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Glassy behaviour and semi-local invariance in Ising model with four-spin interaction

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Abstract. We show that the rapidly quenched high-temperature phase of the 3D Ising model, with four-spin interaction, evolves into the glassy phase with higher energy than in the low-temperature phase which can be reached upon slow cooling. The mechanism which traps the dynamics in the glassy phase is a consequence of a shape dependence of the energy of excitations. The semi-local invariance in this model is lifted by (sufficiently strong) thermal fluctuations to the local gauge invariance.

1. Introduction

With the advent of very-high-speed-cooling techniques almost every fluid can be turned into a glass provided cooling is fast enough [1]. Rapid progress on the experimental side of the physics of glasses ignited their theoretical studies. However, the complex nature of glasses makes their theoretical examination very difficult. It would be desirable to formulate a lattice spin model of glasses since the physics of such models is relatively well understood and many efficient methods have been developed in this area. Since a fluid under slow cooling can be turned into an ordered crystalline phase, a possible candidate for the model of glass should be non-random at the level of the Hamiltonian of the system. Randomness, which is an intrinsic feature of glasses, should be the consequence of the dynamics of the model under special conditions. This is in contrast to spin glasses where randomness is included at the level of the Hamiltonian [2]. Recently, it has been shown that certain non-random models indeed exhibit glassy behaviour [3]. However, these models are usually infinite dimensional and it is not clear if a glassy phase exists in finite dimensional versions of such models.

In this paper we show that the 3D Ising model with four-spin plaquette interaction has a glassy phase. The idea that four-spin interaction yields the glassy phase has been recently examined by Bouchaud and Mézard [4]. However, their model is rather complicated and it is difficult to infer the microscopic mechanism responsible for the trapping of the dynamics in the glassy phase. In contrast, in our model this mechanism can easily be deduced: it is the shape dependence of the energy of excitations. As shown by Shore *et al* [5], basically the same mechanism is responsible for the glassy behaviour in the Ising model with bilinear, competing interactions. Our results suggest that the shape dependence of the energy of excitations might be a more common mechanism responsible for the appearance of a glassy phase.

Models with multi-spin interactions have been frequently studied in the past, also in the context of glassy properties. Certain indications of very slow dynamics in such models

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were noted several years ago by Mouritsen *et al* [6] who studied models with a slightly different version of the four-spin interaction. In their version, interacting spins constitute an elementary tetrahedron. Such a modification leads to important differences: Mouritsen *et al*'s model has a two-fold degenerate ground state while our model with a plaquette interaction has an infinitely degenerate ground state. This study was not motivated by the glassy properties of the model and the authors did not examine this further. More recently, glassy behaviour has been examined in the 1D three-spin model by Kisker *et al* [7]. One should also mention studies of the random (at the level of the Hamiltonian) versions of multispin models by Rieger [8] and by Alvarez *et al* [9].

There is another reason for studying a 3D Ising model with four-spin interaction. Recently, this model, as a particular case of the so-called gonihedric models, drew considerable attention in connection with lattice string theories [10, 11]. Such a connection exists because the energy of excitations in gonihedric models scales linearly with their size (in the ordinary Ising model energy is proportional to the area of an excitation). The thermodynamical properties of gonihedric models has already been examined by mean-field approximations [12], the cluster variational method [13] and by Monte Carlo simulations [12, 14]. For the model with a four-spin interaction, simulations indicate [14] that this model undergoes a first-order phase transition. What is, in our opinion, not quite clear in this model is the nature of the transition. What kind of symmetry is broken in the low-temperature phase and restored in the high-temperature phase? In this paper we give some arguments, supported by Monte Carlo simulations, that the high-temperature phase has a very high symmetry, which is basically the same as in some gauge-invariant models. Thus, we show that in the present model, whose Hamiltonian is invariant only with respect to certain semi-local transformations, the local gauge symmetry is generated by (sufficiently strong) thermal fluctuations. We also show that the square of the spin–spin correlation function might be regarded as an order parameter which distinguishes between the high- and low-temperature phases.

In section 2 we describe the model and examine its symmetries. We also propose a form for the order parameter. In section 3 we study the glassy properties of our model. Section 4 contains a summary of our results.

2. Symmetries of the model and the order parameter

First let us consider the 2D version of this model which is described by the Hamiltonian

$$H = -J \sum S_i S_j S_k S_l \tag{2.1}$$

where $S_i = \pm 1$ and i runs over the sites of the square lattice. Summation in (2.1) is performed over elementary plaquettes of the lattice. In the following we put $J = 1$. The general gonihedric model also contains nearest- and next-nearest-neighbour bilinear interactions but here we examine only the particular case (2.1).

