D.A. Johnston and R.P.K.C. Malmini, “Evidence for a first order transition in a plaquette 3d Ising-like action”, [hep-lat/9607002].

[12] R. Kikuchi, Phys. Rev. 81 (1951), 988.

[13] G. An, J. Stat. Phys. 52 (1988) 727;
T. Morita, J. Stat. Phys. 59 (1990) 819.

[14] A. Pelizzola, Phys. Rev. E49 (1994) R2503.

[15] A. Pelizzola, J. Magn. Magn. Mat. 140-144 (1995) 1491.

[16] A. Pelizzola, Phys. Rev. E53 (1996) 5825.

[17] R. Kikuchi, J. Chem. Phys. 60 (1974) 1071.
[18] A. Pelizzola, Physica A 211 (1994) 107.

[19] E.N.M. Cirillo, G. Gonnella and A. Pelizzola, in preparation.
Figure 1: Solid, dash-dotted and dashed lines represent respectively the free energies $f_F(\beta)$, $f_P(\beta)$ and $f_L(\beta)$ at $\kappa = 1$.

Figure 2: The inverse transition temperature is plotted as a function of the parameter $\kappa$. Dashed and solid lines represent respectively first and second order inverse transition temperatures.
Figure 3: The dash-dotted and the solid lines represent respectively the free energy of the paramagnetic phase and of the coexisting low temperature phases at $\kappa = 0$. 