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LETTER TO THE EDITOR

A solvable multipolar glass

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Abstract. We examine a class of models of fully isotropic uniaxial p-polar glasses with M orientational degrees of freedom and Gaussian-distributed random, infinite-range exchange interactions. The multipolar glass transition was accessed in the large-M limit. A complete solution is obtained for $M \to \infty$ and arbitrary parameter p in the glassy phase within the Parisi *ansatz* with a single step of the replica symmetry breaking.

Orientational glasses have recently attracted much experimental and theoretical attention (see reviews [1, 2]). These include disordered systems with Ising, vector, Potts, quadrupolar, octupolar or higher-order multipolar interactions. Usually, an orientational glass is formed when a solid phase with dynamic orientational disorder can be cooled down to low temperatures without undergoing a transition to a long-range orientationally ordered phase. Examples of orientational glasses include: K(Br, CN) [3], $Ar_{1-x}(N_2)_x$ [4] and para- and ortho-hydrogen $(pH_2)_{1-x}(oH_2)_x$ mixtures[5] (quadrupolar glasses, QG). An example of an octupolar glass is the mixed crystal $Kr_x(CH_4)_{1-x}$ [6]. In contrast to the 'conventional' spin glasses different aspects of orientational disordered systems are not yet satisfactorily explained [7]. For example, there is some controversy about the application of the Parisi replica symmetry breaking (RSB) scheme to the quadrupolar glass problem [8]. Therefore, while attempting to address the question of glassy formation in multipolar glass systems, it appears to have a simple reference model solved exactly at least in some limiting cases.

The unified Hamiltonian, describing multipolar glasses reads [9]:

$$H = \frac{1}{M^{p-1}} \sum_{i<j} J_{ij} A^{\mu_1\ldots\mu_p;\nu_1\ldots\nu_p} X_i^{\mu_1\ldots\mu_p} X_j^{\nu_1\ldots\nu_p}. \qquad (1)$$

The tensor $A^{\mu_1\ldots\mu_p;\nu_1\ldots\nu_p}$ $(\mu, \nu = 1 \ldots M)$ describes the symmetry of the interaction whereas the particle tensors $X_i^{\mu_1\ldots\mu_p}$ describe M-orientational degrees of freedom (the normalizing prefactor in equation (1), $1/M^{p-1}$, has been introduced for convenience). The Hamiltonian (1) generalizes the correlations found in dipolar $(p = 1)$ glasses to those present in multipolar glassy systems of order p. For $p = 2$ we have an example of the quadrupolar glass while for $p > 2$ the Hamiltonian (4) describes other glassy systems including uniaxial hexapolar $(p = 3)$, octupolar $(p = 4)$ or higher-order multipolar systems. To be explicit, we take the matrix J_{ij} which is a random symmetric matrix with independently Gaussian distributed components scaled with N

$$P(J_{ij}) = (N/2\pi J^2)^{1/2} \exp(-NJ_{ij}^2/2J^2). \qquad (2)$$

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If the system is uniaxial with no axes preferred, i.e.

$$A^{\mu_1\ldots\mu_p;\nu_1\ldots\nu_p} = \frac{1}{p!}\sum_{P_\nu}\delta_{\mu_1}^{P(\nu_1)}\ldots\delta_{\mu_p}^{P(\nu_p)} \tag{3}$$

where the summation runs over all permutation P of the indices $\nu_1\ldots\nu_p$ the tensor $X_i^{\mu_1\ldots\mu_p}$ can be replaced by a 'spin' or component product $X_i^{\mu_1\ldots\mu_p} = n_i^{\mu_1}\ldots n_p^{\mu_p}$ and the phase space is more easily accessible in terms of n_i^μ (in the general case, the phase space is described by the set of the rotations $SO(M)$ of the tensor $X_i^{\mu_1\ldots\mu_p}$). Therefore, the Hamiltonian (1) reads

$$H = \frac{1}{M^{p-1}}\sum_{i<j} J_{ij}(\boldsymbol{n}_i\cdot\boldsymbol{n}_j)^p \tag{4}$$

where $\boldsymbol{n}_i\cdot\boldsymbol{n}_j = \sum_\mu n_i^\mu n_j^\mu$.

