LETTER TO THE EDITOR

On the phase diagram of the discrete $\mathbb{Z}_6$ spin models

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Abstract.   We point out some problems with the previously proposed phase diagram of the $\mathbb{Z}_6$ spin models. Consideration of the diagram near to the decoupling surface using both exact and approximate arguments suggests a modification which remedies these deficiencies. With the aid of a new parametrization of the phase space, we study the models numerically, with results which support our conjectures.

The discrete $\mathbb{Z}_6$ spin models describe the behaviour of a collection of spins $S_i = \exp(i\theta_i)$, where the θ_i are integer multiples of $\pi/3$. These spins live on a square two-dimensional lattice and interact according to a reduced Hamiltonian of the form

$$H \equiv \frac{1}{k_B T}\mathcal{H} = \sum_{\langle ij \rangle} V(\theta_i - \theta_j) \tag{1}$$

the sum running over nearest-neighbour pairs of sites $\langle ij \rangle$. Imposing $V(\theta) = V(-\theta)$, a particular system is characterized by the three numbers $V_r = V(\pi r/3) - V(0)$, $r = 1, 2, 3$. A duality transformation maps the space of such models to itself [1–4]: with the couplings parametrized by variables $x_r = \exp(-V_r)$, a sum over the θ_i is equivalent to one over dual variables $\tilde{\theta}_i$, with the triplet of couplings $\{x_r\}$ replaced by the dual set $\{\tilde{x}_r\}$:

$$
\begin{aligned}
\tilde{x}_1 &= (1 + x_1 - x_2 - x_3)/\Delta \\
\tilde{x}_2 &= (1 - x_1 - x_2 + x_3)/\Delta \\
\tilde{x}_3 &= (1 - 2x_1 + 2x_2 - x_3)/\Delta
\end{aligned}
\tag{2}
$$

where $\Delta = 1 + 2x_1 + 2x_2 + x_3$. The transformation leaves invariant points on the line

$$(x_1, x_2, x_3) = (t, \beta - \alpha t, \alpha - 2\beta t) \tag{3}$$

where $\alpha = 3 - \sqrt{6}$ and $\beta = \sqrt{6} - 2$. This self-dual line intersects the line of six-state Potts models at the point $x_1 = x_2 = x_3 = (\sqrt{6} - 1)/5$, denoted P below. There is also a distinguished surface on which the models decouple into independent three-state Potts and

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Ising models [2]. This is revealed on writing each spin S_i as a product of a $\mathbb{Z}_2$ and a $\mathbb{Z}_3$ valued variable:

$$S_i = e^{i\theta_i} = \Sigma_i \sigma_i \qquad \Sigma_i = 1, e^{\pm 2\pi i/3}, \quad \sigma = \pm 1. \tag{4}$$

The pairwise interaction energy can then be written as

$$
\begin{aligned}
V(\theta) &= J_1[1 - \cos(\theta)] + J_2[1 - \cos(2\theta)] + J_3[1 - \cos(3\theta)] \\
&= J_1[1 - \tfrac{1}{2}(S + S^{-1})] + J_2[1 - \tfrac{1}{2}(\Sigma + \Sigma^{-1})] + J_3[1 - \tfrac{1}{2}(\sigma + \sigma^{-1})] \\
&= 3J_1[1 - \delta_{\sigma_i\sigma_j}\delta_{\Sigma_i\Sigma_j}] + \tfrac{3}{2}(J_2 - J_1)[1 - \delta_{\Sigma_i\Sigma_j}] + (2J_3 - J_1)[1 - \delta_{\sigma_i\sigma_j}]
\end{aligned} \tag{5}
$$

where $\theta = \theta_i - \theta_j$, $S = S_i/S_j$, $\Sigma = \Sigma_i/\Sigma_j$, $\sigma = \sigma_i/\sigma_j$, and

$$J_1 = \frac{1}{3}\ln\frac{x_1}{x_2 x_3} \qquad J_2 = \frac{1}{3}\ln\frac{x_3}{x_1 x_2} \qquad J_3 = \frac{1}{6}\ln\frac{x_2^2}{x_1^2 x_3}. \tag{6}$$

The spins Σ_i and σ_i decouple on the surface $J_1 = 0$, $x_1 = x_2 x_3$, on which $\frac{3}{2}J_2$ is the three-state Potts coupling, and $2J_3$ the Ising coupling.

