

## One-step replica symmetry breaking solution of the quadrupolar glass model

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2006 J. Phys. A: Math. Gen. 39 13393

(<http://iopscience.iop.org/0305-4470/39/43/001>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.106

The article was downloaded on 03/06/2010 at 04:53

Please note that [terms and conditions apply](#).

# One-step replica symmetry breaking solution of the quadrupolar glass model

F P Mancini<sup>1</sup> and D Sherrington<sup>2</sup>

<sup>1</sup> Dipartimento di Fisica and Sezione I.N.F.N., Università di Perugia, Via A Pascoli, Perugia 06123, Italy

<sup>2</sup> Rudolf Peierls Centre for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford, OX1 3NP, UK

E-mail: [FrancescoPaolo.Mancini@pg.infn.it](mailto:FrancescoPaolo.Mancini@pg.infn.it) and [D.Sherrington1@physics.oxford.ac.uk](mailto:D.Sherrington1@physics.oxford.ac.uk)

Received 5 July 2006, in final form 12 September 2006

Published 11 October 2006

Online at [stacks.iop.org/JPhysA/39/13393](http://stacks.iop.org/JPhysA/39/13393)

## Abstract

We consider the quadrupolar glass model with infinite-range random interaction. Introducing a simple one-step replica symmetry breaking ansatz we investigate the para-glass continuous (discontinuous) transition which occurs below (above) a critical value of the quadrupole dimension  $m^*$ . By using a mean-field approximation we study the stability of the one-step replica symmetry breaking solution and show that for  $m > m^*$  there are two transitions. The thermodynamic transition at a temperature  $T_D$  is discontinuous but there is no latent heat. At a higher temperature we find the dynamical or glass transition temperature  $T_G$  and the corresponding discontinuous jump  $q_G$  of the order parameter.

PACS numbers: 75.10.Nr, 05.50.+q

## 1. Introduction

In the last decades quadrupolar glasses have found widespread experimental and theoretical interest [1]. Disordered quadrupolar glasses are produced by random dilution of (quadrupolar) molecular crystals with atoms which have no quadrupole moments; well-known examples of such systems are  $\text{K}(\text{CN})_x\text{Br}_{1-x}$  or  $\text{Na}(\text{CN})_x\text{Cl}_{1-x}$ , or  $\text{N}_2\text{Ar}$ ,  $\text{CuCN}$ , or solid hydrogen (see [2] for a review). The success of the Sherrington–Kirkpatrick (SK) model [3] in providing a good theory to describe systems of interacting magnetic or electric dipole moments, suggests to extend to quadrupolar glasses the same kind of analysis. However, there are differences between standard spin-glass systems and quadrupolar glasses; the latter do not have the global inversion symmetry  $S_i \rightarrow -S_i$  for all spins. For several systems without reflection symmetry, and close to the transition temperature, only one step in the Parisi replica symmetry breaking scheme is sufficient to describe the transition para-glass above a lower critical dimension [4].

Indeed, the one-step replica symmetry breaking (1RSB) scheme has proven to provide stable solutions for the Potts glass model [5–7], the spherical  $p$ -spin model [8] and the  $p$ -spin Ising spin-glass model [9]. It is the purpose of the present paper to show that the 1RSB scheme can be applied also to the quadrupolar glass model, and indeed it provides a stable solution in certain regimes.

In the present paper, we shall consider a perturbative evaluation of the free energy by means of a Taylor expansion up to fourth order in the order parameter. It is obvious that the perturbative approach is most reliable near the transition temperature. We shall show that the transition from the replica symmetric (RS) state to the 1RSB occurs either discontinuously or continuously, depending on the value of the quadrupole dimension  $m$ . A similar dependence of the RS to 1RSB transition, though on the value of an external field, is exhibited by the spherical  $p$ -spin model [8] and the Ising  $p$ -spin model [9]. For any  $p > 2$ , the transition is discontinuous (continuous) for fields weaker (larger) than a critical value of the external field  $h_c$ , which depends on  $p$ .

The plan of this paper is as follows: in section 2 we shall use a rather pedagogical approach mainly to review the results obtained in the mean-field analysis of the quadrupolar glass model in the framework of the replica symmetry ansatz [10]. Section 3 is devoted to the study of the 1RSB solutions of the saddle-point equations, assuming all the transitions to be continuous or at worst weakly discontinuous. In section 4 we shall perform the de Almeida–Thouless (AT) stability analysis while the dynamical transition is discussed in section 5. The concluding remarks are given in section 6.

## 2. Uniaxial quadrupolar glass

The infinite-ranged quadrupolar glass model has been first introduced by Goldbart and Sherrington (GS) [10]. The model assumes the quadrupole–quadrupole interaction to be more dominant than the interactions between dipoles. This appears to be the case in several experimental situations, where the quadrupolar species occupy the sites of a regular lattice, but share this lattice with a dilutant without quadrupole moment: argon in the case of interacting  $N_2$ , parahydrogen in the case of interaction with orthohydrogen, and KBr in the case of KCN, etc [2].

