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A SPIN-GLASS-LIKE PHASE IN COMPLEX NONMAGNETIC SYSTEMS. VARIOUS KINDS OF REPLICA SYMMETRY BREAKING

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A brief review of the works of the authors on generalized spin glass models is given. The problem of the dependence of transition scenario on different factors is discussed. A classification of spin glasses behavior as depending on symmetry characteristics of systems is proposed.

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In this report dedicated to the memory of Nikolay Nikolaevich Bogolyubov, we are dealing with spin glass theory. We note that spin glass (SG) theory is an important field of modern statistical mechanics, where, just as in other fields, Bogolyubov's concept of quasi-averages [1] is most important for understanding the essence. While usually quasi-averages are introduced using an external field, the quasi-averages describing replica symmetry breaking (RSB) in SG are defined through infinitesimal interaction between the replicas*.

Our aim now is twofold: first, we show that there exist a number of real complex nonmagnetic physical systems that have much in common with the traditional spin glasses and that can be described using the standard methods of SG theory; second, we use our results to clear some points in the classification of the different kinds of SG behavior. Extending the class of models permits considering the role of different factors in the scenarios for the appearance of SG-type nonergodic states.

The theory of spin glasses appeared as an attempt to describe unordered equilibrium freezing of spins in actual dilute magnetic systems with disorder and frustration. This problem was soon solved in principle by Sherrington and Kirkpatrick, Edwards and Anderson, and Parisi (see [2] for a review). The

*See, e.g., Sec. 12 in *Moskalenko V. A. et al.* The Self-Consistent Field Method in the Theory of Glassy States of Spin and Quadrupole Systems (Kishinev: Shtiintsa, 1990).

Sherrington–Kirkpatrick (SK) Hamiltonian is of the form

$$H = -\frac{1}{2}\sum_{i\neq j} J_{ij} U_i U_j, \tag{1}$$

and describes Ising spins U located at the lattice sites i, j, and the quenched interactions J_{ij} are distributed with Gaussian probability

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

with $J = \tilde{J}/\sqrt{N}$, $J_0 = \tilde{J}_0/N$. To perform averaging over disorder in this case one has to average the quenched free energy F rather than the partition sum Z itself. The standard method for performing such an average is the replica method. After averaging the free energy becomes a function of the order parameters depending on replica indices:

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

The free energy $F(x^\alpha, q^{\alpha\beta})$ has an extremum at replica symmetric (RS) solution when all $q^{\alpha\beta}$ are equals. However, this state is unstable under RSB. Parisi proposed a schema of RSB step by step obtaining as a limit full RSB (FRSB) when $q^{\alpha\beta}$ becomes a continuous function of a parameter x. The results describe the main features of experiments on spin glasses.

So, the problem of theoretical description of SG *per se* was solved in principle and at that time different other models appeared without any connection to real experiments and real physical systems. The main feature of these models was the absence of time reversal symmetry — in contrast to the SK model. The most investigated among those are p-spin models and Potts models, considered in the papers by E. Gardner, A. Crisanti, H.-J. Sommers, D. Thirumalai, T. R. Kirkpatrick, etc. The spherical p-spin model was 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 jumpwise. Although this model was not aimed to describe any actual glass, it occurs to be very interesting because its behavior gives a scenario for real liquid-glass transition: two critical temperatures, the number of metastable states similar to that obtained in numerical modelling. The structure of the dynamical equations for the correlation functions of supercooled liquids in mode-coupling theory and that for p-spin SG model are identical [3].

Based mainly on the investigation of these two models — SK and p-spin spherical — a conclusion appears in the literature attributing a kind of two classes of universality to the models with and without reflection symmetry. As is well known, reflection symmetry plays an important role in characterizing the phase transitions in regular mean-field models without disorder. The presence of cubic terms in the free-energy expansion leads to a first-order phase transition, and their absence results in a second-order phase transition. In several papers where systems with random interaction were studied in the mean-field approximation, attempts were made to formulate a kind of universality rules for disordered case (see, e.g., [3,4]). It is worth noting that the series in order parameter for the free energy in replica approach contains explicitly in addition to that of the reflection symmetrical case

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

the part without reflection symmetry: the terms with 3 equal replica indices:

$$\frac{\Delta F^{ns}}{NkT} = \lim_{n\to 0}\frac{1}{n}\sum\left[\ldots + b_3(\delta q^{\alpha\beta})^3 + \ldots + b_4\delta q^{\alpha\beta}\delta q^{\beta\gamma}\delta q^{\gamma\alpha}\delta q^{\delta\alpha}\ldots\right].$$

So, a natural question arises: whether there can be made a general statement about the behavior of SG models with and without reflection symmetry? do all models of the first type behave in fact as SK model and all models of the second type as p-spin model? Now we try to answer this question.

