Possible instability of one-step replica symmetry breaking in *p*-spin Ising models outside mean-field theory

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The fully connected Ising p-spin model has for $p > 2$ a discontinuous phase transition from the paramagnetic phase to a stable state with one-step replica symmetry breaking (1RSB). However, simulations in three dimension do not look like these mean-field results and have features more like those which would arise with full replica symmetry breaking (FRSB). To help understand how this might come about we have studied in the fully connected p-spin model the state of two-step replica symmetry breaking (2RSB). It has a free energy degenerate with that of 1RSB, but the weight of the additional peak in $P(q)$ vanishes. We expect that the state with full replica symmetry breaking (FRSB) is also degenerate with that of 1RSB. We suggest that finite-size effects will give a nonvanishing weight to the FRSB features, as also will fluctuations about the mean-field solution. Our conclusion is that outside the fully connected model in the thermodynamic limit, FRSB is to be expected rather than 1RSB.

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I. INTRODUCTION

The historical importance of p-spin models [1] was that it was investigations of their properties which led to the random first-order transition theory (RFOT) of structural glasses [2–7]. In this paper we shall once again study the fully connected p-spin glass model described by the Hamiltonian [1]

$$H = -\sum_{1\leqslant i_1<\cdots<i_p\leqslant N} J_{i_1,i_2,\ldots,i_p} S_{i_1} S_{i_2} \cdots S_{i_p}, \tag{1}$$

where S_i is the Ising spin at site i, $i, \ldots, N$, and the bonds $J_{i_1,i_2,\ldots,i_p}$ are independent random variables satisfying the Gaussian distribution with zero mean and variance $p!/(2N^{p-1})$. At high temperatures, there is a replica symmetric (RS) paramagnetic phase. To characterize the nature of a glass phase it is useful to study the distribution $P(q)$ of overlaps q, between two copies A and B of the system, where

$$q = \frac{1}{N}\sum_i S_i^A S_i^B, \tag{2}$$

and $P(q)$ is defined as

$$P(q) = \overline{P_J(q)}. \tag{3}$$

The thermal averaging is done with the Hamiltonians of the two copies, A and B, and the overline denotes an average over the bonds. In the paramagnetic (high-temperature) phase of the Hamiltonian of Eq. (1),

$$P(q) = \delta(q - q_0), \tag{4}$$

where $q_0 = 0$. Much of the work on the p-spin model has focused on the dynamical transition at a temperature T_d, the temperature below which metastable states exist separated by barriers of order N. This has connections with the glass transition T_g of structural glasses. At a lower temperature $T_{\rm 1RSB}^c$ there is a discontinuous phase transition to a state with one-step replica symmetry breaking (1RSB). The distribution of overlaps in the low-temperature phase becomes

$$P(q) = m\delta(q - q_0) + (1 - m)\delta(q - q_1), \tag{5}$$

where $0 \leqslant m \leqslant 1$ and m equals unity at $T_{\rm 1RSB}^c$. The order parameter q_1 is finite at the transition, so the transition is discontinuous, but there is no latent heat at the transition. In the RFOT approach to structural glasses $T_{\rm 1RSB}^c$ becomes the Kauzmann transition temperature T_K [8], and for temperatures below T_K the phase with 1RSB is the ideal glass phase. This paper is about the properties of the p-spin system at temperatures less than $T_{\rm 1RSB}^c$ or structural glasses at temperatures below T_K. Until recently, behavior at temperatures below T_g would have been of only academic interest, but the use of the swap algorithm in simulations [9] and the creation of ultrastable glasses by vapor deposition has changed that situation [9,10].

Gardner pointed out [1] that in the fully connected p-spin model there is a continuous transition (now called the Gardner transition), at a temperature T_G below $T_{\rm 1RSB}^c$, from the state with 1RSB to a state with full replica symmetry breaking (FRSB) [11]. Recently there has been much interest in Gardner transitions in structural glasses, which is reviewed in Ref. [12].

The chief purpose of this paper is to question whether the state which exists between $T_G < T < T_{\rm 1RSB}^c$ really does have 1RSB symmetry breaking. We shall argue that it probably is much more like a state with FRSB. We reached this conclusion from the calculation done in Sec. II, where we have gone beyond 1RSB to 2RSB. A 2RSB calculation has already been done for the p-spin model by Montanari and Ricci-Tersenghi [13], but it was mostly focused on behavior at $T = 0$. In a

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2RSB calculation $P(q)$ has the form

$$P(q) = m_1\delta(q-q_0) + (m_2-m_1)\delta(q-q_1) + (1-m_2)\delta(q-q_2), \tag{6}$$

where the weights $1 \geqslant m_2 \geqslant m_1 \geqslant 0$.