To construct the mean-field theory of a set of uniaxial quadrupoles interacting through randomly quenched and frustrated isotropic exchange one may adopt the Hamiltonian

$$H = - \sum_{(i,j)} J_{ij} \sum_{\mu\nu} S_{\mu}^i S_{\nu}^i S_{\mu}^j S_{\nu}^j = - \sum_{(i,j)} J_{ij} (\mathbf{S}^i \cdot \mathbf{S}^j)^2, \quad (1)$$

where the spin vector  $\mathbf{S}^i$  is defined via the component  $f_{\mu\nu}^i = (S_{\mu}^i S_{\nu}^i - \delta_{\mu\nu}/m)$  of the electric quadrupole moment tensor [10]. The summation  $(i, j)$  runs over all the distinct pairs. Each  $\mathbf{S}^i$  has  $m$  components  $S_{\mu}^i$  ( $\mu = 1, \dots, m$ ) and, for convenience, is assumed to be a vector with fixed length  $|\mathbf{S}^i| = m$ . Of course, taking general  $m$  does not describe the experimental quadrupolar glasses. Rather it is a natural model to consider theoretically for classification. By analogy with SK, the spins are taken to interact via independent random interactions  $J_{ij}$  which are assumed Gaussian distributed:

$$P(J_{ij}) = \left( \frac{N}{2\pi J^2} \right)^{1/2} \exp \left[ - \frac{(J_{ij} - J_0/N)^2}{2J^2/N} \right]. \quad (2)$$

The mean  $J_0$  and the variance  $J$  of the distribution depend on the total number of quadrupoles  $N$  to ensure a meaningful thermodynamic limit ( $N \rightarrow \infty$ ) with an extensive energy:  $J_0 = \tilde{J}_0/N$  and  $J = \tilde{J}/N^{1/2}$ . The Hamiltonian (1) can be seen as the Hamiltonian of an infinite-range model for  $N$  classical vector spins  $\mathbf{S}^i$  and zero external field is assumed.

In [10] it has been shown that in terms of the order parameters

$$\begin{aligned} Q_{\mu\nu\lambda\rho}^{ab} &= \frac{\text{tr}[S_{\mu}^a S_{\nu}^a S_{\lambda}^b S_{\rho}^b \exp L]}{\text{tr}[\exp L]} = \langle S_{\mu}^a S_{\nu}^a S_{\lambda}^b S_{\rho}^b \rangle \\ M_{\mu\nu}^a &= \frac{\text{tr}[S_{\mu}^a S_{\nu}^a \exp L]}{\text{tr}[\exp L]} = \langle S_{\mu}^a S_{\nu}^a \rangle, \end{aligned} \quad (3)$$

the free energy per spin  $f$ —by means of the replica trick—is given by

$$\begin{aligned} -\beta f &= \frac{1}{N} \lim_{n \rightarrow 0} \frac{1}{n} (\overline{Z^n} - 1) = \lim_{n \rightarrow 0} \frac{1}{n} \left[ -\frac{\beta J_0}{2} \sum_a \sum_{\mu\nu} (M_{\mu\nu}^a)^2 \right. \\ &\quad \left. - \left( \frac{\beta J}{2} \right)^2 \sum_{ab} \sum_{\mu\nu\lambda\rho} (Q_{\mu\nu\lambda\rho}^{ab})^2 + \log \text{tr} \exp L \right], \end{aligned} \quad (4)$$

where  $n$  is the number of replicas,  $\beta = 1/k_B T$ , and  $L$  is

$$L = \beta J_0 \sum_a \sum_{\mu\nu} M_{\mu\nu}^a S_{\mu}^a S_{\nu}^a + \frac{(\beta J)^2}{2} \sum_{ab} \sum_{\mu\nu\lambda\rho} S_{\mu}^a S_{\nu}^a S_{\lambda}^b S_{\rho}^b Q_{\mu\nu\lambda\rho}^{ab}. \quad (5)$$

The elements of the order parameters  $Q_{\mu\nu\lambda\rho}^{ab}$  and  $M_{\mu\nu}^a$  are not independent quantities and they can be parameterized in terms of five sets of independent parameters  $A^a$ ,  $B^{ab}$ ,  $C^{ab}$ ,  $D^{ab}$  and  $E^{ab}$ . The nonzero extremal values of the above sets describe possible glass ordering [10].

Upon decreasing the temperature, when one of the parameters becomes different from zero, the high-temperature disordered phase becomes unstable. By assuming continuous transition in the replica symmetric ansatz and provided that the average interaction is not too positive,

$$\frac{J_0}{J} < \frac{-m^2 + m + 8}{m + 4}, \quad (6)$$

there is a transition to an isotropic glass state occurring at the temperature  $T_{\text{RS}} = (2mJ)/[k_B(m+2)]$ . This highest temperature phase transition is associated with the order parameter  $B^{ab}$  acquiring a nonzero value, hinting at the presence of isotropic quadrupolar order [10]. As GS showed, below  $T_{\text{RS}}$  the replica symmetric solution isotropic glass phase is unstable with respect to fluctuations in the space of broken replica symmetric isotropic glass order parameters, the instability being stronger than in conventional systems.

It is worth noting that equation (6) is the equivalent of the condition  $J_0/J < 1$  in the  $SK$  model to ensure a transition from the paramagnet state to spin-glass state. Furthermore, when the numerator on the right-hand side of equation (6) becomes negative, it is necessary to introduce a negative value for  $J_0$  in order to obtain a glass phase at low temperatures; this happens for  $m > 3.37\dots$ . Increasing the negativity of  $J_0$  reduces the temperature of ferromagnetism onset, though it cannot be stopped.