Since model (2.1) is actually a special case of the symmetric eight-vertex model, its properties are known exactly [15]. Namely, the model is paramagnetic at any temperature T. Nevertheless, below, we present a qualitative analysis of this model because our arguments should also apply to a 3D, unsolvable, version of model (2.1).

The following property of the model (2.1) will be of interest to us: Hamiltonian (2.1) is invariant with respect to a semi-local group of transformations which flip the entire row (or column) of spins. Immediate proof follows from the structure of the Hamiltonian (2.1). This group of transformations will be referred to in the following as G.

Now, let us calculate the correlation function $\langle S_i S_j \rangle$:

$$\langle S_i S_j \rangle = \sum_{\{S_k\}} S_i S_j \mathrm{e}^{-\beta H}/Z \qquad Z = \sum_{\{S_k\}} \mathrm{e}^{-\beta H} \tag{2.2}$$

where $i \neq j$ and $\beta = \frac{1}{k_B T}$. To calculate (2.2) note that there must be a row or a column which contains the site i but does not contain the site j. With each configuration $\{S_k\}$ in which $S_i = 1$ let us associate a configuration $\{S_k\}'$ which is obtained from $\{S_k\}$ by flipping all spins along this row or column. Since the contributions to $\langle S_i S_j \rangle$ coming from $\{S_k\}$ cancel with those from $\{S_k\}'$ (both configurations have the same energy) we obtain that $\langle S_i S_j \rangle = 0$.

Since all spin–spin correlation functions vanish we find that the system is a perfect paramagnet with the susceptibility following Curie's law $\chi = \frac{1}{k_B T}$ and no spontaneous magnetization defined as

$$m^2 = \lim_{|i-j|\to\infty} \langle S_i S_j \rangle. \tag{2.3}$$

Note that the vanishing of $\langle S_i S_j \rangle$ is a consequence of the fact that the operator $S_i S_j$ is not invariant with respect to G. It is easy to see that, for example, the product of four operators around an elementary plaquette is invariant and such correlation function does not vanish (at least not due to this symmetry).

The above analysis resembles Elitzur's theorem [16] in lattice gauge theory [17]. This theorem states that quantites which are non-invariant with respect to local gauge symmetry vanish. However, the proof of this theorem is restricted to the local gauge symmetries. This locality ensures that when the thermodynamic limit is taken in the proper way (first the system size $L \to \infty$ and then the external field $h \to 0$) then the non-invariant quantity vanishes. The non-local character of G means that the above 'derivation' of the vanishing of $\langle S_i S_j \rangle$ is not strictly correct and requires important reconsideration.

This problem is related with the ergodicity [18] of the model (2.1). Let us illustrate this problem with a simple example. The $d = 2$ Ising model with bilinear interaction has global up–down invariance. The operator $S_i S_j$ is invariant with respect to this transformation while S_i is non-invariant. The simple argument, as presented above, thus suggests that $\langle S_i S_j \rangle \neq 0$ and $\langle S_i \rangle = 0$. However, we know that only the former statement is correct since at low temperature the model breaks ergodicity and has spontaneous magnetization. But this simple argument is correct at high temperature where ergodicity is restored and, as required by symmetry, the system has no magnetization.

Thus, if the model is ergodic then our results concerning the correlation functions in model (2.1) are correct. Although we cannot provide rigorous analysis of the ergodicity properties of model (2.1) we can present some reasonable, in our opinion, arguments that model (2.1) are indeed ergodic.

Let us consider one of the ground states of (2.1) with $S_i = 1$ at every site. Let us also assume that all spins are kept rigid except spins along a certain row. However, the evolution of spins in this row closely resembles the dynamics of the $d = 1$ Ising model with bilinear coupling. Let us flip a single spin on this row thus creating an excitation which consists of four 'broken' squares. Flipping one of the nearest neighbours of the already flipped spin does not increase the energy but merely shifts the 'broken' squares and exactly the same dynamics governs the 1D Ising model, which is known to be disordered at any temperature. Since freeing the remaining spins can only speed up the escape from this ferromagnetic ground state we thus conclude that the model is ergodic at any positive temperature (evolution starting at any other ground state will proceed with the same energetics).

