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Stability limit of the replica-symmetric phase of a simple quadrupolar glass model

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Using the de Almeida and Thouless method the stability limit of the replica-symmetric phase of the quadrupolar glass described by a simple model is studied without the Landau expansion for the free energy. The temperature dependence of the quadrupolar susceptibility is also calculated.

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 theory some attempts to study the replica-symmetry breaking mechanism have been made.[1–4] However, the analysis of the last problem as well as an investigation of the stability of the replica-symmetric phase have 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 quadrupolar and Potts glasses in the whole range of temperature is rather a complicated task because of the complexity of interactions in those systems. Nevertheless, it would be interesting and desirable to attempt to perform such 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:

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

where $N\to\infty$ denote 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 Hamiltonian, has been used a number years ago[5] (see also Ref. 6) for formulating in a crude approximation the theory of the order-disorder transition in solid hydrogen (in this case $S=1$ denotes the rotational quantum number of quadrupole-bearing molecules of orthohydrogen). For the long-ranged interaction $P\left(J_{ij}\right)$ obeying the Gaussian distribution (not necessary with the zero mean) the model (1) has been solved within the replica-symmetric theory.[7,8] As it was discussed in Ref. 9 the long-ranged version of (1) is not the situation in solid hydrogen, but it is useful in that it does lead to a glasslike ordering for the quadrupoles.

The main purpose of this paper is to investigate the limit of stability of the replica-symmetric solution of the model (1) which should be a first step before further studies. This will be realized in strict analogy to the de Almeida and Thouless stability analysis[10] of the replica-symmetric solution for the famous Sherrington-Kirkpatrick spin-glass model.[11] The replica method and saddle-point treatment[11] applied to the problem with the Hamiltonian (1) yield, for the free energy per site, the expression (see also Refs. 7 and 8)

$$\frac{\beta F}{N}=-(\beta J)^2+\lim_{n\to 0}\frac{1}{n}\left[\frac{(\beta J)^2}{4}\sum_{\alpha\neq\alpha'}q_{\alpha\alpha'}^2 +\frac{(\beta J)^2}{4}\sum_{\alpha}m_\alpha^2-\ln\operatorname{Tr}\exp\left(-\beta H[q,m]\right)\right] \tag{4}$$

with

$$H[q,m]=-\frac{\beta J}{2}\left[\sum_{\alpha\neq\alpha'}q_{\alpha\alpha'}\mathcal{O}_\alpha^0\mathcal{O}_{\alpha'}^0+\sum_\alpha(m_\alpha-2)\mathcal{O}_\alpha^0\right]\ , \tag{5}$$

where α,α' running from 1 to n refer to the replica number and $\mathcal{O}_\alpha^0$ denotes the operator $\mathcal{O}_i^0$ (2) referred to the αth replica of the system at an arbitrary site i. As a result of the saddle-point treatment one obtains the following self-consistent equations:

$$q_{\alpha\alpha'}=\langle\mathcal{O}_\alpha^0\mathcal{O}_{\alpha'}^0\rangle \tag{6a}$$

and

$$m_\alpha=\langle\mathcal{O}_\alpha^0\rangle\ , \tag{6b}$$

where the expectation value $\langle\cdots\rangle$ is taken with respect to the "single-site" Hamiltonian $H[q,m]$. It can be shown that the following relations hold:

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$$[\langle \mathcal{O}_i^0\rangle_T^2]_{\rm av} = \lim_{n\to 0}\frac{1}{n(n-1)}\sum_{\alpha\neq\alpha'} q_{\alpha\alpha'} \tag{7a}$$

and

$$[\langle \mathcal{O}_i^0\rangle_T]_{\rm av} = \lim_{n\to 0}\frac{1}{n}\sum_{\alpha} m_\alpha\ , \tag{7b}$$

where, as usual, $\langle\cdots\rangle_T$ and $[\cdots]_{\rm av}$ denote the thermal and sample averaging, respectively.

The problem now is to determine the stability condition of the replica-symmetric solution $q_{\alpha\alpha'} = q$ and $m_\alpha = m$. For this, as in the spin-glass theory,[10] one must require that, in the limit $n \to 0$, the eigenvalues of the Hessian with the elements

$$G_{\alpha,\alpha'} = \frac{2}{\beta J^2 N}\left(\frac{\partial^2 F}{\partial m_\alpha \partial m_{\alpha'}}\right)_{\{m_\alpha\}\equiv m,\{q_{\alpha\alpha'}\}\equiv q}\ , \tag{8a}$$