First, let us consider a generalized model with reflection symmetry. In this case, it occurs to be possible to prove a kind of a theorem. We consider the Hamiltonian (1) with the interactions given by (2) and arbitrary diagonal operators U. The reflection symmetry means

$$\mathrm{Tr}\left[\hat{U}^{(2k+1)}\right] = 0 \tag{3}$$

for any integer k. The saddle point conditions for the free energy averaged over disorder give the glass order parameter $q^{\alpha\beta} = \mathrm{Tr}\,[U^\alpha U^\beta \exp(\hat\theta)]/\mathrm{Tr}\,[\exp(\hat\theta)]$ and auxiliary order parameter $p^\alpha = \mathrm{Tr}\,[(U^\alpha)^2\exp(\hat\theta)]/\mathrm{Tr}\,[\exp(\hat\theta)]$. Here

$$\hat\theta = \frac{t^2}{2}\sum_\alpha p^\alpha (U^\alpha)^2 + t^2\sum_{\alpha>\beta} q^{\alpha\beta}U^\alpha U^\beta, \tag{4}$$

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

In RS approach one has the trivial solution $q_{\mathrm{RS}} = 0$. The bifurcation condition gives

$$1 - t_c^2 p^2(t_c) = 0. \tag{5}$$

This equation coincides with $\lambda_{\rm repl(RS)} = 0$ (see [2]). It is very important that it is zero solution that bifurcates. Realizing the 1RSB, then 2RSB, 3RSB, and so on, we see that the equations for the glass order parameters always contain the quantity ${\rm Tr}\,[U \exp{(\hat{\theta}_{n\rm RSB})}]/{\rm Tr}\,[\exp{(\hat{\theta}_{n\rm RSB})}]$. Therefore, one of the solutions is trivial at each of the RSB steps, and the appearance of the nRSB solution can be regarded as a bifurcation of the trivial $(n-1)$RSB solution. In this case, the equation $\lambda_{n\rm RSB} = 0$ coincides with the corresponding branching condition (5). This means that in any case, the nRSB 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 free energy as a series in $\delta q^{\alpha\beta}$ near T_c (up to the fourth order of magnitude inclusively), we obtain $q(x) = cx$ in leading approximation (see [5] for details). It is also possible to write free energy in the form of Parisi [2] with the only difference in the boundary conditions for the Parisi function ϕ that now reads

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

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

Let us consider now some examples of models without reflection symmetry and some real physical systems corresponding to such models (see also [6] and the references therein). It is easy to trace how the proof given above fails using the model of [7]. The difference between two cases is already manifested in the RS approximation. In the case when the condition (3) is not fulfilled for the Hamiltonian (1) there is no trivial solution for the order parameters. The disorder smears out the first-order phase transition; 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 $\rm Ar - N_2$. These substances present mixtures of spherically symmetric molecules and momentum bearing molecules. The corresponding glass was described in [8] on the base of the Hamiltonian (1) with $U = Q$, where $Q = 3J_z^2 - 2$, $\mathbf{J} = 1$. The RSB solution branches continuously and smoothly on cooling. Breaking the RS results in a transition to the nonergodic phase of quadrupolar glass.

Another example of a SG-like phase in molecular crystal is presented by pure para-H_2 (or ortho-D_2) under pressure. The possibility of orientational order in systems of initially spherically symmetric molecule states is due to the involving of higher order orbital moments $J = 2, 4, \ldots$ in the physics under pressure. With increasing density the anisotropic interaction potential and the crystal field grow rapidly and the energy of many-body system can be lowered by taking advantage of the anisotropic interactions. The long-range orientational order appears abruptly at a 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 [9] for the numbers of interacting particles $p = 2, 3$. The essential feature of the obtained intermediate phase in both models is the coexistence of orientational glass with long-range orientational order as is seen in the experiment.

For all quadrupolar glass models considered the RSB was performed and the stability of the 1RSB solution against further RSB was checked. The very important result is that in the case of three-particle interaction between quadrupoles with $J = 2$ as well as with $J = 1$ the first stage RSB is stable only in the finite region of temperature and not down to zero temperature.

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 (1) is replaced with continuous functions of angles.

In [10] a model for low-temperature transition to the orientational glass state in solid molecular C_{60} 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 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.

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 the papers [11] we use the microscopic approach based on equations for distribution functions which are in spirit of Bogolyubov hierarchy 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 and there is, hence, 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.

To conclude, we have shown that for arbitrary models with reflection symmetry the Parisi FRSB always takes place. In the absence of reflection symmetry the situation is not so definite. The behavior of the system depends on some additional characteristics. In any case, it is not always similar to that of p-spin spherical model, as is usually believed. We present three counterexamples. We have shown that in this case under certain additional conditions, there exists a finite domain of stability of the 1RSB. This was apparently first shown for simple nonspherical models in our papers [6, 9]. This fact was discovered for the Potts model with three states in [12] earlier.

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