A widely used method to study statistical mechanical models is to increase the number of components M, where it is often found that the new model is exactly solvable in the infinite component limit $M\to\infty$ and that a systematic $1/M$ expansion may be developed. We follow this strategy here and in this letter we study the glassy properties of the multipolar disordered system (4) in the $M\to\infty$ limit by superimposing the spherical constraint $\boldsymbol{n}_i\cdot\boldsymbol{n}_i = M$. We recall that the model (4) for $p=1$ and $M\to\infty$ reduces to the spherical spin glass model considered some time ago [10, 11]. The finite M-component system corresponding to the quadrupolar case ($p=2$) has been studied by Goldbart and Sherrington [8]. The non-random version of the Hamiltonian (4) for $p=2$ was considered for arbitrary M by Ohno *et al* [12] and in the context of RP^{M-1} field theory [13].

In the present letter we show that the system (4) exhibits a glassy transition with a discontinuous RSB. Moreover, we identify the scenario for this spontaneous RSB and prove that the one-step of the replica symmetry breaking (1RSB) within Parisi *ansatz* [14] is the exact solution for the multipolar model for $p\geqslant 2$ in the large-M limit (4)—the order parameter function $q(x)$ is a step function with a break point $x_0\equiv m(T)$ where T denotes temperature. As a consequence, fluctuations about the disordered state should remain finite at the critical temperature T_c, hence nonlinear susceptibilities will *not diverge* as T approaches T_c from the disordered phase. Interestingly, this feature is in striking resemblance to the exactly solvable random energy level model [15] or the 'simplest spin glass', namely the Ising spin glass with p-spin interactions for $p\to\infty$ [16]. However, there are important differences in symmetries and the nature of interactions between the Hamiltonian (4) and the p-spin model: O(M) rotational symmetry and two-body ($p=2$) interactions in equation (4) as opposed to discrete $\mathcal{Z}_2$ symmetry and multi-spin interactions in the p-spin Ising glass. For related quadrupolar systems we emphasize the first-order glass transition found in QG for $M > M_c\approx 3.4$ (see [8]). In the present paper we show that the first-order phase transition persists for arbitrary multipolar glass—an exact statement in the large-M component limit.

Introducing n replicas of the original system, we average the free energy $F=-T\ln Z$ where $Z=\mathrm{Tr}\,\mathrm{e}^{-\beta H}$, ($\beta = 1/k_BT$) over the ensemble of the random interactions $\{J_{ij}\}$ using the identity $[\ln Z]_{av} = \lim_{n\to 0}([Z^n]_{av}-1)/n$, thus reducing the problem to a translationally invariant system. In the process distinct sites are decoupled and the n_i^μ components can be traced out. Finally, the number of sites N is taken to infinity, along with the $M\to\infty$ limit, allowing the exact evaluation of the disorder averaged free energy density $f_{av} = [F/MN]_{av}$ via the saddle point method. Explicitly, $f_{av} = f_{av}^{\text{non-diag}} + f_{av}^{\text{diag}}$ where

$$\beta f_{av}^{\text{non-diag}} = \lim_{n\to 0}\frac{1}{n}\left\{\frac{1}{4}(\beta J)^2(2p-1)\sum_{\alpha\beta} q_{\alpha\beta}^{2p} + \frac{1}{2}\,\mathrm{Tr}_n\ln[\mathbf{1}_n - p(\beta J)^2 R\boldsymbol{\mu}]\right\}$$

$$f_{\rm av}^{\rm diag} = \frac{1}{4}(\beta J)^2(2p-1)R^{2p} + \frac{1}{2}\ln\left[\frac{2z}{J} - p(\beta J)^2 R^{2p-1}\right] - \beta z \qquad (5)$$

contains the natural glass order parameter according to the symmetry of the problem $q_{\alpha\beta} = \langle\langle \boldsymbol{n}_i^\alpha \cdot \boldsymbol{n}_i^\beta\rangle_T\rangle_J$ $(\alpha \neq \beta)$ and measuring the overlap of the configurations of couplings of two replicas while $R = \langle\langle \boldsymbol{n}_i^\alpha \cdot \boldsymbol{n}_i^\alpha\rangle_T\rangle_J$ describes the replica-diagonal correlation in the multipolar system. Here, $\langle\ldots\rangle_T$ and $\langle\ldots\rangle_J$ are the statistical and random averages, respectively. Furthermore, $\mathbf{1}_n$ and $[\boldsymbol{\mu}]_{\alpha\beta} = q_{\alpha\beta}^{2p-1}$ are $n \times n$ matrices with trace Tr_n acting in the replica space. The Lagrange multiplier z superimposes the constraint fixing the length of 'spins' n_i^α.