We shall find in Sec. II that there are two types of solution for the equations which determine m_1, m_2, q_0, q_1, q_2 for the fully connected p-spin model in the limit $N \to \infty$. There is a solution, which we refer to as the type-II 2RSB solution, which has a higher free energy than the 1RSB solution at temperature $T < T_G$ (which in the world of replicas makes it more stable than the 1RSB solution); it is, however, just the 2RSB approximation to the state of FRSB which is expected for $T < T_G$. It has an extension to the region $T > T_G$, but there it has a lower free energy than that of the state of 1RSB.

The other solution will be referred to as the type-I 2RSB solution. It has $m_2 = m_1 = m$, where m is that of the 1RSB solution of Eq. (5). The free energy of this solution is exactly degenerate with that of the 1RSB state, and because $m_2 = m_1$ its $P(q)$ is also identical with that of the 1RSB state: There is no weight in the δ function at $q = q_1$. One would expect that similar states will exist at the K level of replica symmetry breaking, KRSB, all the way up to FRSB. We believe that if one goes beyond the leading term as $N \to \infty$ to include the fluctuations around the mean-field limit then the degeneracy is lifted and the system goes to a state with FRSB, by having (say) $m_2 - m_1$ no longer zero but of order of a small quantity which vanishes as $N \to \infty$.

We can provide two arguments that 1RSB has to be replaced by FRSB. In fact, we believe that there is already evidence that finite N effects do modify 1RSB order to FRSB order in the fully connected model. Billoire *et al.* [14] studied $P(q)$ of the $p = 3$ fully connected model for values of N up to 192. Their $P(q)$ looks remarkably similar to the finite-size form predicted by Mottishaw and Derrida [15] for the generalized random energy model (GREM) when FRSB is present. Unfortunately the treatment in Ref. [15] was not done using replicas, so it is not obvious how it might be extended directly to the finite N fully connected p-spin model.

Our second argument also concerns lifting the degeneracy of the states with KRSB but this time by the fluctuation effects about the mean-field solution. The 1RSB (and the KRSB) state do not have massless modes (null eigenvalues in their Hessian matrix) [16]. For p-spin models with p even and $p/2$ odd (such as $p = 6$) the system has time-reversal invariance and one can calculate the free energy cost of creating a droplet of reversed spins with linear extent R within the state [17]. (The calculations of this reference need to be qualified to make it clear that they are only applicable when p is even with $p/2$ odd.) The droplet free energy cost varies as $\sim \exp(-R/\xi)$, where ξ is the longest length scale in the system. Thus the free energy cost of flipping the spins in a region of size R will vanish for $R \gg \xi$, implying that the state would be unstable against thermal fluctuations. However, in the presence of FRSB, one expects massless modes to occur, i.e., that $\xi \to \infty$ [18]. An example of a state with massless modes is the low-temperature phase of the Ising ($p = 2$) spin glass, which is a phase with FRSB [18] and is stable against excitations of spin-flipped droplets. We would therefore conclude that the state which exists between T_G and T^c_{1RSB} can be stable against such fluctuations only if it has FRSB. (This argument holds only for p even with $p/2$ odd, but we suspect that for other p values droplets—but not simply time-reversed droplets—will exist to destabilize them also.)

In Sec. II we set up the 2RSB calculations and present the main results. In Sec. III we introduce types of $(M-p)$ models which are convenient for describing fluctuation effects when p is even, the "balanced" $(M-p)$ models, and show that among them there is a subset, those with p even and $p/2$ odd, for which the calculations in Ref. [17] are valid. In Sec. IV we speculate what might happen in physical dimensions like $d = 3$, which are a long way away from the mean-field limit of the fully connected model studied in Sec. II. There are simulations in three dimensions which have FRSB-like features [19,20]. It is these studies which suggested to us that the state of 1RSB might just be a feature of the infinite N fully connected p-spin model. We shall also comment on the possible relevance of our work to structural glasses (which is the reason one studies p-spin models) and speculate as to whether the fluctuations remove not only 1RSB but FRSB in three dimensions.