$$G_{(\alpha_1\alpha_2),(\alpha_3\alpha_4)} = \frac{2}{\beta J^2 N}\left(\frac{\partial^2 F}{\partial q_{\alpha_1\alpha_2}\partial q_{\alpha_3\alpha_4}}\right)_{\{m_\alpha\}\equiv m,\{q_{\alpha\alpha'}\}\equiv q}\ , \tag{8b}$$

and

$$G_{\alpha,(\alpha_1\alpha_2)} = \frac{2}{\beta J^2 N}\left(\frac{\partial^2 F}{\partial m_\alpha \partial q_{\alpha_1\alpha_2}}\right)_{\{m_\alpha\}\equiv m,\{q_{\alpha\alpha'}\}\equiv q} \tag{8c}$$

must be positive. After some algebra one obtains

$$G_{\alpha,\alpha} = A = 1 - \frac{(\beta J)^2}{2}\left(2 - \langle \mathcal{O}_\alpha^0\rangle - \langle \mathcal{O}_\alpha^0\rangle^2\right) = 1 - \frac{(\beta J)^2}{2}(2 - m - m^2)\ , \tag{9}$$

$$G_{\alpha,\alpha'} = B = -\frac{(\beta J)^2}{2}\left(\langle \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha'}\rangle - \langle \mathcal{O}_\alpha^0\rangle\langle \mathcal{O}_{\alpha'}^0\rangle\right) = -\frac{(\beta J)^2}{2}(q - m^2) \tag{10}$$

with $\alpha \neq \alpha'$,

$$\begin{aligned}G_{(\alpha\alpha'),(\alpha\alpha')} = P &= 2 - 2(\beta J)^2(4 - 2\langle \mathcal{O}_\alpha^0\rangle - 2\langle \mathcal{O}_{\alpha'}^0\rangle \\ &\quad + \langle \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha'}^0\rangle - \langle \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha'}^0\rangle^2) \\ &= 2 - 2(\beta J)^2(4 - 4m + q - q^2)\end{aligned} \tag{11}$$

with $\alpha \neq \alpha'$,

$$\begin{aligned}G_{(\alpha\alpha_1),(\alpha\alpha_2)} = Q &= -2(\beta J)^2(2\langle \mathcal{O}_{\alpha_1}^0 \mathcal{O}_{\alpha_2}^0\rangle - \langle \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha_1}^0 \mathcal{O}_{\alpha_2}^0\rangle \\ &\quad - \langle \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha_1}^0\rangle\langle \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha_2}^0\rangle) \\ &= -2(\beta J)^2(2q - t - q^2)\end{aligned} \tag{12}$$

with $\alpha_1 \neq \alpha_2$,

$$\begin{aligned}G_{(\alpha_1\alpha_2),(\alpha_3\alpha_4)} = R &= -2(\beta J)^2(\langle \mathcal{O}_{\alpha_1}^0 \mathcal{O}_{\alpha_2}^0 \mathcal{O}_{\alpha_3}^0 \mathcal{O}_{\alpha_4}^0\rangle \\ &\quad - \langle \mathcal{O}_{\alpha_1}^0 \mathcal{O}_{\alpha_2}^0\rangle\langle \mathcal{O}_{\alpha_3}^0 \mathcal{O}_{\alpha_4}^0\rangle) \\ &= -2(\beta J)^2(r - q^2)\end{aligned} \tag{13}$$

with $\alpha_1 \neq \alpha_2 \neq \alpha_3 \neq \alpha_4$,

$$\begin{aligned}G_{\alpha,(\alpha\alpha')} = C &= (\beta J)^2(\langle \mathcal{O}_{\alpha}^0\rangle\langle \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha'}^0\rangle + \langle \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha'}^0\rangle \\ &\quad - 2\langle \mathcal{O}_{\alpha'}^0\rangle) \\ &= (\beta J)^2(q - 2m + qm)\end{aligned} \tag{14}$$

with $\alpha \neq \alpha'$, and

$$\begin{aligned}G_{\alpha_1,(\alpha\alpha')} = D &= -(\beta J)^2(\langle \mathcal{O}_{\alpha_1}^0\rangle\langle \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha'}^0\rangle \\ &\quad - \langle \mathcal{O}_{\alpha_1}^0 \mathcal{O}_\alpha^0 \mathcal{O}_{\alpha'}^0\rangle) \\ &= -(\beta J)^2(t - qm)\end{aligned} \tag{15}$$

with $\alpha_1 \neq \alpha \neq \alpha'$. In the limit $n \to 0$ the parameters r and t entering Eqs. (14)–(16) are defined as

$$t = \frac{8}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-x^2/2}\left(\frac{e^{3\theta}-1}{2e^{3\theta}+1}\right)^3 \tag{16}$$

and

$$r = \frac{16}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-x^2/2}\left(\frac{e^{3\theta}-1}{2e^{3\theta}+1}\right)^4 \tag{17}$$

with

$$\theta = \beta J q^{1/2} x + \frac{(\beta J)^2}{2}(q + m - 2)\ , \tag{18}$$

where the QG order parameter q and quadrupolarization m satisfy the equations[7,8]

$$q = \frac{4}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-x^2/2}\left(\frac{e^{3\theta}-1}{2e^{3\theta}+1}\right)^2 \tag{19a}$$

and

$$m = \frac{2}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-x^2/2}\frac{e^{3\theta}-1}{2e^{3\theta}+1}\ . \tag{19b}$$