Accessing the glassy phase requires proper *ansatz* for the matrix $\mathbf{q}$ in order to perform the $n \to 0$ limit in equation (5). It is customary to start with the replica symmetric (RS) proposition $q^{\alpha\beta} = q$ for all $\alpha \neq \beta$. By examining the stationarity condition $\partial f_{\rm av}/\partial q = 0$ for $p > 1$ we found that the only stable RS solution corresponds to $q = 0$. There are other non-zero (but unstable) RS solution involving a jump in the order parameter q which have to be rejected. Since the solution corresponding to the high-temperature phase ($q = 0$) does not become unstable at low temperatures, the relevant solution cannot be close to it and so there must be a jump in the order parameter at the transition point accompanied by the spontaneous RSB. In order to access the RSB solution we follow Parisi first-step replica symmetry breaking (1RSB) *ansatz* and express $\mathbf{q}$ in terms of a tensor product

$$\mathbf{q} = (q_1 - q_0)\mathbf{1}_{n/m} \otimes \boldsymbol{e}_m \boldsymbol{e}_m^{\rm T} + q_0 \boldsymbol{e}_n \boldsymbol{e}_n^{\rm T} - q_1 \mathbf{1}_n \qquad (6)$$

where $\boldsymbol{e}_n^{\rm T} = (1, 1, \ldots, 1)$ is a transposed column vector with n-elements identical to unity. Here, m is the partitioning parameter which becomes a continuous variable $0 \leqslant m \leqslant 1$ in the $n \to 0$ limit and equation (5) reads

$$\begin{aligned}\beta f_{\rm av}^{\text{non-diag}} = {} & \tfrac{1}{4}(\beta J)^2(2p-1)[(m-1)q_1^{2p} - m q_0^{2p}] \\ & - \frac{1}{2}\frac{p(\beta J)^2 R q_0^{2p-1}}{1 + p(\beta J)^2 R q_1^{2p-1}(1-m) + pm(\beta J)^2 R q_0^{2p-1}} \\ & + \frac{1}{2}\frac{m-1}{m}\ln[1 + p(\beta J)^2 R q_1^{2p-1}] \\ & + \frac{1}{2}\frac{1}{m}\ln[1 + p(\beta J)^2 R q_1^{2p-1}(1-m) + pm(\beta J)^2 R q_0^{2p-1}]. \qquad (7)\end{aligned}$$

The 1RSB involves five parameters q_0, q_1, m, z and R which have to be determined self-consistently. Stationarity with respect to m is not necessarily required in the case of continuous order parameter function $q(x)$ but is requested in the case where there is a discontinuous transition as is happening here. Accordingly,

$$\frac{\partial f_{\rm av}}{\partial q_0} = \frac{\partial f_{\rm av}}{\partial q_1} = \frac{\partial f_{\rm av}}{\partial m} = \frac{\partial f_{\rm av}}{\partial R} = \frac{\partial f_{\rm av}}{\partial z} = 0. \qquad (8)$$

For an arbitrary value of the parameter m the RS solution $q_0 = q_1 = q$ is contained in the 1RSB equations (7) and (8). However, as already pointed out, this is not the correct one and equations (7) and (8) will admit another solution with $q_0 = 0$ and $q_1 \neq 0$ involving a discontinuous jump of q_1 at certain critical temperature $T_{\rm c}$. We found that the free energy of 1RSB solution coincides with the paraorientational RS solution $q = 0$ only at $m = 1$. As a result, the critical line is given as the solution of equation (7) with $m = 1$. The critical temperature of this discontinuous transition is given by

$$k_{\rm B}T_{\rm c}/J = \sqrt{p}\sqrt{1-y}\,y^{p-1}. \qquad (9)$$

At T_c the order parameter jump is

$$q_1 = \frac{(\beta J)^{-\frac{1}{p}} y^{\frac{1}{p}}}{p^{\frac{1}{2p}}(1-y)^{\frac{1}{2p}}}. \tag{10}$$