### 3. One-step replica symmetry breaking theory

The further analysis of GS leads to the conclusion that a replica symmetric ansatz cannot give a stable, and hence physical, solution of the quadrupolar glass model. Thus, one has to resort to a replica symmetry breaking ansatz. Close to the isotropic quadrupolar glass transition, i.e. confining attention to regions of parameter space  $(J_0, J)$  in which the highest transition temperature does correspond to a phase transition in the order parameter  $B^{ab}$ , it is sufficient to consider only this parameter different from zero in the free energy (see [10]). Thus, one

requires  $J_0$  to satisfy the inequality (6) for  $T \lesssim T_{RS}$ , i.e. in the neighbourhood of the transition temperature. The free energy is then given by

$$\beta f = \lim_{n \rightarrow 0} \frac{1}{n} \left\{ \frac{(\beta J)^2}{2} (m-1)(m+2) \sum'_{ab} (B^{ab})^2 + m(\beta J)^2 \sum'_{ab} B^{ab} - \log \text{Tr} \exp \left[ (\beta J)^2 \sum'_{ab} \sum_{\mu\nu} B^{ab} S_\mu^a S_\nu^a S_\mu^b S_\nu^b \right] \right\}. \tag{7}$$

The symbol  $\sum'_{ab}$  stands for a sum which excludes terms with any equal indices; i.e.  $a \neq b$ . The paramagnetic contribution  $\beta f_{PM} = -(\beta J)^2 m(m-3)/2$  has been subtracted as it does not depend on the order parameter. One then looks for a replica symmetry breaking ansatz for  $B^{ab}$ . Here we consider this to the first level in the standard Parisi procedure.

Using the standard procedure of the replica symmetry breaking method, one groups the  $n$  replicas in blocks of  $x$ , where  $x$  is a parameter (between 1 and  $n$ ) to be located by the saddle-point equations. Each block contains  $x$  replicas. Thus, one has

$$B^{ab} = \begin{cases} q & \text{if } I(a/x) = I(b/x) \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

where  $I(y)$  is an integer-valued function: its value is the smallest integer which is greater than or equal to  $y$ . Upon substituting in equation (7), one has

$$\beta f = \frac{(\beta J)^2}{2} (m-1)(m+2)(x-1)q^2 + (\beta J)^2 (x-1)mq + (\beta J)^2 m^2 q - \lim_{n \rightarrow 0} \frac{1}{n} \log \text{Tr} \exp \left[ (\beta J)^2 q \sum_{\mu\nu} \sum_k^{n/x} \left( \sum_{a \in \text{block}(k)} S_\mu^a S_\nu^a \right)^2 \right], \tag{9}$$

where there are  $n/x$  blocks labelled by  $k = 1, \dots, n/x$ . The index  $a$  belongs to block  $k$  if  $I(a/x) = k$ . We shall now perturbatively compute the free energy (9) by Taylor-expanding the free energy up to fourth order in  $q$ . This approximation implies that one is assuming the transitions to be continuous or at worst weakly discontinuous. After some lengthy but straightforward algebra, one obtains the following expression for the free energy:

$$\beta f(q, x) = -\frac{\alpha_2}{2} (x-1) t q^2 - \frac{\bar{\alpha}_3}{3} (x-1) q^3 - \frac{\hat{\alpha}_3}{3} (x-1)(x-2) q^3 - \frac{\beta_1}{12} (x-1)q^4 - \frac{\beta_3}{12} (x-1)(x-2)q^4 - \frac{\beta_5}{12} (x-1)(x-2)(x-3)q^4 + O[q^5], \tag{10}$$

where the coefficients in the free energy expansion are given by

$$\begin{aligned} \alpha_2 &= \frac{(m-1)(m+2)^3}{4m^2(1-t)^2} & \bar{\alpha}_3 &= \frac{(m-1)(m-2)(m+2)^5}{4m^3(m+4)(1-t)^3} \\ \hat{\alpha}_3 &= \frac{(m-1)(m+2)^4}{4m^3(1-t)^3} & \beta_1 &= \frac{3(m-1)(m-4)(m+2)^6(m^2+m-3)}{4m^4(m+4)(m+6)(1-t)^4} \\ \beta_3 &= \frac{3(m-1)(m-2)(m+2)^6}{m^4(m+4)(1-t)^4} & \beta_5 &= \frac{3(m-1)(m+2)^5}{4m^4(1-t)^4}, \end{aligned} \tag{11}$$

and  $t$  is the reduced temperature, defined as  $t = 1 - (T^2/T_C^2)$ , where

$$T_C = \frac{2mJ}{(m+2)k_B}. \tag{12}$$

For  $m$  less than a critical value  $m^*$ , discussed below, the transition is continuous, with the same  $T_C$  as predicted by RS theory [10]. In this case one may use the saddle-point method to evaluate the extremal values of the parameters  $q$  and  $x$ . These saddle-point equations are

$$\frac{\partial f}{\partial q} = \frac{\partial f}{\partial x} = 0,$$

from which one has

$$\begin{aligned} 0 &= 3t\alpha_2 + 3q(\bar{\alpha}_3 + (x-2)\hat{\alpha}_3) + q^2[\beta_1 + (x-2)(\beta_3 + (x-3)\beta_5)] \\ 0 &= 6t\alpha_2 + 4q(\bar{\alpha}_3 + (2x-3)\hat{\alpha}_3) + q^2[\beta_1 + (2x-3)\beta_3 + (3x^2 - 12x + 11)\beta_5]. \end{aligned} \quad (13)$$