II. THE FULLY CONNECTED p-SPIN GLASS MODEL

In this section, we study the fully connected p-spin glass model described by the Hamiltonian of Eq. (1) in the limit when the number of spins N goes to infinity. The replicated partition function averaged over the random couplings at inverse temperature β can be expressed [1] as integrals over the auxiliary fields q_{ab} and λ_{ab} as

$$\langle Z^n \rangle = e^{nN\beta^2/4} \int \prod_{a<b} dq_{ab} \int \prod_{a<b} d\lambda_{ab} \exp[-NG(q_{ab}, \lambda_{ab})], \tag{7}$$

where the q_{ab} and λ_{ab} are symmetric matrices with the replica indices $a, b = 1, 2, \ldots, n$ with zero diagonal part and

$$G(q_{ab}, \lambda_{ab}) = -\frac{\beta^2}{4} \sum_{a\neq b} q_{ab}^p + \frac{1}{2} \sum_{a\neq b} \lambda_{ab} q_{ab} - \ln \mathrm{Tr}_{S_a} \exp\left[\frac{1}{2} \sum_{a\neq b} \lambda_{ab} S_a S_b\right]. \tag{8}$$

In the large-N limit, the integral in Eq. (7) is given by the saddle-point values of q_{ab} and λ_{ab} The free energy per site of the p-spin spin glass model is then given by

$$\frac{F}{N} = \frac{1}{\beta} \lim_{n\to 0} \frac{1}{n} G[q_{ab}, \lambda_{ab}] - \frac{\beta}{4}, \tag{9}$$

where the saddle-point values of q_{ab} and λ_{ab} are assumed to be used.

If we take the replica symmetric form, $q_{ab} = q$ and $\lambda_{ab} = \lambda$ for $a \neq b$, the solution to the saddle-point equations are given by $\lambda = q = 0$, and the free energy per site is just

$$\frac{F_{\mathrm{RS}}}{N} = -\frac{\beta}{4} - \frac{\ln 2}{\beta}. \tag{10}$$

The entropy per site is then given by

$$\frac{S_{\rm RS}}{N} = \ln 2 - \frac{\beta^2}{4}, \tag{11}$$

which becomes negative for temperature $T < T_* \equiv 1/(2\sqrt{\ln 2}) \simeq 0.601$.

A. One-step replica symmetry breaking

We now consider the case where the saddle-point values of q_{ab} and λ_{ab} take the 1RSB form, where q_{ab} and λ_{ab} is equal to q and λ on n/m diagonal blocks of size m and q_0 and λ_0 outside the blocks, respectively. The detailed derivations can be found elsewhere [1,16], and we present the relevant results in the following.

In the absence of an external field, the 1RSB saddle points are given by $q_0 = \lambda_0 = 0$. The other parameters are determined by

$$\lambda = \frac{\beta^2}{2} p q^{p-1} \tag{12}$$

and

$$q = \frac{\int Dy\ \cosh^m(\sqrt{\lambda}y)\tanh^2(\sqrt{\lambda}y)}{\int Dy\ \cosh^m(\sqrt{\lambda}y)}, \tag{13}$$

where

$$\int Dz \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz\ e^{-z^2/2}. \tag{14}$$

The free energy for the 1RSB solution is given by

$$\frac{F_{\rm 1RSB}}{N} = -\frac{\beta}{4}[1 + (1-m)(p-1)q^p - pq^{p-1}] - \frac{\ln 2}{\beta} - \frac{1}{\beta m} \ln \int Dy\ \cosh^m(\sqrt{\lambda}y). \tag{15}$$

There is another saddle-point equation which is obtained by varying the free energy with respect to m:

$$0 = \frac{\beta^2}{4} q^p (p-1) + \frac{1}{m^2} \ln \int Dy\ \cosh^m(\sqrt{\lambda}y) - \frac{1}{m} \frac{\int Dy\ \cosh^m(\sqrt{\lambda}y) \ln[\cosh(\sqrt{\lambda}y)]}{\int Dy\ \cosh^m(\sqrt{\lambda}y)} = 0. \tag{16}$$

We note that when $m = 1$, $F_{\rm 1RSB}$ becomes equal to $F_{\rm RS}$ in Eq. (10). We determine the temperature $T^c_{\rm 1RSB}$ at which the two free energies are equal to each other by setting $m = 1$ in Eqs. (13) and (16) and by solving the equations for β. We have $T^c_{\rm 1RSB} \simeq 0.651$ for $p = 3$.

As noted by Gardner in Ref. [1], the 1RSB solution is stable only when

$$\frac{q}{(p-1)\lambda} > \frac{\int Dy\ \cosh^{m-4}(\sqrt{\lambda}y)}{\int Dy\ \cosh^m(\sqrt{\lambda}y)}. \tag{17}$$

If we use the 1RSB solution, this equation translates into $T > T_G$, where $T_G \simeq 0.24$ for $p = 3$.

