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LETTER TO THE EDITOR

Simplest quadrupolar glass

K Walasek

Institute of Physics, Pedagogical University of Zielona Góra, Plac Słowiański 6, 65-069, Poland

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Abstract. The quadrupolar glass model with p-quadrupole interactions, exactly solvable in the limit $p \to \infty$ is presented. It has been shown that for $p \to \infty$ the energy levels of the system are statistically independent, which gives a quadrupolar counterpart of the spin random energy model. Using the Parisi scheme of replica symmetry breaking it has been calculated that the quadrupolar glass parameter function is a step function for $p \to \infty$ as well as for large p.

Quadrupolar glasses (QGs) have recently attracted much experimental and theoretical attention (see reviews [1]). However, in contrast to spin glasses, different aspects of the behaviour of QGs are not yet satisfactorily explained. For example there is controversy about the application of the Parisi replica symmetry breaking (RSB) scheme [2]. Thus it appears to be a quite important to have a simple model solved exactly, at least, in some limiting cases in order to gain a better understanding of QG problem. In the spin glass theory such exactly solvable model, known as the random energy model (REM), has been formulated by Derrida [3]. In this letter we present a quadrupolar counterpart of the REM. The proposed model describes a system of N quadrupoles interacting via p-body interaction. It is defined by the Hamiltonian

$$H = -\sum_{i_1 \cdots i_p} \sum_{\mu_1 \cdots \mu_p = 0,2} J_{i_1 \cdots i_p}^{\mu_1 \cdots \mu_p} Q_{i_1,\mu_1} \cdots Q_{i_p,\mu_p} \tag{1}$$

where the $Q_{i,\mu}$ are spin or pseudospin operators defined as

$$Q_{i,0} = 1 - \tfrac{3}{2} \left(S_i^z\right)^2 \tag{2a}$$

$$Q_{i,2} = \tfrac{1}{2}\sqrt{3} \left[\left(S_i^x\right)^2 - \left(S_i^y\right)^2\right] \tag{2b}$$

with $S = 1$ and the sum $(i_1 \cdots i_p)$ runs over all distinct clusters of p quadrupoles. The random couplings $J_{i_1 \cdots i_p}^{\mu_1 \cdots \mu_p}$ are independent variables distributed according to

$$P\left(J_{i_1 \ldots i_p}^{\mu_1 \cdots \mu_p}\right) = \left(N^{p-1}/J^2 \pi p!\right) \exp\left[-\frac{\left(J_{i_1 \ldots i_p}^{\mu_1 \cdots \mu_p}\right)^2 N^{p-1}}{J^2 p!}\right] . \tag{3}$$

Obviously the $Q_{i,\mu}$ commute and satisfy the relation

$$Q_{i,0}^2 + Q_{i,2}^2 = 1 . \tag{4}$$

For $p = 2$ and short-range electric quadrupole–quadrupole couplings $J_{ij}^{\mu,\nu}$ the model (1) has been used in the theory of QG behaviour of solid hydrogen with the concentration of the orthohydrogen less than 55% [4, 5]. In this case S_i^x, S_i^y and S_i^z denote the components of angular momentum operator in the local coordinate system of the orthohydrogen molecule [6].

In strict analogy with the Derrida [3] and Gross and Mezard [7] analysis it can be shown that in the limit $p \to \infty$ the Hamiltonian (1) describes the quadrupolar REM. Indeed, the probability distribution $P(E, Q^{(1)})$ that a given configuration $Q^{(1)}$ of quadrupoles (understood as a given set $\{Q^{(1)}_{i,\mu}\}$ of the eigenvalues of the $Q_{i,\mu}$) has energy E is

$$P\left(E, Q^{(1)}\right) = \left[\delta\left(E - H\left\{Q^{(1)}\right\}\right)\right]_{\mathrm{av}} = \frac{1}{\sqrt{\pi N J^2}} \exp\left(-\frac{E^2}{N J^2}\right) \tag{5}$$