According to the value of the quadrupole dimension  $m$ , the transition from the higher temperature RS phase can occur either continuously or discontinuously. The transition is continuous in  $q$  for  $m < m^* \simeq 3.37$ , i.e. when the coefficient  $\hat{\alpha}_3$  becomes larger than  $\bar{\alpha}_3$ .  $q$  and  $x$  satisfy the following equations that express the extremum of the free energy functional (10)

$$t < 0: \quad \begin{cases} q = 0 \\ x \text{ undetermined} \end{cases} \quad (14a)$$

$$t > 0: \quad \begin{cases} q = -\frac{t\alpha_2}{2(\bar{\alpha}_3 - \hat{\alpha}_3)} + \frac{t^2\alpha_2}{48(\bar{\alpha}_3 - \hat{\alpha}_3)^3 \hat{\alpha}_3^2} \{(\bar{\alpha}_3^2 + 4\bar{\alpha}_3\hat{\alpha}_3 - 15\hat{\alpha}_3^2)\beta_5 \\ \quad + \hat{\alpha}_3[-5\beta_1\hat{\alpha}_3 + \beta_3(7\hat{\alpha}_3 - 2\bar{\alpha}_3)]\} + O[t^3], \\ x = \frac{\bar{\alpha}_3}{\hat{\alpha}_3} + \frac{t\alpha_2[\hat{\alpha}_3^2(-\beta_1 + \beta_3) + \beta_5(\bar{\alpha}_3^2 - 2\bar{\alpha}_3\hat{\alpha}_3 - \hat{\alpha}_3^2)]}{4(\bar{\alpha}_3 - \hat{\alpha}_3)\hat{\alpha}_3^3} + O[t^2]. \end{cases} \quad (14b)$$

Close to the transition temperature  $T_C$ , i.e. when  $t \gtrsim 0$ , solution (14b) is valid only for  $2 < m \leq m^* \simeq 3.37$  within 1RSB subspace. At  $m^*$  the cubic term in the free energy functional (10) changes the sign. This coincides with  $x = 1$ . Thus, above  $m^*$ , the transition is no longer continuous. The parameters  $q$  and  $x$  are plotted for  $m = 3$  within this approximation in figure 1. By substituting equation (14b) in equation (10) one finds the free energy of the glass phase close to the transition, to be

$$\beta f = \frac{\alpha_2^3 t^3}{24\hat{\alpha}_3(\hat{\alpha}_3 - \bar{\alpha}_3)} + O[t^4] = -\frac{(m-1)(m+2)(m+4)t^3}{96(m^2 - m - 8)} + O[t^4]. \quad (15)$$

Below the transition the free energy is larger than that of the paramagnetic phase.

On the other hand, when  $m > m^*$  there is still a glass solution to the saddle-point equations but with a discontinuous onset of  $q$  from the higher temperature RS phase. The transition may be found with the additional requirement that the free energy in the paramagnetic phase is equal to the one in the glass phase with break point  $x$  equal to 1. Denoting this transition temperature by  $T_D$ , to the quartic order in  $q$  for the free energy, one finds that

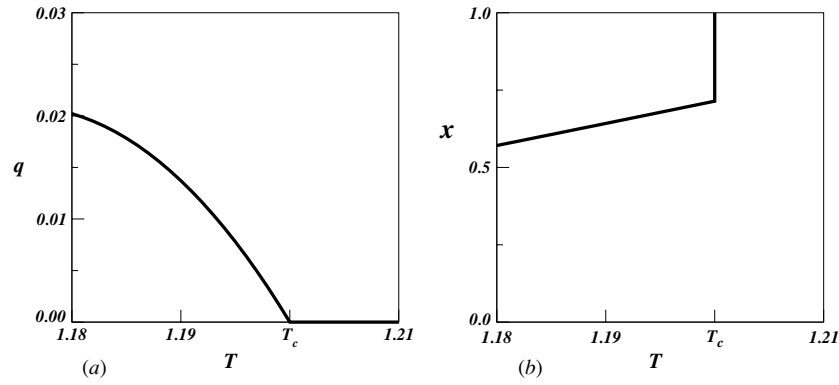
$$t_D = \frac{2(\bar{\alpha}_3 - \hat{\alpha}_3)^2}{3\alpha_2(\beta_1 - \beta_3 + 2\beta_5)} = \frac{2(m+6)(m^2 - m - 8)^2}{9(m+4)(168 + 34m - 35m^2 - 5m^3 + m^4)}, \quad (16)$$

where  $t_D = 1 - (T_D/T_C)^2$ . There is a discontinuous jump in the order parameter at  $T_D$  from zero to

$$q_D = -\frac{2(\bar{\alpha}_3 - \hat{\alpha}_3)}{\beta_1 - \beta_3 + 2\beta_5} = -\frac{2m(m+6)(m^2 - m - 8)(1 - t_D)}{3(m+2)(168 + 34m - 35m^2 - 5m^3 + m^4)}, \quad (17)$$

where  $q_D = q(T = T_D^-)$ . In the neighbourhood of the transition temperature  $T_D$  one finds that  $(x-1) \propto (t - t_D)$  and that the free energy of the quadrupolar glass phase is given by

$$\beta f = q_D(t - t_D)^2 + O[(t - t_D)^3].$$



**Figure 1.** (a) Plot of the one-step parameter  $q$  as a function of the temperature  $T$  (in units of  $k_B/J$ ); (b) Plot of the one-step breaking parameter  $x$  as a function of the temperature  $T$  (in units of  $k_B/J$ ). Both plots are drawn for  $m = 3$  and within the quartic approximation for the free energy (10).