This can also be described in the following way. Model (2.1) has a 2^{2L}-degenerate ground state, where L is the linear size of the lattice. However, these ground states are not well separated: each ground state is connected with other $2L$ ground states by the interface of dimension $D = 0$ ($2L$ is the total number of columns and rows). A standard argument [18] shows that such interfaces are low-energy barriers and cannot trap the system and at any positive temperature the system will visit the entire phase space.

Now consider the 3D version of model (2.1) on the simple cubic lattice. It is easy to see that in this case the Hamiltonian (2.1) is invariant, but only with respect to the flipping of whole planes of spins. Using the same arguments as in the 2D case, we find that if the model is ergodic then all spin–spin correlation functions vanish. But the situation is now very different. Namely, to go from one ground state to the other, the system has to flip an entire plane of spins and thus it has to overcome much higher energy barriers. Free energies of such barriers will most likely increase linearly with the system size L (since the interface is one dimensional) and should be capable of breaking the ergodicity and trapping the system at sufficiently low temperature. Thus, we expect that $\langle S_i S_j \rangle = 0$ but only at sufficiently high temperature (it is natural to expect that the temperature which separates these two regimes is the same as the temperature of the discontinuous transition). Note that the vanishing of $\langle S_i S_j \rangle$ due to Elitzur's theorem is a characteristic feature of gauge invariant systems [17]. Thus, as far as correlation functions are concerned, model (2.1) at high temperature is equivalent to gauge-invariant models. Moreover, our arguments apply to the general gonihedric model (whose model (2.1) is only a particular case) as well because in this model the semi-local invariance considered above also holds. This is particularly interesting for some other values of parameters where the gonihedric models are known to have a second-order transition. In such a case the model is expected to have a well defined continuum limit which corresponds to the string theory.

To confirm this scenario we performed the standard, importance sampling Monte Carlo simulations [19]. Such studies of this model have already been performed by Espriu *et al* [14]. Measuring Binder's energy cumulant they found that the model has a first order phase transition at $T_c \sim 3.96$ (in our units). For lattices of size $L = 8, 12, \ldots, 24$ we measured susceptibility χ defined as the sum of all spin–spin correlation functions. We do not present detailed data but our results clearly confirm that above T_c we have $\chi = T^{-1}$. The behaviour of χ for $T < T_c$ requires more careful analysis. Provided we start the simulations from the ferromagnetic ground state, we observe, as expected, that $\chi \sim L^3$. However, magnetized ground states constitute only a small portion of all ground states [11]. It is thus more appropriate to choose the low-temperature phase in a more representative way. One possibility is to choose it randomly by cooling the system from the high-temperature phase. Doing so we found that χ again follows Curie's law but this time with much larger fluctuations. We expect that due to some self-averaging the susceptibility follows Curie's law even though spin–spin correlation functions are non-zero. Our explanation of this fact is that, since cooling selects the ground state randomly, correlation functions in this ground state are most likely to acquire random values which cancel out and eventually we obtain Curie's law. If so, then two-spin correlation functions $\langle S_i S_j \rangle$ might be used to construct an order parameter r which would distinguish between high- and low-temperature phases. However, because $\langle S_i S_j \rangle$ assumes random values in the low-temperature phase, we have to take its square:

$$r(\delta) = \sum_i \langle S_i S_{i+\delta} \rangle^2. \tag{2.4}$$

For an arbitrary finite lattice vector δ the order parameter should be zero in the high-temperature phase and non-zero in the low-temperature phase.

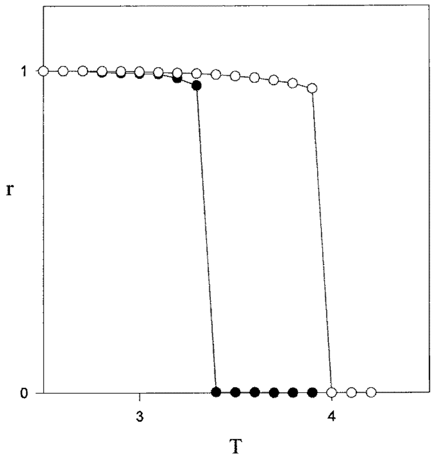

Figure 1. The order parameter r as a function of temperature. Open and full circles correspond to heating and cooling, respectively. The results are obtained for $L = 24$ and for each temperature we made runs of 20 000 Monte Carlo steps.