with

$$[\cdots]_{\mathrm{av}} = \int \prod_{i_1\mu_1,\ldots,i_p\mu_p} \mathrm{d}J^{\mu_1\cdots\mu_p}_{i_1\ldots i_p}\, P(J^{\mu_1\cdots\mu_p}_{i_1\ldots i_p}) \cdots \tag{6}$$

whereas for the probability distribution $P\left(E_1, E_2, Q^{(1)}, Q^{(2)}\right)$ that two given configurations of quadrupoles $Q^{(1)}$ and $Q^{(2)}$ have, respectively, energies E_1 and E_2 one obtains

$$\begin{aligned} P\left(E_1, E_2, Q^{(1)}, Q^{(2)}\right) &= \left[\delta\left(E_1 - H\left\{Q^{(1)}\right\}\right) \delta\left(E_2 - H\left\{Q^{(2)}\right\}\right)\right]_{\mathrm{av}} \\ &= \frac{1}{\sqrt{\pi J^2 N(1-q^p)}} \frac{1}{\sqrt{\pi J^2 N(1+q^p)}} \\ &\quad \times \exp\left[-\frac{(E_1 - E_2)^2}{2J^2 N(1-q^p)} - \frac{(E_1 + E_2)^2}{2J^2 N(1+q^p)}\right] \end{aligned} \tag{7}$$

where

$$q = \frac{1}{N} \sum_{i=1}^{N} \sum_{\mu=0,2} Q^{(1)}_{i,\mu} Q^{(2)}_{i,\mu} \tag{8}$$

is the overlap between two configurations. Since $|q| < 1$ in the limit $p \to \infty$, we have

$$P\left(E_1, E_2, Q^{(1)}, Q^{(2)}\right) = P(E_1)P(E_2) \tag{9}$$

so that the energy levels are uncorrelated. We find also the critical tempertu re T_c which for $p \to \infty$ is

$$T_c = 1/(2\sqrt{\ln 3})\,. \tag{10}$$

Below T_c the system gets stuck in the lower available level with energy $E_0 = -NJ\sqrt{\ln 3}$. The entropy is

$$S(T) = \begin{cases} N\left(\ln 3 - \dfrac{J^2}{4T^2}\right) & \text{for } T > T_c \\ 0 & \text{for } T \leqslant T_c \end{cases} \tag{11}$$

whereas the free energy has the form

$$F(T) = \begin{cases} -N\left(\dfrac{J^2}{4T} + T\ln 3\right) & \text{for } T > T_c \\ -\sqrt{\ln 3} & \text{for } T \leqslant T_c. \end{cases} \tag{12}$$

Now we will show results obtained by the replica method for $p \to \infty$ and for large p. After calculations similar to those performed for the spin glass with p-spin interactions [7, 8] we get the free energy in the form

$$\beta F = -\frac{(\beta J)^2}{4n} \sum_{\alpha \neq \alpha'} q^p_{\alpha\alpha'} + \frac{1}{2n} \sum_{\alpha \neq \alpha'} \lambda_{\alpha\alpha'} q_{\alpha\alpha'} - \frac{1}{n} \ln \operatorname{Tr} \exp\left(\frac{1}{2} \sum_{\alpha \neq \alpha'} \lambda_{\alpha\alpha'} \hat{q}_{\alpha\alpha'}\right) - \frac{(\beta J)^2}{4} \tag{13}$$

where $\alpha, \alpha' = 1 \ldots n$ $(n \to 0)$ are replica indices

$$\hat{q}_{\alpha\alpha'} = \sum_{\mu=0,2} Q^{\alpha}_{i,\mu} Q^{\alpha'}_{i,\mu} \tag{14}$$

in which $Q^{\alpha}_{i,\mu}$ is the αth replica of the operator $Q_{i,\mu}$ referred to an arbitrary site i, and the $q_{\alpha\alpha'}$ and $\lambda_{\alpha\alpha'}$ respectively denote the QG parameters and Lagrange multipliers controlling the condition

$$q_{\alpha\alpha'} = \frac{1}{N} \sum_{i=1}^{N} \sum_{\mu=0,2} Q^{\alpha}_{i,\mu} Q^{\alpha'}_{i,\mu} \, .$$