Even though the transition is discontinuous in the order parameter  $q$ , there is no discontinuity in any thermodynamic quantities. Moreover, there is no latent heat at the transition. This behaviour is qualitatively common to a whole class of mean-field models of spin glasses e.g. the  $p > 2$  spin model beneath a critical field [9] and the Potts glass model above the critical Potts dimension  $p = 4$  [5, 6, 12].

Since the order parameter has a discontinuous jump at the transition temperature when  $m > m^*$ , the perturbative approach should no longer be valid. However, one may control the approximation by setting  $m = m^* + \varepsilon$ , where  $\varepsilon \ll 1$ . Thus, one obtains a quadrupolar glass phase with broken replica symmetry appearing below  $t_D \propto \varepsilon^2$ , with  $q_D \propto \varepsilon$  and  $x(T \rightarrow T_D^-) \rightarrow 1$ . Explicitly, to leading order, one has

$$q_D(m = m^* + \varepsilon) = \frac{2m^*g(m^*)(m^* + 4)(1 - 2m^*)}{m^* + 2}\varepsilon + O[\varepsilon^2], \quad (18a)$$

$$t_D(m = m^* + \varepsilon) = 4g(m^*)(m^{*2} - m^* - 5/2)\varepsilon^2 + O[\varepsilon^3], \quad (18b)$$

where  $g(m^*) = (m^* + 6)/[3(m^* + 4)(m^{*4} - 5m^{*3} - 35m^{*2} + 34m^* + 168)] < 0$ . In the next section, we shall investigate the stability of the 1RSB solution found against small further RSB fluctuations.

#### 4. Stability analysis

In order to study the stability of the 1RSB ansatz one introduces 1RSB-breaking fluctuations

$$B^{ab} = q\delta_{G_a G_b} + \eta^{ab}, \quad (19)$$

and expands the free energy to second order in the fluctuations  $\eta^{ab}$  [13]. The group Kronecker delta  $\delta_{G_a G_b}$  is unity if  $a$  and  $b$  belong to the same group and zero otherwise [6]. One has to compute the second derivatives of the free energy (7) with respect to  $\{B^{ab}\}$  at the 1RSB solution. The Taylor expansion of the free energy around the 1RSB solution is

$$f = f(q_D\delta_{G_a G_b}) + \frac{\partial f}{\partial B^{ab}}\eta^{ab} + \frac{\partial^2 f}{\partial B^{ab}\partial B^{cd}}\eta^{ab}\eta^{cd} + \dots \quad (20)$$

The quadratic form

$$\Delta = \frac{\partial^2 f}{\partial B^{ab} \partial B^{cd}} \eta^{ab} \eta^{cd} \tag{21}$$

should be positive definite for a stable solution of the problem. It is easy to see that the only non-vanishing terms are those where  $a, b, c$  and  $d$  all belong to the same group and those where  $a$  and  $c$  belong to group  $k$ , and  $b$  and  $d$  belong to group  $k'$ . The Hessian matrix  $S$  associated with the quadratic form (21) factorizes in  $n/x$  identical submatrices of dimension  $x(x-1)/2 \times x(x-1)/2$  which couple intragroup fluctuations and  $(n/x) [(n/x) - 1]/2$  identical submatrices of dimension  $x^2 \times x^2$  which couple intergroup fluctuations. We shall give details only on the intragroup matrices, because lengthy computations show that the intergroup matrices always have positive eigenvalues in the range of validity of the solution (see also [6]).

If the 1RSB is stable thermodynamically, all of the eigenvalues of the stability matrix should be positive. The intragroup matrices  $S^{(ab)(cd)}$  have three different types of matrix element:

$$S^{(ab)(ab)} = -2\alpha_2 t - 4\bar{\alpha}_3 B^{ab} - 2\beta_1 (B^{ab})^2 - \frac{1}{3}\beta_3 \sum_{k \neq a \neq b} B^{bk} B^{ka}$$

$$S^{(ab)(ac)} = -2\hat{\alpha}_3 B^{bc} - \frac{1}{6}\beta_3 [(B^{bc})^2 + 2B^{ab} B^{bc} + 2B^{bc} B^{ca}] - \frac{2}{3}\beta_5 \sum_{k \neq a \neq b \neq c} B^{kb} B^{ck}$$

$$S^{(ab)(cd)} = -\frac{2}{3}\beta_5 (B^{bc} B^{da} + B^{ac} B^{db}),$$

where  $a \neq b \neq c \neq d$ . Since  $a, b, c$  and  $d$  belong to the same group

