Replica symmetry breaking for a simple model of a quadrupolar glass

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The first stage of the replica symmetry breaking for a simple quadrupolar glass model using the Parisi ansatz has been performed in a wide range of temperatures including $T=0$. It has been obtained that the entropy of the system increases considerably compared to that calculated within the replica symmetric theory. [S0163-1829(96)05326-X]

Much effort has been dedicated in recent years to the clarification of the nature of nonmagnetic frustrated systems such as Potts and quadrupolar glasses (QG's).[1] Though these systems have been considered mostly within the replica symmetric (RS) theory some attempts to study the replica symmetry-breaking (RSB) mechanism have been made.[1–6,8] However, despite the success of the Parisi RSB scheme[8] for magnetic systems with the spin-reversal symmetry (the Ising and m-vector model) a convincing theory does not exist for richer models of disordered systems. The analysis of the RSB problem for quadrupolar and Potts glasses has been performed using the simplified Landau free energy of the system expanded up to fourth order into the glassy order parameter. Such an approach is limited to the range where the order parameter is sufficiently small, but it is not adequate for the study of the system at lower temperatures. In general, the study of properties of such systems in the whole range of temperature (without Landau expansion) is rather a complicated task because of the complexity of interactions which makes it difficult to express the free energy in a closed form. Nevertheless, it would be interesting and desirable to attempt to perform RSB investigations for a possible simplest model. We have in mind the quadrupolar system with strong anisotropy in the z direction described by the following $S=1$ spin (or pseudospin) Hamiltonian:

$$H=\sum_{i,j} J_{ij}\mathcal{O}_i^0\mathcal{O}_j^0\,, \tag{1}$$

where J_{ij} denotes the coupling between quadrupoles located at sites i,j and

$$\mathcal{O}_i^0=3(S_i^z)^2-2\,. \tag{2}$$

It is assumed that J_{ij}'s are quenched random interactions of infinite range independently distributed according to the probability distribution:

$$P(J_{ij})=\sqrt{\frac{N}{2\pi J^2}}\,\exp(-NJ_{ij}^2/2J^2), \tag{3}$$

where $N\rightarrow\infty$ denotes the number of spins (pseudospins).

The short-ranged version of the Hamiltonian (1) with the nonrandom couplings J_{ij}'s, called otherwise the truncated electric quadrupole-quadrupole (EQQ) Hamiltonian, has been used a number of years ago[9] for formulation in a crude approximation of the theory of the order-disorder transition in solid orthohydrogen ($o-H_2$). In this case $S=1$ denotes the rotational quantum number of quadrupole-bearing molecule of $o-H_2$. However, as it was discussed in Ref. 10 some insight into the nature of the quadrupolar glassy freezing of randomly distributed molecules of $o-H_2$ in a matrix of spherical parahydrogen species can be obtained from the model (1) [for the concentration of $o-H_2$ smaller than 55% the system forms a QG (Refs. 10 and 11)]. Of course, the Hamiltonian (1) does not describe exactly the situation in solid hydrogen but for its relative simplicity is a good theoretical laboratory for exploring some crucial aspects which would be much harder to access from the more realistic quantum EQQ Hamiltonian.[10,12]

The model (1), with a mean of J_{ij} not necessarily equal to zero, has been solved within the RS theory.[13,14] In Ref. 15 the stability limit of the RS phase of the model (1) has been studied. It has been found that above some temperature $T_c=1.367J/k_B$ the RS phase is stable, whereas at $T<T_c$ becomes unstable. This means that as the temperature is lowered and reaches T_c the system undergoes a transition from ergodic to nonergodic phase with multiple minima of free energy characteristic of the glassy state with the broken replica symmetry. However, this is not a phase transition in an usual thermodynamic sense since the QG order parameter increases continuously with the decreasing of temperature.[13,14] Such a situation is observed in solid ortho-parahydrogen mixtures.[10] The order parameter is not a small quantity near T_c. Hence in order to study our system we cannot use, in the region of temperature (except maybe very high temperatures), the Landau expansion for the free energy. According to the knowledge of the authors, existing investigations about RSB in QG's have used the Landau expansion.[1–7]

The aim of the present paper is to study the RSB theory for the model (1) in the wide region of temperature, that is for $0\leqslant T\leqslant T_c$, using the Parisi ansatz.[8] Since an explicit calculation for an arbitrary stage of RSB is a difficult problem and rather unfeasible practically we restrict ourselves to the first stage. We expect that even this simplest approach will give us some insight into the RSB mechanism in QG's. Moreover, as it will be seen, even the theory with RSB at the first level leads to essential improvements on the thermodynamic properties of the system compared to the RS approach.[13,14]