Equations (19a) and (19b) have no trivial solutions $q = 0$ and $m = 0$ at finite temperature (for numerical solution of these equations, see, Refs. 7 and 8). Therefore the model (1) does not lead to any sharp phase transition.

Now, following strictly the procedure of Ref. 10, we obtain that the eigenvalues of our Hessian reduce for $n = 0$ to

$$\lambda_\pm = \frac{1}{2}\left\{(A - B + P - 4Q + 3R) \pm [(A - B - P + 4Q - 3R)^2 - 8(C - D)^2]^{1/2}\right\} \tag{20}$$

and

$$\lambda = P - 2Q + R\ . \tag{21}$$

It can be shown that $\infty > \lambda_+ \geq 2$ as T varies from 0 to ∞, respectively, with the low-temperature asymptotic behavior $\lambda_+ \sim J/T$. For λ_- we have $0 \leq \lambda_- \leq 1$ as $0 \leq T < \infty$, respectively, and when the temperature tends to 0 vanishes as $\lambda_- \sim T/J$. In addition, numerical

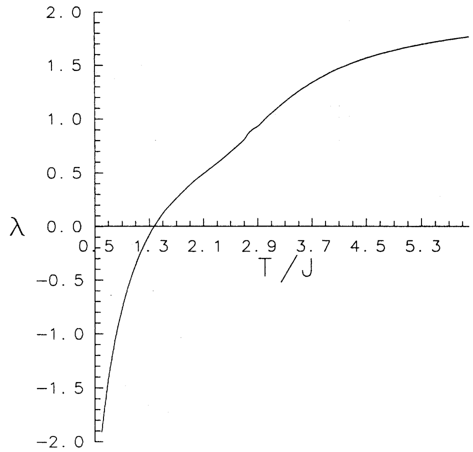

FIG. 1. The eigenvalue λ of the Hessian as a function of temperature.

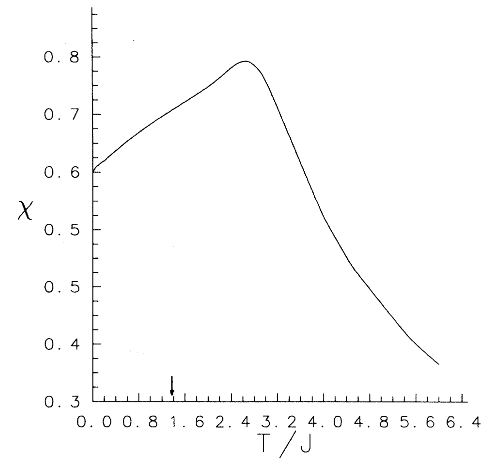

FIG. 2. The variation of the quadrupolar susceptibility χ with temperature. The arrow indicates $T_c \approx 1.367J$.

analysis shows that there is no region in which $\lambda_\pm$ would be negative.

Another situation emerges for λ, which is negative for $T < T_c$ and positive for $T > T_c$ with $T_c \approx 1.367J$. Therefore as the temperature is lowered and reaches T_c the system undergoes the transition from ergodic to nonergodic phase with multiple minima of the free-energy characteristic of the glassy state with the broken replica symmetry. In Fig. 1 the plot λ against T/J is presented.

It would be interesting to investigate the temperature dependence of the quadrupolar susceptibility $\chi = (\partial m/\partial h)_{h=0}$, where h denotes the reaction field. The quadrupolar susceptibility may be obtained adding an extra contribution βh to θ (18) and differentiating (19a) and (19b) with respect to h. In the limit $h \to 0$ one obtains

$$\chi = \frac{2T}{J^2}\left[\frac{P-4Q+3R}{(A-B)(P-4Q+3R)+2(C-D)^2}-1\right] . \tag{22}$$

In Fig. 2 the variation of $J\chi$ with T/J is shown. It is seen that the susceptibility exhibits a broad hump with the maximum at $T \approx 2.75J$ rather far from the temperature T_c.

The next step in the study of our model would be to clarify the applicability of Parisi's replica-symmetry breaking scheme[12] without the Landau expansion for the free energy. This problem is currently in progress.

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