Here, y is the solution of $F(m=1, p, y) = 0$ where

$$\begin{aligned} F(m, p, y) = &-\frac{1}{2m^2}\ln\left(\frac{\sqrt{m^2y^2+(2m-4)y+1}-my+1}{\sqrt{m^2y^2+(2m-4)y+1}+my+1}\right) \\ &+\frac{(2p-1)y^2}{2p\sqrt{m^2y^2+(2m-4)y+1}+(2m-4)py+2p} \\ &-\frac{y}{m\sqrt{m^2y^2+(2m-4)y+1}-m^2y+m} \end{aligned} \tag{11}$$

is the universal function dependent only on the break-point m and the parameter p. We have computed numerically T_c for several values of the parameter p. The results are presented in table 1. It is seen that the critical temperature decreases rather rapidly with increase of the parameter p.

Table 1. Multipolar glass transition temperature T_c as a function of the parameter p. The case $p = 1$ corresponnds to the critical temperature of the spherical dipolar model (RS solution, see [10, 11]).

p	$y(m=1, p)$	$k_\mathrm{B}T_\mathrm{c}(p)/J$
1	—	1
2	0.804 522	0.503 039
3	0.002 334 58	$9.429\,08 \times 10^{-6}$
4	0.001 537 77	$7.267\,30 \times 10^{-9}$
5	0.001 543 55	$1.268\,34 \times 10^{-11}$
6	0.001 545 81	$2.160\,33 \times 10^{-14}$

An important question is whether the 1RSB solution presented above is exact or whether it is just a good approximation. Instead of performing the stability analysis in a form of fluctuation expansion about the 1RSB solution we have rather decided to look at the problem with arbitrary k step of the RSB. For the generic kRSB the matrix

$$\begin{aligned} \mathbf{q} = &(q_k - q_{k-1})\mathbf{1}_{n/m_k} \otimes \boldsymbol{e}_{m_k}\boldsymbol{e}_{m_k}^\mathrm{T} + (q_{k-1} - q_{k-2})\mathbf{1}_{n/m_{k-1}} \otimes \boldsymbol{e}_{m_{k-1}}\boldsymbol{e}_{m_{k-1}}^\mathrm{T} \\ &+ \cdots + q_0\boldsymbol{e}_n\boldsymbol{e}_n^\mathrm{T} - q_k\mathbf{1}_n \end{aligned} \tag{12}$$

is given in terms of the parameters

$$\begin{aligned} &m_0 = n \geqslant m_1 \geqslant m_2 \geqslant \cdots \geqslant m_k \geqslant 1 \\ &q_0 \leqslant q_1 \leqslant q_2 \cdots \leqslant q_{k-1} \leqslant q_k \end{aligned} \tag{13}$$

which determine the order parameter function at each level of the Parisi ultrametric *ansatz* [14]. The matrix $\mathbf{q}$ can be parametrized by the function $x(q)$ which measures the fraction of pairs of replicas with overlap $q_{\alpha\beta} \leqslant q$, where

$$x(q) = n + \sum_{r=0}^{k}(m_{r+1} - m_r)\theta(q - q_r) \tag{14}$$

with $m_{r+1} \equiv 1$ and $\theta(q)$ as the step function. Assuming that the RSB goes to the arbitrary k level, the function $0 \leqslant x(q) \leqslant 1$ becomes continuous in the $n \to 0$ limit and equation (5) transforms into integral expression of the form

$$\begin{aligned}
\beta f_{\mathrm{av}}^{\text{non-diag}} = {} & \frac{1}{2}\ln[1 + p(\beta J)^2 R q^{2p-1}(1)] - \frac{1}{2}\frac{p(\beta J)^2 R q^{2p-1}(0)}{1 + p(\beta J)^2 R[\int_0^1 \mathrm{d}y\, q^{2p-1}(y)]} \\
& - \int_0^1 \mathrm{d}x\, \frac{(2p-1)(\beta J)^2}{4} q^{2p}(x) \\
& - \frac{1}{2}\int_0^1 \mathrm{d}x\, \frac{p(2p-1)(\beta J)^2 R q^{2p-2}(x) q'(x)}{1 + p(\beta J)^2 R[x q^{2p-1}(x) + \int_x^1 \mathrm{d}y\, q^{2p-1}(y)]}.
\end{aligned} \tag{15}$$