To confirm this scenario using Monte Carlo simulations we calculated $r(\delta)$. Our results, for δ equal to the lattice unit vector, are shown in figure 1, clearly confirm the vanishing of r in the high-temperature phase (at the same time it confirms the restoration of ergodicity in this phase). We also measured r for some other values of δ and similar behaviour was observed. Thus, the transition at T_c might be regarded as the freezing of correlation functions. Let us also note a similarity with the ordinary Ising model where the one-spin correlation function (magnetization) is an order parameter and the two-spin interaction enters the Hamiltonian.

3. Glassy behaviour

There is yet another reason for studying model (2.1). Namely, when suddenly cooled the high-temperature phase does not evolve into the low-temperature phase but to a phase with considerably higher energy. This phase is referred to in the following as a glassy phase. The temperature dependence of the internal energy is shown in figure 2. We simulated a lattice of size $L = 24$ and at each temperature we made runs of $\sim 10^4$ Monte Carlo steps. Strong hysteresis confirms that a model undergoes a discontinuous transition (Espriu *et al*'s estimation of $T_c(\sim 3.96)$ is at the high-temperature end of our hysteresis). From this figure one can see that the glassy phase extends up to $T \sim 3.4$ which is approximately the same as the low-temperature end of the hysteresis. Thus, in the temperature range $T_G \sim 3.4 < T < T_c$ our model is in a supercooled liquid phase. The time evolution of energy under such a quench is shown in figure 3. Stability of the glassy phase is most pronounced for $L = 16$ and $T = 3.0$, where during almost the whole run the energy of the system remains nearly constant. From visual inspection of figure 3 one can see that the evolution into the glassy phase (aging) becomes slower for larger system size and lower temperature but of course more extensive analysis of these effects would be desirable. Moreover, our results suggest only slight size dependence of the energy of the glassy phase. We made runs of 2×10^5 Monte Carlo steps also for $L = 32$ and $T = 3.0$ and the limiting energy $U = -2.91$ is, within (small) error, the same as the energy for $L = 24$ (for $L = 16$ this energy is $U = -2.92$).

What is the mechanism which traps the dynamics in the glassy phase? This problem is a consequence of the shape dependence of the energy of excitations in the present model. Let us consider again model (2.1) in the 2D case. For simplicity, let us choose the ferromagnetic

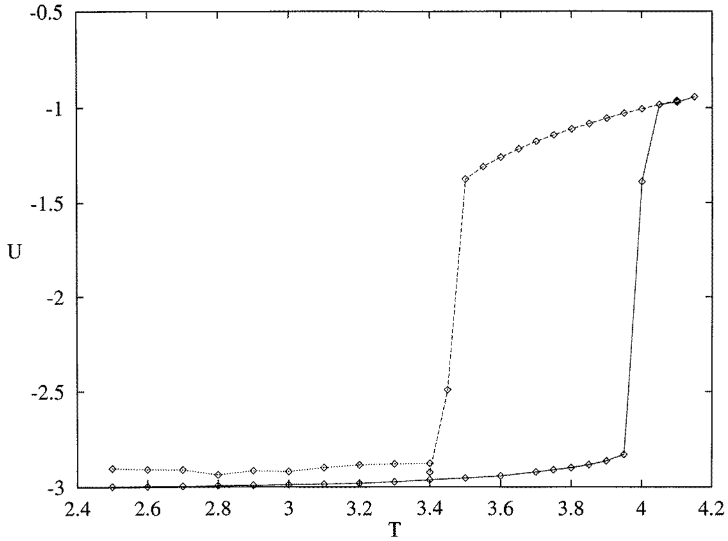

Figure 2. Internal energy U as a function of temperature T ($k_B = 1$). Full and broken curves correspond to heating and cooling, respectively. The dotted curve shows the energy of the glassy phase obtained from cooling a random configuration ($T = \infty$). Heating starts from the ferromagnetic configuration ($S_i = 1$ at every i) but for quantities like internal energy the choice of the ground state is not important.

