

Full versus first-stage replica symmetry breaking in spin glasses

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A short survey is presented on spin-glass-like states characteristics in complex nonmagnetic systems. We discuss the interplay of the interaction structure and symmetry with the classification of scenarios of the replica symmetry breaking. It is shown that the kind of the transition to the nonergodic state depends not only on the presence or absence of the reflection symmetry but on the number of interacting operators and their individual characteristics.

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I. INTRODUCTION

The reflection symmetry plays a crucial role defining the character of phase transition in nonrandom mean-field (MF) models.¹ Generally speaking the presence of the terms without reflection symmetry usually results in the first-order phase transition while in the absence of such terms the transition is of the second order. In the case of random MF systems the absence of reflection symmetry also leads to a special form of the free-energy functional that differs from the symmetrical case. As a consequence, the scenarios of replica symmetry breaking (RSB) are different for these two cases.

However, not only the symmetry determines the transition to nonergodic state. Extending the class of models permits considering the role of different factors in scenarios of appearance of spin-glass- (SG-) type states.

In this paper we try to use our recent results for different models of spin-glass-like states in complex nonmagnetic systems (see Ref. 2 for a review) to investigate how the interaction type correlates with the SG behavior.

The theory of spin glasses has been developed as an attempt to describe unordered equilibrium freezing of spins in actual dilute magnetic systems with disorder and frustration. This problem was soon solved at the mean-field level [Edwards and Anderson,³ Sherrington and Kirkpatrick,⁴ Almeida and Thouless,⁵ and Parisi^{6,7} (see Ref. 8 for a review)]. The Sherrington-Kirkpatrick (SK) approach to the spin-glass theory starts with the Hamiltonian

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} U_i U_j. \quad (1)$$

It describes Ising spins U located on the lattice sites i . The quenched interactions J_{ij} are distributed with the Gaussian probability

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi J}} \exp\left[-\frac{(J_{ij} - J_0)^2}{2J^2}\right], \quad (2)$$

where $J = \tilde{J}/\sqrt{N}$, $J_0 = \tilde{J}_0/N$, and N is the number of sites. To perform averaging over disorder in this case one has to average the quenched free energy F rather than the partition sum Z itself. Such averaging is usually performed using the

replica method. The free energy becomes the function of the order parameters that depend on replica indices

$$F = F(x^\alpha, q^{\alpha\beta}), \quad (3)$$

$$x^\alpha = \frac{1}{N} \sum_{i=1}^N U_i^\alpha, \quad q^{\alpha\beta} = \frac{1}{N} \sum_{i=1}^N U_i^\alpha U_i^\beta. \quad (4)$$

The free energy $F(x^\alpha, q^{\alpha\beta})$ has a stationary point for the RS solution when all $q^{\alpha\beta}$ are equal. However this state is unstable under RSB. Parisi^{6,7} proposed a method of performing RSB step by step with the limit of so-called full RSB (FRSB) when $q^{\alpha\beta}$ becomes a continuous function of a parameter x . This approach allowed to describe main results of experiments on spin glasses. Namely, in the framework of the equilibrium approach, the spin-glass phase with qualitatively correct boundaries was obtained and the difference in the behavior of magnetic susceptibility in field-cooled and zero-field-cooled cases was explained.

So, the problem of theoretical description of SG per se was solved, in principle, on MF level. Ever since different other models appeared without any connection to real experiments and real physical systems. The main feature of these models was the absence of reflection symmetry—in contrast to the SK model. The most investigated models among those are the p -spin models and the Potts models, considered, for example, in Refs. 9–12. The spherical p -spin model (see, e.g., Ref. 13) was for a long time believed to be a generic for this class of models. From the point of view of RSB the main feature of this model is the stability of the first step of RSB (1RSB) down to zero temperature. Also, the order parameter behaves stepwise. Although this model was not aimed to describe any real glass it appeared to be very interesting because its behavior gave a scenario for real liquid-glass transition: two critical temperatures, the number of metastable states similar to that obtained in numerical simulations. It should be noted that the structure of the dynamical equations for the correlation functions is identical for both the supercooled liquids in the mode-coupling theory and for the p -spin spherical SG model.¹⁰

Based mainly on investigations of these two models—SK and p -spin spherical—a conclusion appears in the literature attributing two classes of universality to models with and

without reflection symmetry. In the disordered case a number of attempts were made to formulate a kind of universality rules based on the mean-field investigation of the model systems with random interactions.^{9,10}