Now we are in a position to show that Parisi's ansatz for the RSB [9] is valid in our model and a possible solution for the SG order parameter function for large p is simply a step function. This means that, similarly as in the spin glass with p-spin interaction [7, 8], the first-order breaking of the replica symmetry is exact.

Following Parisi's procedure [9], in the general kth order RSB, we introduce a sequence of variables

$$0 \leqslant q_0 \leqslant q_1 \leqslant \cdots \leqslant q_{k-1} \leqslant q_k$$

and

$$0 \leqslant \lambda_0 \leqslant \lambda_1 \leqslant \cdots \leqslant \lambda_{k-1} \leqslant \lambda_k$$

where k is an arbitrary integer, which are related to the parameters $q_{\alpha\alpha'}$ and $\lambda_{\alpha\alpha'}$, respectively. Then, we can rewrite equation (13) with $n \to 0$ in the form

$$\beta F = \frac{(\beta J)^2}{4} \sum_{l=0}^{k} (m_{l+1} - m_l) q_l^p - \frac{1}{2} \sum_{l=0}^{k} \lambda_l q_l + \frac{\lambda_k}{2} - \ln S - \frac{(\beta J)^2}{4} \tag{15}$$

where $m_0 = n, m_1, \ldots, m_k, m_{k+1} = 1$ are the tree branch parameters [9] satisfying the inequalities

$$m_0 \leqslant m_1 \leqslant \cdots \leqslant m_{k-1} \leqslant m_k \leqslant 1$$

as $n \to 0$. In expression (15)

$$S = G_0 \left(G_1 \left(\cdots \left(G_{k-1} \left(G_k Z_0^{m_k}(h_1, h_2) \right)^{m_{k-1}/m_k} \right)^{m_{k-2}/m_{k-1}} \cdots \right)^{m_1/m_2} \right)^{n/m_1} \Bigg|_{h_1 = h_2 = 0} \tag{16}$$

where the differential operators G_l $(l = 0, 1, \ldots, k)$ are defined by

$$G_l = \exp\left[\frac{1}{2} (\lambda_l - \lambda_{l-1}) \sum_{\mu=0,2} \frac{\partial^2}{\partial h_\mu^2} \right] \tag{17}$$

assuming $\lambda_{-1} = 0$ when $l = 0$, and

$$Z_0(h_0, h_2) = \operatorname{Tr} \exp\left(\sum_{\mu=0,2} h_\mu Q_\mu \right) . \tag{18}$$

The stationary condition $\partial F / \partial q_l = 0$ gives

$$\lambda_l = \frac{(\beta J)^2}{2} p q_l^{p-1} \, . \tag{19}$$

If we assume $q_l < 1$ for $l = 0, 1, \ldots, k-1$ and $q_k = 1$ in the limit $p \to \infty$, we have that λ_l $(l = 0, 1, \ldots, k-1)$ are very small and λ_k is large for large p. Then, expanding S, equation (16), to first order in $\lambda_{l<k}$, for large p, we get the free energy in the form

$$\beta F = \frac{(\beta J)^2}{4}\sum_{l=0}^{k}(m_{l+1}-m_l)\,q_l^p - \frac{1}{2}\sum_{l=0}^{k-1}\lambda_l\,(m_{l+1}-m_l)\,(q_l - a) + \frac{\lambda_k m_k}{2}$$
$$-\frac{1}{m_k}\ln I_k - \frac{(\beta J)^2}{4} + \mathcal{O}\left(\lambda_{l<k}\lambda_{l'<k}\right) \qquad (20)$$