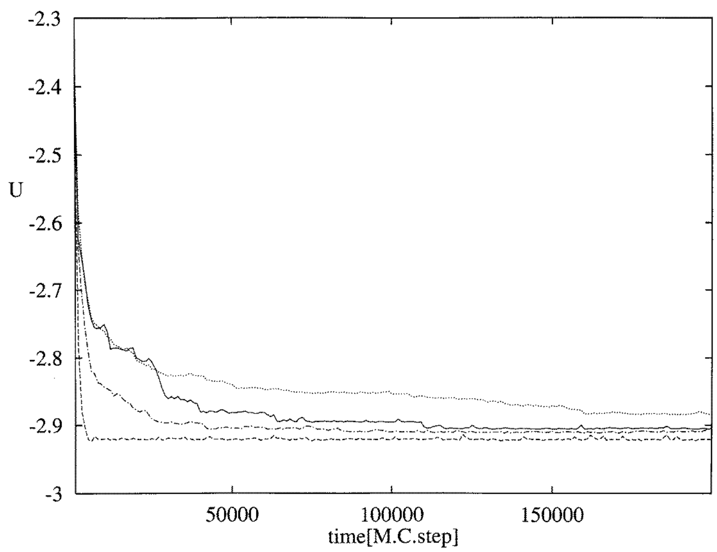

Figure 3. The time evolution of energy under cooling to temperature (a) $T = 2.5$; the dotted and full curves correspond to $L = 24$ and $L = 16$, respectively. (b) $T = 3.0$; the chain and broken curves correspond to $L = 24$ and $L = 16$, respectively. The initial configuration is random ($T = \infty$). Averaging was made every 1000 Monte Carlo steps.

ground state; for any other ground state the same considerations can be made. An elementary excitation, obtained by flipping a single spin, increases the energy by 8 J. But it is easy to note that every excitation which is rectangular increases in energy by the same amount (see

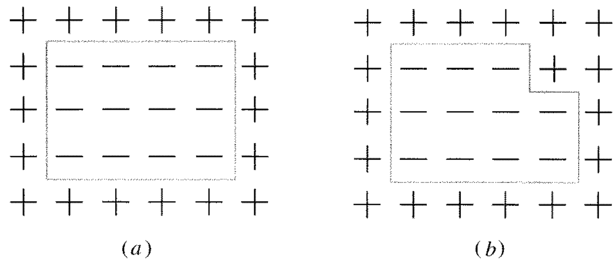

Figure 4. (*a*) A rectangular excitation. (*b*) A higher energy excitation.

figure 4(*a*)). One can immediately realize that it is not the total perimeter of an excitation which determines its energy, as in an ordinary (two-spin) Ising model, but merely the number of its corners. Such energetics of excitations is very peculiar. It gives rise to a large class of low-energy, effectively tensionless, excitations ('Goldstone mode'). The existence of these low-energy excitations provides yet another way to understand why model (2.1) for 2D is disordered for any T.

Let us assume that we prepared our system at high temperature and then we cooled it suddenly. At high temperature, excitations of arbitrary shape and size are present. After reducing the temperature, the system reduces its energy by eliminating excitations. The key point of our argument is that to eliminate excitations such as those shown in figure 4(*a*) one has to create an excitation of the shape shown in figure 4(*b*); but such excitation has more corners and thus its energy is larger. Consequently, to remove such excitations, the system has to climb certain energy barriers. It is natural to expect that removing such excitations is very slow especially at low temperature. Note that in the ordinary Ising model both excitations shown in figure 4 would have the same energy. In this case we would not have to climb any barrier and the process of elimination of excitations would be much faster.

Is this mechanism capable of trapping the 2D model? Our Monte Carlo results show that the answer is negative. Although slowly, especially at low temperature, the model evolves to the equilibrium (disordered) phase. Since in 2D the model has only the disordered phase thus the lack of the glassy phase is an expected feature. Later, we will mention some dimensional arguments on the non-existence of the glassy phase in 2D as suggested by Shore *et al* [5].

Now let us consider the 3D case. In this case the energetics of excitations changes. It is easy to show that, for example a cubic excitation of size M increases energy by $24M$ J: energy is determined by the total length of edges of the cube; in our case $12M$. Although not tensionless, such size dependence is again different than in the ordinary Ising model where the energy of an excitation of size M is proportional to M^2 and not to M. However, in the 3D case a similar trapping mechanism operates. Namely, to remove a cubic excitation of size M, initially we have to increase the total length of its edges and thus climb some energy barrier. In 3D this mechanism requires more careful consideration. In 2D, to reduce the excitation by one row, we had to climb some finite energy barrier, then further evolution did not require any additional increase of energy (essentially it would be a random walk). Note that in 3D this is not the case. Let us remove an elementary cube from a corner (the most vulnerable place) of our cubic excitation of size M. A step which is created in such a way is not free (as for $d = 2$) and to move it we have to further increase the energy (to change the position of this step we have to remove other elementary cube(s) but this increases the total length of edges and thus the energy). In order to diminish our cubic excitation by one layer we have to climb an energy barrier $\delta E \sim M$, but the average time needed to climb such barriers grows exponentially with M, i.e. $\tau \sim \lambda^M$, $\lambda > 1$ [18]. This means that excitations of large size, which should appear in the process of evolution after sudden cooling, are actually trapped.