The more general phase structure of these models has been studied by various authors over the years (see, for example, [2–5]). The question is an interesting exercise in its own right, and is also of wider relevance—to, for example, the effect of hexagonal symmetry-breaking on the isotropic planar model [2, 6], the behaviour of the cubic model [2, 7], and the spectra of Heisenberg antiferromagnetic spin chains [8]. An initial phase diagram was suggested by Domany and Riedel in [2], with the three-dimensional thermodynamic phase space partitioned into four domains, one disordered and the others exhibiting $\mathbb{Z}_2$, $\mathbb{Z}_3$ and $\mathbb{Z}_6$ ordering. The existence of an additional massless phase was then demonstrated, first [9] along the Villain [10] line, and then [3] throughout a whole three-dimensional region. This phase was incorporated into the Domany–Riedel diagram by Alcaraz and Koberle in [4], its endpoint on the self-dual line later being identified with a particular integrable point C on the phase diagram [11] (further support for such an identification can be found in [12, 13]).

However, there are reasons to believe that the story is not yet complete. We give two examples.

(i) In the diagrams of [2, 4], the point P touches surfaces of transition from the disordered phase into regions of $\mathbb{Z}_2$ and $\mathbb{Z}_3$ order. Such transitions are expected to be of second order, and so the correlation length on these surfaces should be infinite. This contradicts the known behaviour of the six-state Potts model at P, where the correlation length remains finite [14], albeit large [15].

(ii) On the decoupling surface $J_1 = 0$, there is a line of Ising transitions, $J_3 = \frac{1}{2}\ln[1 + \sqrt{2}]$, and a line of three-state Potts transitions, $J_2 = \frac{2}{3}\ln[1 + \sqrt{3}]$. These lines cross at a renormalization group fixed point D, the product of a critical Ising model and a critical three-state Potts model. Three $\mathbb{Z}_6$-invariant operators at this point are the Ising and three-state Potts energy densities ϵ and $\mathcal{E}$, and their product $\epsilon\mathcal{E}$. Since their scaling dimensions are 1, $\frac{4}{5}$ and $\frac{9}{5}$ respectively, all are relevant and the fixed point is triply unstable. This corrects the approximate (Migdal) renormalization group result used in [2], which gave D as being doubly unstable.

We can take this second point a little further, using continuum field theory arguments which are valid in the scaling region around the point D. The fixed point itself is described by a product of $c = \frac{1}{2}$ and $c = \frac{4}{5}$ conformal field theories, and nearby points by perturbations of this product $c = \frac{13}{10}$ conformal field theory by combinations of the continuum operators ϵ, $\mathcal{E}$ and $\epsilon\mathcal{E}$. The first two are anti-self-dual under (2), while the third is self-dual and moves the model away from D along the line (3). Minimal models coupled by local operators have

received a fair amount of attention (see, for example, [16]) but this particular instance does not seem to have been studied in any detail. However, Zamolodchikov's counting argument [17] can be used to show that the $\epsilon\mathcal{E}$ perturbation preserves at the very least conserved charges of spins ± 3 and ± 5. The perturbed (continuum) theory should therefore be integrable [18] and we can hope to obtain information about the scaling region of the self-dual line near to D via the thermodynamic Bethe ansatz (TBA) technique [19]. This method expresses the finite-volume 'effective central charge' $c(r)$, $r = mR$, of a model with bulk length scale $1/m$ confined to a circle of circumference R in terms of the solutions $\varepsilon_a(\theta)$ to a set of coupled integral equations. A candidate system for this case has already been identified: in [20] it was observed that the following TBA system for the functions $\varepsilon_1, \ldots, \varepsilon_7$:

$$\varepsilon_a(\theta) = \delta_{a1} r \cosh\theta - \frac{1}{2\pi} \sum_{b=1}^{7} l_{ab}^{[E_7]} \phi * \ln(1 + e^{-\varepsilon_b})(\theta)$$

$$c(r) = \frac{3}{\pi^2} \int_{-\infty}^{\infty} d\theta \, r \cosh\theta \ln(1 + e^{-\varepsilon_1(\theta)}) \tag{7}$$

predicts an ultraviolet central charge of $\frac{13}{10}$, and a small-r behaviour of $c(r)$ compatible with an expansion in even powers of a coupling λ to an operator of dimension $\frac{9}{5}$. (Here $*$ denotes the convolution, $f*g(\theta) = \int_{-\infty}^{\infty} d\theta' \, f(\theta - \theta')g(\theta')$, $\phi(\theta) = 1/\cosh\theta$, and $l_{ab}^{[E_7]}$ is the incidence matrix of the E_7 Dynkin diagram, with 1 labelling the node at the end of the middle-length arm.) This is the behaviour expected of the perturbation of the product Ising and three-state Potts conformal field theory by its $\epsilon\mathcal{E}$ operator. (On dimensional grounds, m will be related to λ as $m \propto \lambda^5$, but we do not attempt to find the constant of proportionality here.) Assuming that the TBA is correct, it can be used to extract a non-trivial prediction about the vacuum structure of the perturbed model, using arguments described in section 4.3 of [13]. The system (7) implies the following asymptotic for the ground state energy $E(m, R)$:

$$E(m, R) = -\frac{\pi}{6R} c(mR) \sim -\frac{\sqrt{6}m}{\pi} K_1(mR) \tag{8}$$

where K_1 is the modified Bessel function of order one and the prefactor $\sqrt{6}$ can be interpreted as the Perron–Frobenius eigenvalue of the incidence matrix for single kinks interpolating degenerate vacua of the perturbed theory [13]. These vacua must support a representation of the global $\mathbb{Z}_6$ symmetry, and we find that the simplest incidence matrices compatible with both this fact and the eigenvalue implied by (8) are the following:

$$I^a = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad I^b = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{pmatrix}. \tag{9}$$

The first is consistent with the coexistence of disordered and $\mathbb{Z}_6$ ordered phases, the second with coexistence of $\mathbb{Z}_2$ and $\mathbb{Z}_3$ ordered phases. This leads us to the first part of our proposal for the resolution of points (i) and (ii) above: we suggest that the entire segment of the self-dual line from D to C, which includes the six-state Potts transition point P, lies on a surface of first-order transitions separating disordered and fully-ordered regions, and in the scaling region near to D is described by an integrable scattering theory with kink incidence matrix I^a. (In the massive scaling region near to C, the vacuum structure comes as the $N = 6$ case of the results of [13], and is also given by I^a.) It is natural to suppose that the matrix I^b describes
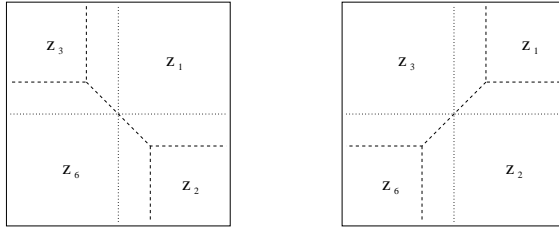
Figure 1. Schematic pictures of slices through the phase diagram just below and just above the decoupling surface.

the vacuum structure on the opposite side of the point D, and support for this idea comes from the following argument.

Consider the behaviour of the model near to the decoupling surface $J_1 = 0$, taking either $J_2 \gg 1$ or $J_3 \gg 1$. In the first case, the effect will be to freeze out the three-state Potts spins Σ_i, and all terms $\delta_{\Sigma_i \Sigma_j}$ can be approximated by 1 in the final line of (5). The result is an effective interaction for the remaining unfrozen spins, equal to $2(J_3 + J_1)[1 - \delta_{\sigma_i \sigma_j}]$. Thus the only effect of a non-zero J_1 in this 'Σ-frozen' region is to replace J_3 with $J_3 + J_1$. The line of Ising transitions on the decoupling surface was at $J_3 = J_3^c = \frac{1}{2} \ln[1 + \sqrt{2}]$; we now conclude that a small non-zero J_1 in the region $J_2 \gg 1$ simply shifts this line to $J_3 = J_3^c - J_1$. A similar argument shows that the line of three-state Potts transitions, situated at $J_2 = J_2^c = \frac{2}{3} \ln[1 + \sqrt{3}]$ on the decoupling surface, is shifted to $J_2 = J_2^c - J_1$ in the region $J_3 \gg 1$ where the σ spins are frozen. Finally, duality can be used to see that in the opposite regimes $J_2 \ll 1$ and $J_3 \ll 1$, the critical lines move in the opposite senses when J_1 shifts away from zero. This line of argument has nothing to say directly about the central region where the Ising and three-state Potts spins are both near their critical points, but the simplest hypothesis, also consistent with the continuum results of the last paragraph, is to continue the lines in from the asymptotic regions as in figure 1.