$$S^{(ab)(ab)} = -2\alpha_2 t - 4\bar{\alpha}_3 q - 2\beta_1 q^2 - \frac{1}{3}\beta_3 (x-2)q^2$$

$$S^{(ab)(ac)} = -2\hat{\alpha}_3 q - \frac{5}{6}\beta_3 q^2 - \frac{2}{3}\beta_5 (x-3)q^2$$

$$S^{(ab)(cd)} = -\frac{4}{3}\beta_5 q^2.$$

The eigenvalues of the intragroup matrices, to order  $q^2$ , are given by

$$\lambda_1 = -2t\alpha_2 - 4q[\bar{\alpha}_3 + (x-2)\hat{\alpha}_3] - 2q^2[\beta_1 + (x-2)\beta_3 + (x^2 - 5x + 6)\beta_5]$$

$$\lambda_2 = -2t\alpha_2 - 2q[2\bar{\alpha}_3 + (x-4)\hat{\alpha}_3] - \frac{1}{6}q^2[12\beta_1 - (24 - 7x)\beta_3 + 4(x^2 - 9x + 18)\beta_5] \tag{22}$$

$$\lambda_3 = -2t\alpha_2 + 4q(\hat{\alpha}_3 - \bar{\alpha}_3) - \frac{1}{3}q^2[6\beta_1 + (x-7)\beta_3 - 4(x-4)\beta_5].$$

The behaviour of the eigenvalues in the ordered phase is obtained by substituting into the above equations the values of the parameters  $q$  and  $x$  pertinent to the continuous or discontinuous transition. Close to the continuous transition temperature, one finds that the first two eigenvalues are positive in the range of validity of the solution  $2 < m < m^*$ :

$$\lambda_1 = \frac{(m-1)(m+2)^3}{2m^2} t + O[t^2]$$

$$\lambda_2 = \frac{(m+2)^3(m^3 - 3m^2 - 10m + 12)}{4m^2(m^2 - m - 8)} t + O[t^2]. \tag{23}$$

The last one, to order  $t^2$ ,

$$\lambda_3 = \frac{(m-1)(m+2)^3(2m^5 + 15m^4 - 8m^3 - 104m^2 - 32m + 96)}{16m^2(m+6)(m^2 - m - 8)^2} t^2 + O[t^3], \tag{24}$$

is positive only for  $m > m_2^* \simeq 2.46$ . Thus, one finds a 1RSB stable mean-field theory with a continuous transition only in the range  $m_2^* < m < m^*$ . This lower limit is the same as given in



[4] and obtained by means of a complementary calculation based on the full replica symmetry breaking (FRSB) ansatz near  $T_C$  with a perturbation treatment. For  $m > m^*$  the behaviour of the eigenvalues in the ordered phase is obtained by setting  $x = 1$  and by substituting  $q$  with the value  $q_D$  obtained in equation (18a). Upon inserting these values, one easily finds that all the fluctuations around the ordered 1RSB phase are finite and positive:

$$\begin{aligned}\lambda_1 = \lambda_3 &= \frac{g(m^*)(m^* - 1)(m^* + 2)^3(-10m^{*2} + 10m^* + 3)}{m^{*2}} \varepsilon^2 > 0 \\ \lambda_2 &= \frac{g(m^*)(m^* - 4)(m^* - 1)(m^* + 2)^3(2m^* - 1)(2m^* + 5)}{m^{*2}} \varepsilon > 0.\end{aligned}\quad (25)$$

Thus, within our approximation, one finds a 1RSB stable mean-field theory with a discontinuous transition when  $m > m^*$ .

## 5. Dynamical transition

Generally, disordered systems with a discontinuous transition have a temperature  $T_G$  where a dynamic instability appears. This temperature is called the glass temperature and is higher than the transition temperature  $T_D$  where the replica symmetry breaks thermodynamically, if the latter breaking is discontinuous.

In the soft spin version of the Potts glass model [14] it has been shown—by means of dynamical studies of the mean-field theory—that indeed there is another transition at temperature  $T_G > T_D$  as in the  $p$ -spin model for  $p > 2$  [15]. Both static and dynamic transitions in the Potts ( $p > 4$ ) case have also been found in [6, 7, 12]. In the study of the thermodynamics of the quadrupolar glass,  $T_G$  can be computed by means of marginal stability [16]. By requiring the vanishing of the first and second derivative of the free energy (10) with respect to  $q$

$$\left(\frac{\partial f}{\partial q}\right)_{q=q_G} = 0, \quad \left(\frac{\partial^2 f}{\partial q^2}\right)_{q=q_G} = 0, \quad (26)$$

one finds, within our approximation, the dynamical transition temperature  $T_G$  and corresponding discontinuous jump  $q_G$  of the quadrupolar glass model

$$t_G = \frac{3(\bar{\alpha}_3 - \hat{\alpha}_3)^2}{4\alpha_2(\beta_1 - \beta_3 + 2\beta_5)} = \frac{(m+6)(m^2 - m - 8)^2}{4(m+4)(168 + 34m - 35m^2 - 5m^3 + m^4)} \quad (27)$$

and

$$q_G = -\frac{3(\bar{\alpha}_3 - \hat{\alpha}_3)}{2(\beta_1 - \beta_3 + 2\beta_5)} = -\frac{m(m+6)(m^2 - m - 8)(1 - t_G)}{2(m+2)(168 + 34m - 35m^2 - 5m^3 + m^4)}, \quad (28)$$