We start from the free energy calculated, using the replica method in Ref. 15. At the first stage of RSB the elements $q_{\alpha\alpha'}$ of the $n\times n$ matrix, which are QG order parameters, take only two different values q_0 and q_1.[8] Proceeding in the strict analogy to the RSB scheme[8] we get

$$\sum_{\alpha\neq\alpha'}^{n} q_{\alpha\alpha'}^2 = -(\overline{x}-n)q_0^2-(1-\overline{x})q_1^2 \tag{4}$$

and

$$\sum_{\alpha\neq\alpha'}^{n} q_{\alpha\alpha'}\mathcal{O}_\alpha^0\mathcal{O}_{\alpha'}^0 = q_0\left(\sum_{\alpha=1}^{n}\mathcal{O}_\alpha^0\right)^2 + (q_1-q_0)\sum_{l=1}^{n/\overline{x}}\left(\sum_{\alpha=1}^{\overline{x}}\mathcal{O}_{\alpha,l}^0\right)^2 - q_1\sum_{\alpha=1}^{n}(\mathcal{O}_\alpha^0)^2. \tag{5}$$

We assume that the quadrupolar long-ranged order parameter (defined in Ref. 15) is the same for each replica, that is $m_\alpha = m$. Finally, we obtain in the limit $n\to 0$ the free energy, at the first stage of RSB, in the form

$$\frac{F}{N}=\frac{\beta J^2\overline{x}}{4}(q_1^2-q_0^2)-\frac{\beta J^2}{4}(q_1+m-2)(q_1-m-2) - \frac{1}{\beta\overline{x}}\int_{-\infty}^{\infty}dP_{q_0}(y)\ln\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}} \tag{6}$$

with

$$dP_a(\xi)=\frac{1}{\sqrt{2\pi a}}\exp\left(-\frac{\xi^2}{2a}\right)d\xi \tag{7}$$

and

$$Z_0 = 2e^{\vartheta}+e^{-2\vartheta} \tag{8}$$

where

$$\vartheta = \beta J(y+z)-\frac{(\beta J)^2}{2}(2-m-q_1). \tag{9}$$

In Eq. (6) $q_1 > q_0$ and $\overline{x}$ is understood as a real number in the interval between 0 and 1.

Stationarity of F with respect to the variables q_1, q_0, m and $\overline{x}$ gives the following set of self-consistent equations:

$$q_1 = 4\int_{-\infty}^{\infty}dP_{q_0}(y) \times\frac{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}[(e^{3\vartheta}-1)/(2e^{3\vartheta}+1)]^2}{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}}, \tag{10a}$$

$$q_0 = 4\int_{-\infty}^{\infty}dP_{q_0}(y) \times\left(\frac{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}[(e^{3\vartheta}-1)/(2e^{3\vartheta}+1)]}{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}}\right)^2, \tag{10b}$$

$$m = 2\int_{-\infty}^{\infty}dP_{q_0}(y) \times\frac{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}[(e^{3\vartheta}-1)/(2e^{3\vartheta}+1)]}{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}}, \tag{10c}$$

and

$$\frac{(\beta J)^2}{4}(q_1^2-q_0^2)+\frac{1}{\overline{x}^2}\int_{-\infty}^{\infty}dP_{q_0}(y)\ln\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}} - \frac{1}{\overline{x}}\int_{-\infty}^{\infty}dP_{q_0}(y)\frac{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}\ln Z_0}{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}}=0\,. \tag{10d}$$

Obviously as $q_1=q_0$ we get from Eqs. (10a)–(10d) the formulas of the RS theory.[13,14] At $T=0$ Eqs. (10a)–(10d) becomes ineffective to a numerical analysis because of indeterminate terms entering them. Nevertheless it is possible to transform analytically (10a)–(10d), in the limit $T=0$, to that form which is suitable to numerical computations. It is convenient in this case to introduce the parameter σ defined as

$$\sigma=\frac{\beta J}{2}(2-m-q_1). \tag{11}$$

It will be seen that at $T=0$ σ is finite. The variable ϑ (9) can be rewritten in the form

$$\vartheta=\beta J(y+z-\sigma). \tag{12}$$

Combining (10a) with (10c) we get the equation

$$\sigma = 9\beta J\int_{-\infty}^{\infty}dP_{q_0}(y)\frac{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}[e^{3\vartheta}/(2e^{3\vartheta}+1)^2]}{\int_{-\infty}^{\infty}dP_{q_1-q_0}(z)Z_0^{\overline{x}}}. \tag{13}$$