Much of our numerical work has been devoted to the confirmation of this picture. Before we describe this, we pause to introduce a third set of coordinates on the thermodynamic phase space. First, notice that the parameter K defined by

$$K(x_1, x_2, x_3) = (x_1 - x_2 x_3)/\Delta \tag{10}$$

is mapped into itself by duality: $\tilde{K} = K$. Therefore, surfaces of constant K in phase space are mapped into themselves by duality; $K = 0$ is the decoupling surface. Points with $K > 0$ lie 'below' this surface, on the same side as the six-state Potts point P. It is easy to check that the two parameters

$$y_2 = \ln \frac{1 + 2x_2}{\sqrt{3 - 6K}} \qquad y_3 = \ln \frac{1 + x_3}{\sqrt{2 - 4K}} \tag{11}$$

have the simple duality transformation rule

$$\tilde{y}_2 = -y_2 \qquad \tilde{y}_3 = -y_3. \tag{12}$$

It is convenient to use (K, y_2, y_3) as coordinates in phase space: on any fixed-K surface the point $(K, 0, 0)$ is the self-dual point and duality is just the reflection in this point. The origin $(0, 0, 0)$ is the fixed point D on the decoupling surface, and the six-state Potts transition point P is at $(K_P, 0, 0)$ with $K_P = (\sqrt{6} - 1)^2/25 \approx 0.084$. On the decoupling surface, y_2 and y_3 are functions of the Ising and Potts couplings, respectively.

A cluster algorithm appears to be the ideal choice to simulate the relevant regions of the phase diagram, since it is reasonable to expect large correlation lengths even when the

transitions are only first-order. Since cluster algorithms are especially simple to implement for $\mathbb{Z}_2$ and $\mathbb{Z}_3$ models, we exploited the possibility of writing the Hamiltonian as in (5): the algorithm we used performs alternate cluster updates of the σ_i and Σ_i variables, where those which are not being updated provide effective, site-dependent couplings for the others. For example, suppose we are updating the $\mathbb{Z}_2$ variables: the effective coupling to be used on the link $\langle ij \rangle$ is then $J_3 + J_1 \left(\Sigma + \Sigma^{-1} \right) /2$ with $\Sigma = \Sigma_i / \Sigma_j$, while when updating the $\mathbb{Z}_3$ variables the effective coupling is $J_2 + J_1\sigma$ with $\sigma = \sigma_i / \sigma_j$. Similar algorithms were introduced in [21] for the Ashkin–Teller model, defined as two coupled Ising models.

The fact that the effective couplings are site-dependent does not pose a problem for the cluster updates. However, the effective $\mathbb{Z}_2$ and $\mathbb{Z}_3$ couplings can become negative, i.e. antiferromagnetic. This will happen for the effective $\mathbb{Z}_2$ coupling whenever $J_3 + J_1 < 0$ or $J_3 - J_1/2 < 0$, and for the $\mathbb{Z}_3$ coupling whenever $J_2 + J_1 < 0$ or $J_2 - J_1 < 0$. Negative couplings on some links can in turn lead to frustrations, which in principle can make the cluster algorithm highly ineffective. However, it is easy to convince oneself that the $\mathbb{Z}_3$ model is never actually frustrated: for every configuration of the $\mathbb{Z}_2$ spins there exists a configuration of the $\mathbb{Z}_3$ ones such that all the links are satisfied. Therefore the possibility of frustrations exists only for $J_1 < -J_3$ or $J_1 > 2J_3$. These relations are never satisfied in the regions we considered.

We explored several fixed-K surfaces and mapped the various phases and their boundaries using the Binder cumulants method [22]. In our case, we define two cumulants, one for each order parameter:

$$Q_\sigma = \frac{3}{2} - \frac{1}{2} \frac{\langle m_\sigma^4 \rangle}{\langle m_\sigma^2 \rangle^2} \qquad Q_\Sigma = 2 - \frac{\langle m_\Sigma^4 \rangle}{\langle m_\Sigma^2 \rangle^2} \tag{13}$$

where m_σ and m_Σ are the $\mathbb{Z}_2$ and $\mathbb{Z}_3$ magnetizations per site. For each surface we measured the $\mathbb{Z}_2$ and $\mathbb{Z}_3$ Binder cumulants on a grid of points around the self-dual point $(K, 0, 0)$ for two different lattice sizes $L_1 \times L_1$ and $L_2 \times L_2$. For every fixed value of y_2 we estimated the value of y_3 where each Binder cumulant remains constant when the lattice size is increased, i.e. the transition point. This allows us to determine a set of points belonging to the transition lines for the $\mathbb{Z}_2$ and $\mathbb{Z}_3$ variables. These are the points plotted in figures 2–4 for the
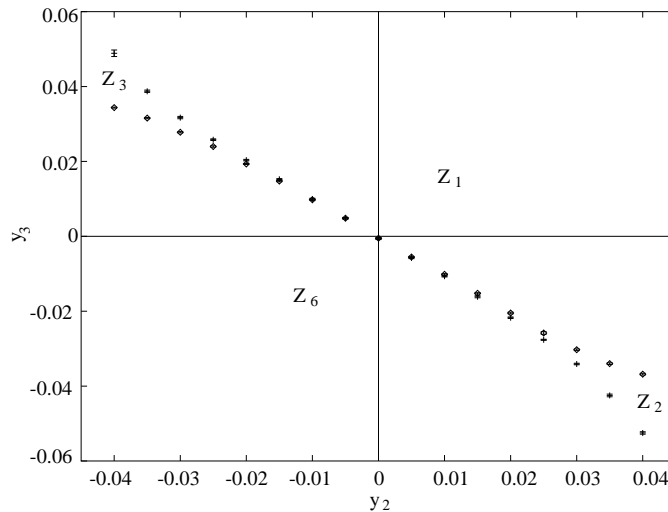