Looking now, in general, at the free-energy series over the glass order parameter we see that the series contain explicitly the terms which can be classified by the reflection symmetry. In general case in addition to the reflection-symmetrical part¹⁴

$$\frac{\Delta F^s}{NkT} = \lim_{n \rightarrow 0} \frac{1}{n} \sum [\dots + a_3 \delta q^{\alpha\beta} \delta q^{\beta\gamma} \delta q^{\gamma\alpha} + a_4' (\delta q^{\alpha\beta})^4 + a_4 \delta q^{\alpha\beta} \delta q^{\beta\gamma} \delta q^{\gamma\delta} \delta q^{\delta\alpha} \dots] \quad (5)$$

there is a part without the reflection symmetry, namely, the terms with odd number of identical replica indices

$$\frac{\Delta F^{ns}}{NkT} = \lim_{n \rightarrow 0} \frac{1}{n} \sum [\dots + b_3 (\delta q^{\alpha\beta})^3 + \dots + b_4 \delta q^{\alpha\beta} \delta q^{\beta\gamma} \delta q^{\gamma\alpha} \delta q^{\delta\alpha} \dots]. \quad (6)$$

The coefficients a_i contain only averages of even degrees of the operator U while in each of b_i enter some averages of the odd ones. Thus, a natural question arises: whether there can be made a general statement regarding the behavior of SG models with and without reflection symmetry? Do all models of the first-type behave in fact like the SK model and all models of the second type like the p -spin spherical model? In this paper we try to answer this question. We prove that for arbitrary models with reflection symmetry the Parisi FRSB always holds. In the absence of reflection symmetry the situation is not so definite and the behavior of the system depends on some additional characteristics. In any case it is not always similar to that of the p -spin spherical model, as it was usually believed: we give the counterexamples that present a generalization of p -spin model to three-quadrupole glasses with momenta $J=1, 2$.

II. GENERALIZED SK MODEL: FRSB

A. SK model with reflection symmetry

In this case it occurs to be possible to prove a kind of a theorem. We consider a generalized model with reflection symmetry defined by the Hamiltonian (1) with the interactions distributed according to Eq. (2) and with arbitrary diagonal operators U . The reflection symmetry implies that for any integer k

$$\text{Tr}[U^{(2k+1)}] = 0. \quad (7)$$

The saddle point conditions for the free energy averaged over disorder define the glass order parameter

$$q^{\alpha\beta} = \text{Tr}[U^\alpha U^\beta \exp(\theta)] / \text{Tr}[\exp(\theta)] \quad (8)$$

and the auxiliary order parameter

$$w^\alpha = \text{Tr}[(U^\alpha)^\gamma \exp(\theta)] / \text{Tr}[\exp(\theta)]. \quad (9)$$

Here

$$\theta = \frac{t^2}{2} \sum_{\alpha} w^\alpha (U^\alpha)^2 + t^2 \sum_{\alpha > \beta} q^{\alpha\beta} U^\alpha U^\beta, \quad (10)$$

where $t = \tilde{J}/kT$ and we choose $J_0=0$ for simplicity.

In the RS approximation we find the solution q_{RS} that is zero at high temperature. The bifurcation condition in this case is

$$1 - t_c^2 w_{\text{RS}}^2(t_c) = 0. \quad (11)$$

This equation coincides with $\lambda_{\text{repl(RS)}}=0$ (see, e.g., Ref. 8). It is zero high-temperature solution that bifurcates. At $T < T_c$ certain nontrivial 1RSB solutions appear but they are unstable.

Investigating 1RSB, 2RSB, 3RSB, ..., n RSB, and so on, we see that the equations for the glass order parameters always contain the quantity

$$\text{Tr}[U \exp(\theta_{n\text{RSB}})] / \text{Tr}[\exp(\theta_{n\text{RSB}})]. \quad (12)$$