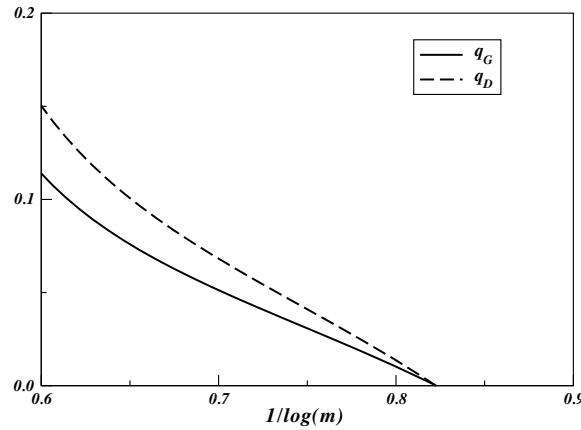
where  $t_G = 1 - (T_G/T_C)^2$  and  $q_G = q(T = T_G^-)$ . Again, by assuming the jump  $q_G$  near the temperature  $T_G$  to be small, one can control the approximation by letting  $m = m^* + \varepsilon$ ,  $\varepsilon \ll 1$ . Thus, one has

$$q_G(m = m^* + \varepsilon) = \frac{3m^*g(m^*)(1 - 2m^*)(m^* + 4)}{2(m^* + 2)} \varepsilon + O[\varepsilon^2], \quad (29a)$$

$$t_G(m = m^* + \varepsilon) = \frac{9}{2}g(m^*)(m^{*2} - m^* - 5/2)\varepsilon^2 + O[\varepsilon^3]. \quad (29b)$$

Within the approximation used, one finds

$$\frac{q_G}{q_D} = \frac{3}{4} + \frac{3}{16}g(m^*)(-2m^{*2} + 2m^* + 5)\varepsilon^2 + O[\varepsilon^3]. \quad (30)$$



**Figure 2.** The static  $q_D = q(T = T_D^-)$  and dynamic  $q_G = q(T = T_G^-)$  order parameter as a function of  $1/\log(m)$ . The dotted line is for the static value, the bold line is for the dynamical one.

It is worth noting that, to the leading order, exactly the same value for this ratio has been obtained for the Potts glass in [6, 7, 12], suggesting a sort of universality related to the same general structure of the free energy for both quadrupolar and Potts glass models (see also [4]). The results for  $q_D$  and  $q_G$  as a function of  $1/\log(m)$  are shown in figure 2. The ratio between the two transition temperatures  $T_G/T_D$  is very close to one

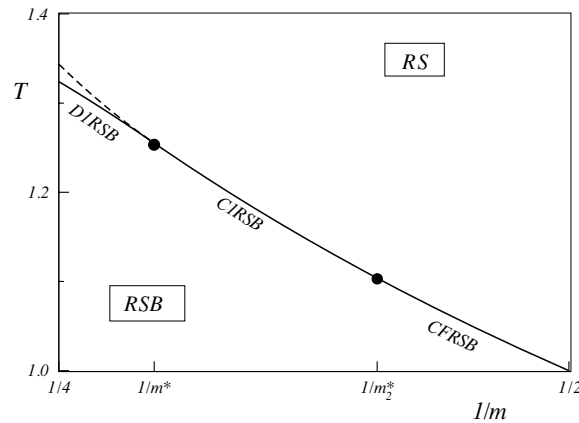
$$\frac{T_G}{T_D} = 1 + \frac{1}{8}g(m^*)(-2m^{*2} + 2m^* + 5)\varepsilon^2 + O[\varepsilon^3], \quad (31)$$

with  $T_G$  always bigger than  $T_D$ , as shown in figure 3. For  $m = 4$  (the smallest integer value of  $m$  compatible with a discontinuous transition) one finds that

$$\begin{aligned} q_D &= 0.056\dots, & T_D &= 1.342\dots, \\ q_G &= 0.042\dots, & T_G &= 1.343\dots \end{aligned} \quad (32)$$

Of course, a naive extension of our result to include large  $m$  results is not possible since we have assumed all the transitions to be at worst weakly discontinuous, implying the possibility of exploring only the range  $m$  close to  $m^*$ . However, since the mean-field theory of the Potts glass is qualitatively very similar to that of the quadrupolar glass, one may have an idea of the large  $m$  limit by considering the large  $p$  limit in the Potts glass model. There, the ratio  $q_G/q_D$  stays close to  $3/4$  for a large range of  $p$ , though it increases for very large  $p$ , approaching unity. The ratio  $T_G/T_D$  grows very slowly with  $p$  [7]. This behaviour is different from the case of the  $p$ -spin model, where the ratio  $q_G/q_D$  is not close to  $3/4$  even for small values of  $p$  and, in the limit  $p \rightarrow \infty$ , it converges to unity. Moreover, the ratio  $T_G/T_D$  grows faster with  $p$  than in the Potts problem [7].