Figure 2. Phase diagram on the $K = 0.06$ surface. Phases are labelled according to the nature of their ordering. Binder cumulants for lattice sizes $L_1 = 15$ and $L_2 = 30$ were used.
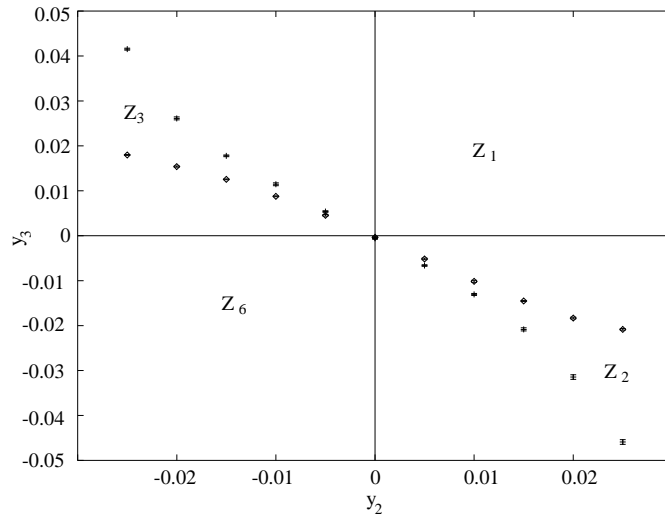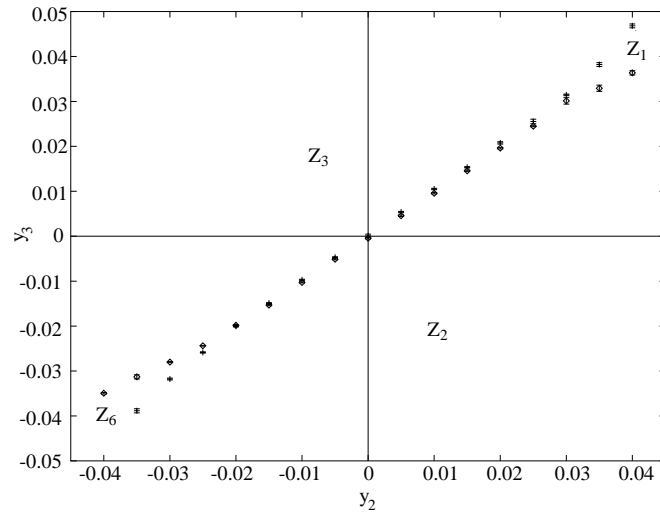
Figure 3. Same as figure 2 for $K = 0.04$.

Figure 4. Same as figure 2 for $K = -0.08$. The lattice sizes used here were $L_1 = 45$ and $L_2 = 60$.

$K = 0.06, 0.04, -0.08$ surfaces, respectively. The consistency of the procedure was checked by repeating it with the roles of y_2 and y_3 inverted. Finite-size effects are signaled by violations of the duality symmetry, that is, in our coordinates, symmetry under reflection in the origin. Small violations are visible in our figures; we checked that they become smaller when the lattice sizes are increased. These effects turned out to be much larger in the $K < 0$ region. In fact we observed that to control them satisfactorily in the $K > 0$ region lattice sizes as small as $L_1 = 15$, $L_2 = 30$ sufficed, while for $K < 0$ we had to use $L_1 = 45$, $L_2 = 60$.

The numerical results confirm the qualitative picture shown in figure 1, and our claim that the decoupling point D on the self-dual line marks a change from the coexistence of disorder and $\mathbb{Z}_6$ order to the coexistence of $\mathbb{Z}_2$ and $\mathbb{Z}_3$ order. The reduced length of the first-order

segment at $K = 0.04$ is consistent with scaling predictions, though we are not close enough to the point D to see a complete collapse of data. In conclusion, we have proposed a significant modification to the previously accepted phase diagram of the $\mathbb{Z}_6$ spin models, and this has been supported by a detailed numerical study.

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