In the limit $\beta\to\infty$ we have

$$Z_0^{\overline{x}} = 2^{\overline{x}}\theta(y+z-\sigma)e^{\beta J\overline{x}(y+z-\sigma)} + \theta(\sigma-y-z)e^{-2\beta J\overline{x}(y+z-\sigma)}, \tag{14a}$$

$$\frac{e^{3\beta J(y+z-\sigma)}-1}{2e^{3\beta J(y+z-\sigma)}+1}=\frac{1}{2}\theta(y+z-\sigma)-\theta(\sigma-y-z), \tag{14b}$$

and

$$\ln Z_0 = [\ln 2\overline{x}+\beta J\overline{x}(y+z-\sigma)]\theta(y+z-\sigma) - 2\beta J\overline{x}(y+z-\sigma)\theta(\sigma-y-z), \tag{14c}$$

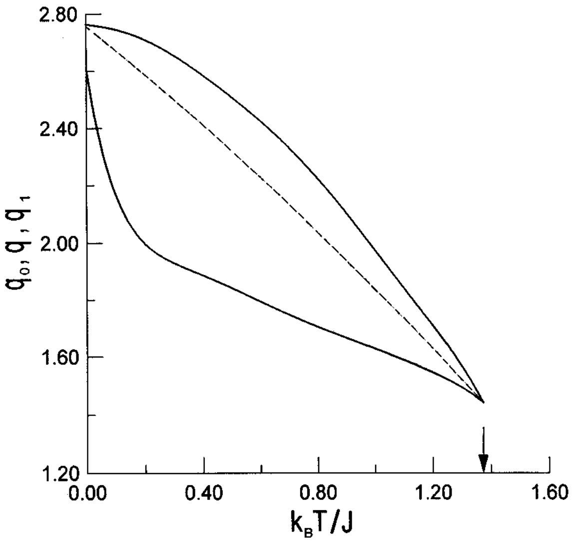

FIG. 1. The temperature dependence of the quadrupolar glass order parameters q_1 upper solid line, q_0 lower solid line, and q (replica symmetric theory) dashed line.

where $\theta(\xi)$ is the Heaviside step function. Concerning Eq. (13) we must expand $e^{3\vartheta}/(e^{2\vartheta}+1)^2$ into the power series with respect to $e^{-3\vartheta}$ and $e^{3\vartheta}$ when $y+z-\sigma>0$ and $y+z-\sigma<0$, respectively.

It turns out that a reasonable solution of our problem at $T=0$ can be obtained assuming that $\overline{x}$ is proportional asymptotically to T as $T\to 0$, that is we have

$$\overline{x}=xT. \tag{15}$$

With above simplifications the integration in Eqs (10a), (10b), (10d), and (13) over the variable z can be performed explicitly and one obtains for $T=0$

$$q_1=1+3\int_{-\infty}^{\infty} dP_{q_0}(y)\frac{B(y)}{A(y)+B(y)}, \tag{16a}$$

$$q_0=\int_{-\infty}^{\infty} dP_{q_0}(y)\left[\frac{A(y)-2B(y)}{A(y)+B(y)}\right]^2, \tag{16b}$$

$$\sigma=\frac{3}{\sqrt{2\pi(q_1-q_0)}}\int_{-\infty}^{\infty} dP_{q_0}(y)\frac{\exp[-(y-\sigma)^2/2(q_1-q_0)]}{A(y)+B(y)}, \tag{16c}$$

and

$$\frac{1}{x^2}\int_{-\infty}^{\infty} dP_{q_0}(y)\ln[A(y)+B(y)]-\frac{\ln 2}{x^2}-\frac{3}{4}(q_1^2-q_0^2)$$
$$-\frac{\sigma}{x}(2-3q_1)=0, \tag{16d}$$

where

$$A(y)=\exp\left[(q_1-q_0)\frac{x^2}{2}+x(y-\sigma)\right]$$
$$\times\left\{1-\mathrm{erf}\left[\frac{\sigma-y-(q_1-q_0)x}{\sqrt{2(q_1-q_0)}}\right]\right\} \tag{17a}$$

and

$$B(y)=\exp[2(q_1-q_0)x^2-2x(y-\sigma)]$$
$$\times\left\{1+\mathrm{erf}\left[\frac{\sigma-y+2(q_1-q_0)x}{\sqrt{2(q_1-q_0)}}\right]\right\}. \tag{17b}$$

Here $\mathrm{erf}(\xi)$ denotes the error function. Solutions of (16a) – (16d) are $q_1=2.763$, $q_0=2.611$, $\sigma=0.001$, and $x=4.709$.