Here $\theta_{n\text{RSB}}$ are the analogs of Eq. (10) for higher stages of RSB (see Ref. 16 for details). Therefore, one of the solutions of these equations is trivial at each of the RSB steps and the appearance of the n RSB solution can be regarded as the bifurcation of the trivial $(n-1)$ RSB solution. In this case, the equation $\lambda_{n\text{RSB}}=0$ coincides with the corresponding branching condition in Eq. (11). This means that in any case, the n RSB solutions at different stages of the symmetry breaking can exist at the temperature $T < T_c$ determined by this bifurcation condition and so we always can look for FRSB solution. Writing the free energy as a series over $\delta q^{\alpha\beta}$ near T_c (up to the fourth order for so-called truncated model, see Refs. 8 and 15) we obtain $q(x)=cx$ in the leading approximation (a similar procedure was described in details in Ref. 16). It is important that it is the zero solution that bifurcates. This enables one to obtain analytically the FRSB solution. It is possible to write the free energy in the form of Parisi with the only difference in the boundary conditions for the Parisi function ϕ that now reads

$$\phi(1, y) = \ln \text{Tr} \left\{ \exp \left[tyU + \frac{t^2}{2} (w - q(1)) U^2 \right] \right\}. \quad (13)$$

Thus we have shown that in the case of systems with reflection symmetry, the infinite FRSB holds at the very point at which the RS solution becomes unstable. In particular, our result means that magnetic systems of arbitrary spin with the interaction between the z components behave in the same way.

B. SK model without reflection symmetry

We consider below several models without reflection symmetry. These models correspond to some real physical systems. Let us note that it is easy to trace how the proof given above fails using the model proposed in Ref. 17. Now we have the same Hamiltonian (1) but without the condition (7) for the operators U .

The difference between two cases is already manifested in the RS approximation. In the case when the condition (7) is not fulfilled for the Hamiltonian (1) the order parameters x_{RS}

and q_{RS} are nonzero everywhere in temperature. The disorder smears out the first-order phase transition which takes place in regular systems without disorder. Hence, instead of a transition, there is a smooth increase in the order parameters (both glass and regular) as the temperature decreases. This situation is seen in experiments on orientational glass phase in *ortho-para*-hydrogen mixed crystals and in Ar-N₂.¹⁸ These substances present mixtures of spherically symmetric molecules and momentum-bearing molecules. The corresponding glass was investigated on the base of the Hamiltonian (1) with $U=Q$, where $Q=3J_z^2-2$, $\mathbf{J}=1$.¹⁹ The RSB solution branches continuously and smoothly on cooling breaking the RS results in a transition to the nonergodic phase of the quadrupolar glass.

Another example of a SG-like phase in molecular crystal is presented by pure *para*-H₂ (or *ortho*-D₂) under pressure.²⁰ The possibility of orientational order in systems of initially spherically symmetric molecule states is due to the involving of higher order orbital moments $J=2,4,\dots$ in the physics under pressure. With increasing density the anisotropic interaction potential and the crystal field grow rapidly and the energy of the many-body system can be lowered taking advantage of the anisotropic interactions. The long-range orientational order appears abruptly at some fixed value of pressure through the first-order phase transition just as it takes place in *ortho-para* mixtures when the concentration of moment-bearing molecules achieves certain fixed value. In the intermediate concentration range the frustration and disorder give the basis to the investigation of quadrupole glass with $J=2$. Such a theory was constructed in Ref. 21. The essential feature of the obtained intermediate phase is the coexistence of orientational glass phase with long-range orientational order as it is seen in the experiment.

Let us consider two more models describing SG-like states in real complex nonmagnetic systems, namely, in systems of clusters. Although they are not mixtures of different kinds of particles with different interactions, one can find frustration and disorder, that is the background to consider the systems in the spirit of SG theory. Now the operator U in Eq. (1) is to be replaced with continuous functions of angles.

In Ref. 22 a model for low-temperature transition to the orientational glass state in solid molecular C₆₀ was developed. Although the molecules have nearly spherical shape, at low temperature there are two pronounced minima in the anisotropic part of intermolecular interaction energy. It is possible to trace an analogy with the mixtures by studying the role of mutual molecular orientations of different types. As a result, a model is constructed where the role of spin is played by certain combinations of cubic harmonics. The results agree well with the experimental data: the coexistence of the glass state and the long-range orientational order and the existence of a wide maximum on the curve for the orientational part of the heat capacity. Moreover, the above model permits considering the pressure dependence of orientational transitions for small pressures.²³

The other model we would like to mention is the SG-like freezing of clusters of different symmetries in supercooled liquids that gives a possible description of liquid-glass transition. In Ref. 24 we used a microscopic approach based on equations for the distribution functions which in spirit of

Bogoliubov hierarchy gave us a possibility to analyze the intercluster interaction. We show that there exists a region of densities and temperatures where this interaction changes sign as a function of the cluster radius generating therefore the frustration in the system. This is the base to write a Hamiltonian of the form (1) with different point group harmonics for U and use standard methods of SG theory to describe real glasses.