We have performed a Monte Carlo simulation to estimate the average time $\tau(M)$ needed to remove an excitation of size M. The initial ferromagnetic configuration ($S_i = 1$) contained a cubic excitation ($S_i = -1$) of the size $M = 3, 4, 5, 6, 7$. The size of the lattice was $L = 2M$ but for small $M(= 3, 4)$ we had to use larger L. We measured the time needed to bring the system to the ground state. The temperature was set at $T = 2.75$ ($T < T_G$), which is sufficiently low to ensure that the process of elimination of the initial excitation sets the only slow timescale (once this excitation is removed the system very quickly reaches the ground state). Our results are averages over 1000 measurements, except $M = 7$ where only 100 measurements were made. We obtained: $\tau(3) = 144$, $\tau(4) = 915$, $\tau(5) = 5433$, $\tau(6) = 30\,843$, $\tau(7) = 155\,400$. In our opinion, these results, which increase roughly by the same factor, strongly support the predicted exponential divergence of τ. Fitting $\tau \sim M^{\phi}$ gives systematically increasing and unrealistically large values of $\phi(\sim 10)$. Recall that in the ordinary $d = 3$ Ising model one expects $\phi = 2$ [20].

Is the existence of the glassy phase restricted to the pure four-spin interaction or does it also appear in the Ising model where both bilinear and four-spin interactions are present? In our opinion the glassy phase should exist in such models as well. The reason is that although the energy of excitations depends on the area (due to the bilinear terms) it still depends on the shape (four-spin terms) and basically the same arguments should apply. However, there might be some important differences as well. Namely, in the model with both kinds of interaction it is possible that the thermodynamic transition is a continuous one. In such a case close to the critical point large fluctuations should be more effective in destroying the trapped domain pattern. The situation should be very similar to that which appears in the ferromagnetic Ising model with small antiferromagnetic next-nearest-neighbour interactions [5]. For that model Shore *et al* found that there is a certain temperature T_{cr} (corner-rounding temperature) below a thermodynamic critical point and such that the trapping mechanism is effective but only below T_{cr}. For larger T thermal fluctuations roughen the domains and the usual (with $\phi = 2$) coarsening mechanism is restored. However, it has been argued [5] that because at T_{cr} the energy barriers go to zero and the transition at T_{cr} is not a true glassy transition. Shore *et al* also explain why in 2D models there in no glassy phase. This is because in 2D, thermal fluctuations roughen the corners of domains at arbitrary positive temperature and quickly coarsening (with $\phi = 2$) brings the system to the low-temperature phase.

Is our T_G a kind of corner-rounding critical temperature? Much more extensive Monte Carlo simulations would be needed to answer this question definitively but one can argue that it need not neccessarily be so. Namely, the important difference is that in our model (2.1) the phase transition is discontinuous while in the model examined by Shore *et al* it is continuous. It has already been argued that at least in some models [21] the roughness of an interface is related to the character of the phase transition and, in particular, it is usually rough at continuous transitions and flat at discontinuous transitions. Since the transition in model (2.1) at T_c is discontinuous, one might expect the interface to be flat at T_G which might imply the non-vanishing of energy barriers at T_G. However, the roughness of the corner constitutes another kind of interfacial phenomenon and applicability of these arguments is at present unclear.

Another interesting question is whether one can construct an order parameter which can distinguish between glassy, crystal and liquid phases of the model. A possible candidate might be the order parameter $r(\delta)$ or rather its δ-dependence. Our preliminary results (not presented here) indicate that in the glassy phase the parameter $r(\delta)$ becomes substantially smaller for increasing δ. However, further calculations would be needed to check whether indeed, the δ-dependence of $r(\delta)$ might distinguish the glassy phase from the crystal phase.

4. Summary

We have found that a relatively simple 3D Ising model has a glassy phase. The stability of this phase is a consequence of the shape-dependence of the energy of excitations in this model. The fact that the glassy behaviour appears in both the model with four-spin interaction and the Shore *et al* model with competing interaction might qualitatively explain the apparent abundance of glasses in real systems because in such systems these interactions are likely to exist. Another interesting feature of this model, which was recently examined in the context of the string theory, is that thermal fluctuations induce the local gauge invariance, even though there is no such symmetry in the low-temperature phase. Although the physics of glasses and the physics of strings have little in common, we should not reject beforehand the possibility of some deeper relationships.

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