Now, we prove that for a general kRSB the only saddle point corresponding to the 1RSB survives. By requiring stationarity of equation (15) with respect to the variations

$$\delta x(q) = \sum_r (\delta m_{r+1} - \delta m_r)\theta(q - q_r) - \sum_r (m_{r+1} - m_r)\delta(q - q_r)\delta q_r \tag{16}$$

one gets

$$\begin{aligned}
& q_r^{2p-2}\phi(q_r) = 0 \qquad 0 \leqslant r \leqslant k \\
& \int_{q_{r-1}}^{q_r} \mathrm{d}q\, \phi(q) q^{2p-2} = 0 \qquad 1 \leqslant r \leqslant k
\end{aligned} \tag{17}$$

where

$$\begin{aligned}
\phi(q) = {} & (\beta J)^2 q - \int_{q(0)}^{q} \mathrm{d}q'\, \frac{p(2p-1)(\beta J)^4 R^2 (q')^{2p-2}}{[1 + p(\beta J)^2 R A_p(q', q(1))]^2} - \frac{p(\beta J)^4 R^2 q^{2p-1}(0)}{[1 + p(\beta J)^2 R A_p(q(0), q(1))]^2} \\
A_p(q', q'') = {} & (q'')^{2p-1} - (2p-1)\int_{q'}^{q''} \mathrm{d}q\, x(q) q^{2p-2}
\end{aligned} \tag{18}$$

so that $\phi(q_r) = 0$, $0 \leqslant r \leqslant k$ and since q^{2p-2} is increasing $\phi(q)$ must change sign for $q_{r-1} \leqslant q \leqslant q_r$, possessing at least two extrema within each interval $[q_{r-1}, q_r]$ obeying $\phi'(\xi) = 0$ for $\xi = q_r^{\mathrm{ex}}$. Thus, for the kRSB we expect not less then $2k$ stationary points as solutions of the equation

$$\frac{\mathrm{d}\phi(\xi)}{\mathrm{d}\xi} = 0 \Rightarrow \kappa_{\mathrm{L}}(\xi) = \kappa_{\mathrm{R}}(\xi) \tag{19}$$

within the domain $0 \leqslant q(0) \leqslant \xi \leqslant q(1)$, where

$$\begin{aligned}
\kappa_{\mathrm{L}}(\xi) &= q^{2p-1}(1) - (\beta J)^{-1}\left[p\xi^{p-1} - \frac{1}{(2p-1)\beta J R}\right] \\
\kappa_{\mathrm{R}}(\xi) &= \int_{\xi}^{q(1)} \mathrm{d}q\, x(q) q^{2p-2}.
\end{aligned} \tag{20}$$

Let us observe now that equation (20) and the property

$$\frac{\mathrm{d}^2\kappa_{\mathrm{R}}(\xi)}{\mathrm{d}\xi^2} = -(2p-2)\xi^{2p-3}x(\xi) - \xi^{2p-2}P(\xi) < 0 \tag{21}$$

where $P(\xi) > 0$ is the probability distribution of thermodynamic states $P(\xi) = \mathrm{d}x(\xi)/\mathrm{d}\xi$, implies that $\kappa_{\mathrm{R}}(\xi)$ is monotonically decreasing concave function, whereas $\kappa_{\mathrm{L}}(\xi)$ for $p > 1$ is convex. Consequently, there are no more than *two* solutions of the stationary equation (19) implying that the only solution for multipolar system involves one step of the replica symmetry breaking.

The important question which arises is: what happens beyond mean field in finite range systems? Physically, the weight of the 1RSB solution is the probability for occurrence of non-zero overlap. There is no reason why it should be constant and one would thus expect that it fluctuates. Therefore, it would be useful to study the loop expansion about the 1RSB solution. Finally, even in the $M = \infty$ infinite-range limit 1RSB is expected to produce ergodicity breaking and ageing effects with non-trivial non-equilibrium relaxations [17]. Further dynamical study of the problem seems of great interest.

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