So, we have considered a set of models with two-particle interaction where the absence of reflection symmetry is caused by the characteristics of the operators U themselves. In this case the RSB solution bifurcates from the RS solution smoothly, without a jump, and the coexistence of glass order with long-range regular order takes place.

III. GENERALIZED p -SPIN MODEL

Let us consider now a generalization of well-known p -spin model¹² of Ising spins to the case of arbitrary operators. The Hamiltonian has the form

$$H = - \sum_{i_1 \leq i_2 \leq \dots \leq i_p} J_{i_1, \dots, i_p} U_{i_1} U_{i_2} \dots U_{i_p}, \quad (14)$$

where $i=1,2,\dots,N$, p is the number of interacting particles and U is an arbitrary traceless diagonal operator. This means that U can take some k values $U=U_1, U_2, \dots, U_k$ and the sum $\text{Tr } U \equiv \sum_1^k U_k = 0$. We do not specify its form here, in order to use general formulas further. Independent interactions have the Gaussian distribution

$$P(J_{i_1, \dots, i_p}) = \frac{\sqrt{N^{(p-1)}}}{\sqrt{p! \pi \tilde{J}}} \exp \left[- \frac{(J_{i_1, \dots, i_p})^2 N^{(p-1)}}{p! \tilde{J}^2} \right]. \quad (15)$$

Using the standard procedure of replica approach we obtain the (effective) free energy and the equations for the order parameters in Eqs. (8) and (9) but now with

$$\theta = p \frac{t^2}{2} \sum_{\alpha > \beta} (q^{\alpha\beta})^{(p-1)} U^\alpha U^\beta + p \frac{t^2}{4} \sum_{\alpha} (w^\alpha)^{(p-1)} (U^\alpha)^2. \quad (16)$$

We perform the first stage RSB (n replicas are divided into n/m_1 groups each containing m_1 replicas) and obtain the free energy in the form

$$F_{1RSB} = -NkT \left[m_1 t^2 (p-1) \frac{r_1^p}{4} + (1-m_1)(p-1) t^2 \frac{(r_1 + v_1)^p}{4} - t^2 (p-1) \frac{w_1^p}{4} + \frac{1}{m_1} \int dz^G \ln \int ds^G [\text{Tr} \exp \theta_{1RSB}]^{m_1} \right]. \quad (17)$$

Here $q^{\alpha\beta} = r_1$ if α and β are from different groups and $q^{\alpha\beta} = r_1 + v_1$ otherwise

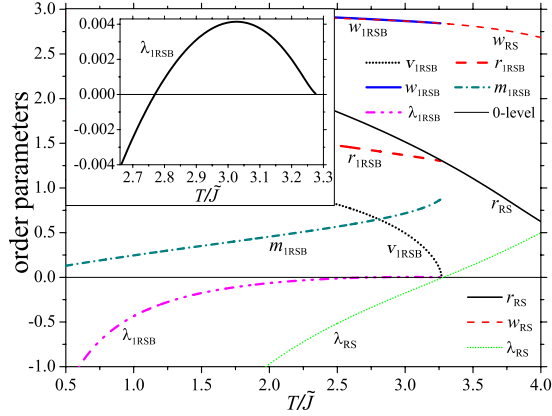


FIG. 1. (Color online) Temperature dependence of the glass order parameters for the quadrupole glass with three particle interaction for $J=1$. The RSB occurs at the temperature corresponding to the condition $\lambda_{(\text{RS})\text{repl}}=0$.

$$\theta_{\text{IRSB}} = zt \sqrt{\frac{pr_1^{(p-1)}}{2}} U + st \sqrt{\frac{p[(r_1 + v_1)^{(p-1)} - r_1^{(p-1)}]}{2}} U + t^2 \frac{p[w_1^{(p-1)} - (r_1 + v_1)^{(p-1)}]}{4} U^2. \quad (18)$$