where

$$I_k = I_k\,(h_0 = 0, h_2 = 0) \qquad (21)$$

and

$$a = \frac{1}{m_k^2}\sum_{\mu=0,2} I_k^{-2}\left[\frac{\partial I_k\,(h_0,h_2)}{\partial h_\mu}\right]^2\Bigg|_{h_0=h_2=0} \qquad (22)$$

with

$$I_k\,(h_0,h_2) = \tilde{G}_k Z_0^{m_k}\,(h_0,h_2) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\;\mathrm{d}y\;\exp\left(-\frac{x^2+y^2}{2}\right)$$
$$\times\left\{\exp\left(h_0 + \lambda_k^{1/2}x\right) + 2\exp\left(-\frac{h_0+\lambda_k^{1/2}x}{2}\right)\cosh\left[\frac{\sqrt{3}}{2}\left(h_2 + \lambda_k^{1/2}y\right)\right]\right\} \qquad (23)$$

where

$$\tilde{G}_k = \exp\left(\frac{1}{2}\lambda_k\sum_{\mu=0,2}\frac{\partial^2}{\partial h_\mu^2}\right)\,.$$

The asymptotic form of $I_k\,(h_0,h_2)$ for large λ_k (large p) is

$$I_k\,(h_0,h_2) = \mathrm{e}^{\lambda_k m_k^2/2}\left\{\mathrm{e}^{h_0 m_k} + 2\mathrm{e}^{-h_0 m_k/2}\cosh\left(\frac{\sqrt{3}}{2}h_2 m_k\right)\left[1 - \frac{3\xi\,(m_k)\exp\left(-\frac{3}{8}\lambda_k m_k^2\right)}{2\lambda_k^{1/2}}\right]\right\} \qquad (24)$$

where

$$\xi(x) = \left(\frac{2}{3}\right)^{3/2}\frac{1}{\sqrt{\pi}}\int_0^1\frac{\mathrm{d}z}{z}\left\{z^x - \left[(1+z)^x - 1\right]z^{-x}\right\}\,. \qquad (25)$$

Note that $\xi(x) \geqslant 0$ for $0 \leqslant x \leqslant 1$ with $\xi(1) = 0$.

From the stationary conditions $\partial F/\partial\lambda_l = 0$ and $\partial F/\partial m_k = 0$ and assuming that p is large we obtain

$$q_{l<k} = \frac{\xi^2\,(m_k)}{2(\beta J)^2 p}3^{-3p/4} \qquad (26)$$

$$q_k = 1 - \frac{3}{4}\frac{m_k\xi\,(m_k)}{1-m_k}\frac{3^{-3p/4}}{\sqrt{\frac{1}{2}(\beta J)^2 p}} \qquad (27)$$

and

$$m_k = \frac{T}{T_c}\left[1 - \frac{3}{8}\frac{T}{T_c}\xi\left(\frac{T}{T_c}\right)\sqrt{\frac{2p}{\ln 3}}3^{-3p/4}\right] \qquad (28)$$

with

$$T_c = \frac{J}{2\sqrt{\ln 3}} \left[1 + \sqrt{\frac{\pi}{3(\ln 3)^3 p}} 3^{-3p/4} \right] . \tag{29}$$

The results (26)–(28) show that the Parisi (RSB) scheme [9] can be applied without any modifications to our QG model, for large p at least. The QG parameter function $q(x)$ is a step function with the jump at $x = m_k$. It is interesting that in contrast to the p-spin interaction spin glass model, where $q_{l<k} = 0$ for $p \to \infty$ as well as for large p [8], in the present model the $q_{l<k}$ vanish only in the limit $p \to \infty$. This is a strict consequence of the lack of spin reversal symmetry in a quadrupolar system, which determines such a form of $I_k(h_0, h_2)$, equation (23), that $I_k(h_0, h_2) \neq I_k(-h_0, -h_2)$ and hence a, equation (22) vanishes only in the limit $p \to \infty$.

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