To study the effect of this first stage RSB on the thermodynamic properties of the system we will calculate the entropy

$$\frac{S}{N}=-\frac{\partial}{\partial T}\left(\frac{F}{k_BN}\right). \tag{18}$$

Inserting into Eq. (18) F/N (6) with the help of Eqs. (10a) and (10b) one obtains

$$\frac{S}{N}=-\frac{3(\beta J)^2\overline{x}}{4}(q_1^2-q_0^2)+\frac{(\beta J)^2}{4}(q_1+m-2)$$
$$\times(3q_1-3m+2)$$
$$+\frac{1}{x}\int_{-\infty}^{\infty} dP_{q_0}(y)\ln\int_{-\infty}^{\infty} dP_{q_1-q_0}(z)Z_0^{\overline{x}}. \tag{19}$$

At $T=0$ the expression for the entropy considerably simplifies. With the help of Eq. (10d) we get

$$\frac{S(T=0)}{N}=-\sigma^2+\frac{4-q_1}{3}\ln 2. \tag{20}$$

From (20) it is seen that at $T=0$ the entropy does not depend on the parameter q_0. The results of the RS theory for entropy[13,14] can be easily reproduced if in Eqs. (19) and (20) we put $q_1=q_0=q$.

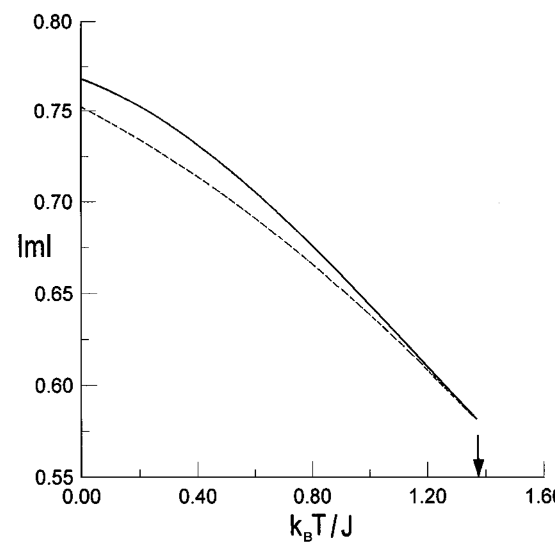

FIG. 2. The $|m|$ as a function of temperature. The first stage of replica symmetry breaking (solid line) and replica symmetry theory (dashed line).

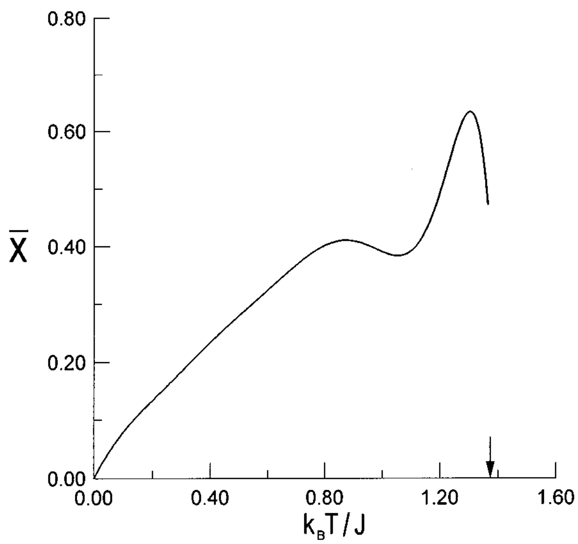

FIG. 3. A variation of $\overline{x}$ with the temperature.

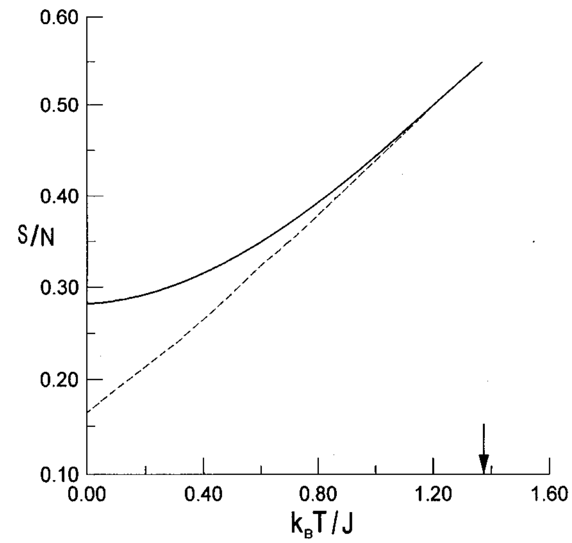

FIG. 4. The temperature dependence of the entropy S. The solid and dashed lines refer to the replica symmetry broken and replica symmetry solutions, respectively.