A useful and new representation of the phase diagram is obtained by plotting the phase boundary line in the plane  $(T, 1/m)$ . One may identify three stable phases, RS paramagnetic and both 1RSB and FR SB glasses. In figure 3, the phases are labelled by their symmetry breaking and the manner of the onset from the paramagnet. The 1RSB transition is continuous between  $m_2^* \leq m \leq m^*$ , whereas it is discontinuous above  $m^*$ . Note that, at  $m = m^*$ , the transition from RS passes continuously from continuous 1RSB (C1RSB) to discontinuous 1RSB (D1RSB) within the one-step RSB phase. The dotted line in the figure corresponds to the  $m > m^*$  dynamical transition temperature given in equation (27). The situation is



**Figure 3.** Phase diagram of the quadrupolar glass model in the  $(T, 1/m)$  plane.  $T$  is in units of  $k_B/J$ . For  $2 < m < m_2^*$  the transition from the higher temperature RS phase occurs within the full replica symmetry breaking mechanism. For  $m < m^*$  the thermodynamic and dynamical transitions coincide. For  $m > m^*$  the dynamical transition, denoted by the dotted line, is higher than the thermodynamic one (solid line). The plot is shown within the quartic approximation for the free energy expansion in  $q$ .

analogous to that of the Potts glass model which shows a crossover from the continuous transition to the discontinuous transition as the number of Potts states increases [5, 6]. The  $p > 2$ -spin Ising and spherical spin glasses also show transitions from C1RSB to D1RSB as an applied field is reduced but differ from the present problem in that the critical field makes also a maximum in the transition temperature, in contrast to the present monotonic variation with  $1/m$ . For  $m < m_2^*$  the transition is continuous to full replica symmetry breaking. A phase line (not shown, but continuous) separates the one-step and full replica symmetry breaking phases within the RSB region.

## 6. Concluding remarks

In this paper we have investigated the quadrupolar glass model in the framework of the replica method. Upon introducing a simple one-step replica symmetry breaking ansatz, one may find a stable mean-field theory with a continuous or discontinuous transition, according to the value of the quadrupole dimension  $m$ . The transition is continuous to one-step replica symmetry breaking in the range of the quadrupolar dimension  $2.46 < m < 3.37$ . For the discontinuous transition ( $m > 3.37$ ) there are two different transition temperatures. We have computed the ratio  $q_G/q_D$ , where  $q_G$  and  $q_D$  are the order parameters associated, respectively, with the dynamic and thermodynamic transition. The ratio between the two transition temperatures  $T_G/T_D$  is also computed. Within the approximation used, the values of these ratios,  $q_G/q_D = 3/4$  and  $T_G/T_D \simeq 1$  (to leading order), are the same as those found in [6, 7, 12] for the Potts glass model.

The results we have obtained confirm the general wisdom that the properties of the quadrupolar glass, with continuous ( $m < m^*$ ) and discontinuous transitions ( $m > m^*$ ), are similar to those of the  $p < 4$  and  $p > 4$  Potts glass well studied in the literature [5–7, 12, 15]. Although the investigation focused on the quadrupolar glass phase, in the wider  $(J_0, J, T)$  space there should exist different types of ferromagnet, collinear and canted; see e.g. [10].

The full phase diagram should include also another curve which may be captured by complexity arguments. In analogy with the  $p$ -spin spin glass there should be another critical line  $T^{\text{compl}}$  associated with the onset of macroscopic complexity [17].

### Acknowledgments

We thank P M Goldbart for the benefit of stimulating discussions. We also thank the EPSRC for financial support in Oxford under grants GR/R83712/01 and 97304299 and ESF programme SPHINX for the opportunity to meet to continue this work.

### References

- [1] Höchli U T, Knorr K and Loidl A 2002 *Adv. Phys.* **51** 589
- [2] Binder K and Reger J D 1992 *Adv. Phys.* **41** 547
- [3] Sherrington D and Kirkpatrick S 1975 *Phys. Rev. Lett.* **35** 1792
- [4] Goldbart P and Elderfield D 1985 *J. Phys. C: Solid State Phys.* **18** L229
- [5] Gross D J, Kanter I and Sompolinsky H 1985 *Phys. Rev. Lett.* **55** 304
- [6] Cwiliich G and Kirkpatrick T R 1989 *J. Phys. A: Math. Gen.* **22** 4971
- [7] De Santis E, Parisi G and Ritort F 1995 *J. Phys. A: Math. Gen.* **28** 3025
- [8] Crisanti A and Sommers H-J 1992 *Z. Phys. B* **87** 341
- [9] Gardner E 1985 *Nucl. Phys. B* **257** 747
- [10] Goldbart P and Sherrington D 1985 *J. Phys. C: Solid State Phys.* **18** 1923
- [11] Goldbart P 1985 *PhD Thesis* Imperial College, London
- [12] Kirkpatrick T R and Wolynes P G 1987 *Phys. Rev. B* **36** 8552
- [13] de Almeida J R L and Thouless D J 1978 *J. Phys. A: Math. Gen.* **11** 983
- [14] Kirkpatrick T R and Thirumalai D 1988 *Phys. Rev. B* **37** 5342
- [15] Kirkpatrick T R and Thirumalai D 1987 *Phys. Rev. B* **36** 5388
- [16] Sommers H-J 1983 *Z. Phys. B* **50** 97
- [17] Kondor I and De Dominicis C 1986 *Europhys. Lett.* **2** 617
- [17] Cavagna A, Garrahan J P and Giardinà I 1999 *J. Phys. A: Math. Gen.* **32** 711