We performed detailed calculations for two models with $p=3$ and U being the quadrupolar moments for $J=1$ and for $J=2$ cases. The results of calculations are illustrated in Fig. 1 ($J=1$) and Fig. 2 ($J=2$). At the point T_{bif} the RS solution bifurcates. In the case $J=1$ (Fig. 1) the new solution goes left (with T), $m(T_{\text{bif}}) < 1$ and the transition is continuous. In the case $J=2$ (Fig. 2) $m(T_{\text{bif}}) > 1$, the new solution goes right and makes a loop giving rise to a jumpwise behavior of the glass order parameter at $m=1$. The stability of the 1RSB solution against further RSB was checked in the standard way^{2,21} looking at the positive values of $\lambda_{(\text{1RSB})\text{repl}}$ (defined as the bifurcation point where the nonzero order parameter v_2 in 2RSB appears)

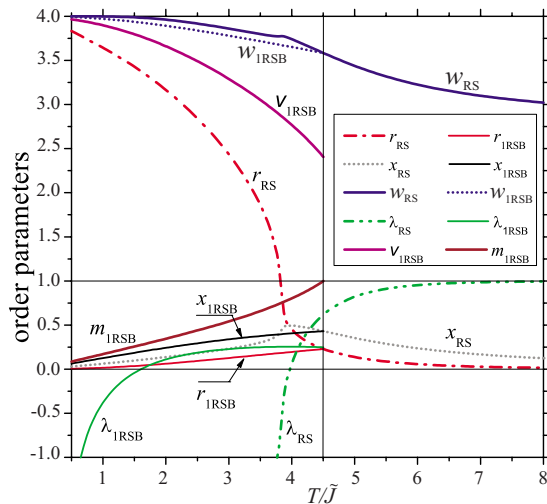


FIG. 2. (Color online) Temperature dependence of the order parameters for the quadrupole glass with three particle interaction for $J=2$. The transition RS-1RSB takes place at the point defined by the condition $m=1$. The glass order parameter v_1 has the jump at this point. Here x is the regular orientational order parameter.

$$\lambda_{(\text{1RSB})\text{repl}} = 1 - \frac{t^2}{2} p(p-1)(r_1 + v_1)^{(p-2)} \times \int dz^G \int ds^G [\text{Tr exp } \theta_{\text{1RSB}}]^{m_1} \times \left\{ \frac{\text{Tr}(U^2 \exp \theta_{\text{1RSB}})}{\text{Tr exp } \theta_{\text{1RSB}}} - \left[\frac{\text{Tr}(U \exp \theta_{\text{1RSB}})}{\text{Tr exp } \theta_{\text{1RSB}}} \right]^2 \right\}^2 \times \left\{ \int ds^G (\text{Tr exp } \theta_{\text{1RSB}})^{m_1} \right\}^{-1}. \quad (19)$$

So, it turns out that in the case of the three-particle interaction between quadrupoles with $J=2$ as well as with $J=1$ the first stage RSB is stable only in a finite temperature region (as was first showed in Ref. 12 for p -spin model) and not down to zero temperature. This is one of our key results. As concerns the models with multiple interactions, this property was investigated for the Potts model with three states in Ref. 25 (see, also Ref. 26) and for more complicated models with two interactions in Refs. 27–30.

IV. CONCLUSION

We have considered several examples of behavior of complex spin-glass-like systems. The set of physical systems described by such generalized models is very wide. On the other hand, all of them can be divided into two classes depending on whether reflection symmetry is present or not.

We have shown that in the case of systems with reflection symmetry, the infinite FRSB in the sense of Parisi takes place at the very point at which the RS solution becomes unstable. Such behavior is well known for the SK spin model. In particular, our result means that magnetic systems of arbitrary spin with interaction between z spin components behave in the same way.

If there is no reflection symmetry, then the situation is not so definite. The behavior of a particular system depends on some additional characteristics. An important factor in studying such systems is the absence of a trivial RS solution. We have considered a set of models with the two-particle interaction where the absence of reflection symmetry was caused by the characteristics of the operators U themselves. In this case the RSB solution bifurcates from the RS solution smoothly, without a jump. The jump appears in the three-quadrupole glass model with $J=2$. The coexistence of the glass order with the long-range regular order takes place in both cases.

The properties of the models considered in our paper are not similar to those of the p -spin spherical model as follows from the counterexamples (Figs. 1 and 2). We have shown that in these cases under certain additional conditions, there exists a finite domain of stability for the 1RSB state. This was apparently first shown for the simple nonspherical models in Refs. 2 and 21. Let us note that it is easy to trace how the proof given above fails using the model proposed in Ref. 17. This effect was discovered for the Potts model with three states in Ref. 25 earlier. We believe that the FRSB is attained as a result of several successive transitions occurring as the temperature decreases.

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