In order to obtain the temperature dependence (T dependence) of the parameters q_1, q_0, m, and $\overline{x}$ we have solved numerically Eqs. (10a)–(10d) for the finite $T<T_c$ and $T\approx T_c$. To these data we have included the zero-temperature results. A variation of QG parameters q_1 and q_0 with T is presented in Fig. 1. For a comparision the T dependence of the QG parameter obtained within the RS theory[13,14] is also given in this figure. In Fig. 2 the absolute value of the quadrupolarization (the quadrupolarization is always negative) as a function of the temperature is shown for the RSB as well as for RS theory.[13,14] Figure 3 contains the T dependence of $\overline{x}$. It is seen that $\overline{x}$ has physical non-negative values but as T approaches T_c this variable slightly oscillates. At the present stage of the theory it is difficult to explain that behavior, however we have no clear physical reasons to exclude it *a priori*. Finally in Fig. 4 the entropies calculated within the RSB and RS theories are given. It is seen that the first stage of RSB leads to the considerable increasing of entropy, particularly at low temperatures, compared to the RS result. This means that RSB solutions are closer to a physical reality than the ones obtained within the RS scheme.[13,14]

Up to now for quadrupolar systems, where a glassy phase transition takes place in the Landau sense, an investigation of RSB theory has been performed only near the transition point,[1–7] but no explicit information for lower temperatures have been obtained because of the complexity of the analyzed models. The present paper contains an attempt to formulate a theory of RSB at the first stage for a simple model of QG without the Landau expansion. In general, the obtained results seem to be reasonable physically. Our solutions give the Parisi QG parameter function in the form:

$$q(x)=q_0\theta(\overline{x}-x)+q_1\theta(x-\overline{x}), \qquad (21)$$

where $0\leqslant x\leqslant 1$. It has been shown for some models of QG's, in which a QG phase transition in the Landau sense takes place, that such a type of solution is stable near the critical point.[6,7] Therefore it would be interesting to perform a stability analysis of our RSB solution in the wide interval of temperature $0\leqslant T\leqslant T_c$. We hope to return to this problem in a future work.

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[1] K. Binder and J.D. Reger, Adv. Phys. **41**, 547 (1992), and references therein.
[2] D. J. Elderfield and D. Sherrington, J. Phys. C **16**, L495 (1983); **16**, L971 (1983); **16**, L1169 (1983).
[3] A. Erzan and E. J. S. Lage, J. Phys. C **16**, L555 (1983).
[4] P. M. Goldbart and D. Sherrington, J. Phys. C **18**, 1923 (1985).
[5] P. Goldbart and D. Elderfield, J. Phys. C **18**, L229 (1985).
[6] P. M. Goldbart, Ph. D. thesis, University of London (1985).
[7] E. A. Lutchinskaia and E. E. Tareeva, Teor. Mat. Fiz. **91**, 157 (1992) (in Russian).
[8] M. Mezard, G. Parisi, and M. A. Virasoro, *Spin Glass Theory and Beyond*, World Scientific Lecture Notes in Physics, Vol. 9 (World Scientific, Singapore, 1987).
[9] J. C. Raich and R. D. Etters, Phys. Rev. **161**, 493 (1967); A. B. Harris, Phys. Rev. B **1**, 1881 (1970).
[10] N. S. Sullivan, Can. J. Chem. **66**, 908 (1988).
[11] N. S. Sullivan, M. Devoret, and D. Estève, Phys. Rev. B **30**, 4935 (1984); Can. J. Phys. **65**, 1463 (1987).
[12] K. Walasek, Phys. Rev. B **46**, 14 480 (1992).
[13] E. A. Lutchinskaia, V. N. Ryzhov, and E. E. Tareyeva, J. Phys. C **17**, L665 (1984).
[14] E. A. Lutchinskaia, V. N. Ryzhov, and E. E. Tareyeva, Teor. Mat. Fiz. **67**, 463 (1986) (in Russian).
[15] K. Walasek, Phys. Rev. B **51**, 9314 (1995).