B. Two-step replica symmetry breaking

We now consider the case where q_{ab} takes the two-step replica symmetry breaking (2RSB) form with values q_0, q_1, and q_2 specified by the parameters m_1 and m_2. There are n/m_1 diagonal blocks of size m_1 denoted by B_i, $i = 1, \ldots, n/m_1$. Outside B_i, $q_{ab} = q_0$. Inside each B_i, $q_{ab} = q_1$ except for m_1/m_2 diagonal blocks of size m_2 denoted by B_i^j, $j = 1, \ldots, m_1/m_2$, where $q_{ab} = q_2$. λ_{ab} takes the same form with λ_0, λ_1, and λ_2. The terms in the free energy are now given by

$$\sum_{a\neq b} q_{ab}^p = n\big[(m_2-1)q_2^p + (m_1-m_2)q_1^p + (n-m_1)q_0^p\big], \tag{18}$$

$$\sum_{a\neq b} \lambda_{ab} q_{ab} = n[(m_2-1)\lambda_2 q_2 + (m_1-m_2)\lambda_1 q_1 + (n-m_1)\lambda_0 q_0], \tag{19}$$

and

$$\frac{1}{2}\sum_{a\neq b} \lambda_{ab} S_a S_b = \frac{\lambda_0}{2} \sum_{a\neq b}^{n} S_a S_b + \frac{1}{2}(\lambda_1 - \lambda_0) \sum_{i=1}^{n/m_1} \sum_{\substack{a,\, b\in B_i \\ a\neq b}} S_a S_b + \frac{1}{2}(\lambda_2 - \lambda_1) \sum_{i=1}^{n/m_1} \sum_{j=1}^{m_1/m_2} \sum_{\substack{a,\, b\in B_i^j \\ a\neq b}} S_a S_b. \tag{20}$$

We then decouple the terms containing spins with two different replica indices using the Hubbard-Stratonovich transformation. After taking the trace over the spins, we obtain the expression for the 2RSB free energy as

$$\frac{F_{\rm 2RSB}}{N} = -\frac{\beta}{4}\big[1 + (m_2-1)q_2^p + (m_1-m_2)q_1^p - m_1 q_0^p\big] + \frac{1}{2\beta}[(m_2-1)\lambda_2 q_2 + (m_1-m_2)\lambda_1 q_1 - m_1\lambda_0 q_0] + \frac{\lambda_2}{2\beta} - \frac{\ln 2}{\beta} - \frac{1}{\beta m_1} \int Dz\ \ln \int Dy \left\{ \int Dw\ \cosh^{m_2}[\eta(z,y,w)] \right\}^{m_1/m_2}, \tag{21}$$

where

$$\eta(z,y,w) = \sqrt{\lambda_0}z + \sqrt{\lambda_1 - \lambda_0}y + \sqrt{\lambda_2 - \lambda_1}w. \tag{22}$$

Varying the free energy with respect to q_i, we obtain $\lambda_i = \beta^2 p q_i^{p-1}/2$ for $i = 0$, 1, and 2.

The saddle-point equation obtained from varying λ_0 gives

$$q_0 = \int Dz \left[\frac{\int Dy \, \{\int Dw_1 \, \cosh^{m_2}[\eta(z,y,w_1)]\}^{\frac{m_1}{m_2}-1} \int Dw_2 \, \cosh^{m_2}[\eta(z,y,w_2)] \tanh[\eta(z,y,w_2)]}{\int Dy \, \{\int Dw \, \cosh^{m_2}[\eta(z,y,w)]\}^{\frac{m_1}{m_2}}} \right]^2. \tag{23}$$

We can show that $q_0 = 0$ and $\lambda_0 = 0$ are solutions to the above equation and set them to zero from now on. Varying the free energy with respect to λ_1 and λ_2 gives, respectively,

$$q_1 = \frac{\int Dy \, \{\int Dw_1 \, \cosh^{m_2}[\zeta(y,w_1)]\}^{\frac{m_1}{m_2}-2} \{\int Dw_2 \, \cosh^{m_2}[\zeta(y,w_2)] \tanh[\zeta(y,w_2)]\}^2}{\int Dy \, \{\int Dw \, \cosh^{m_2}[\zeta(y,w)]\}^{\frac{m_1}{m_2}}} \tag{24}$$

and

$$q_2 = \frac{\int Dy \, \{\int Dw_1 \, \cosh^{m_2}[\zeta(y,w_1)]\}^{\frac{m_1}{m_2}-1} \int Dw_2 \, \cosh^{m_2}[\zeta(y,w_2)] \tanh^2[\zeta(y,w_2)]}{\int Dy \, \{\int Dw \, \cosh^{m_2}[\zeta(y,w)]\}^{\frac{m_1}{m_2}}}, \tag{25}$$

where

$$\zeta(y,w) = \sqrt{\lambda_1} y + \sqrt{\lambda_2 - \lambda_1} w. \tag{26}$$

Using $q_0 = \lambda_0 = 0$, we can rewrite the free energy, Eq. (21), as

$$\frac{F_{\rm 2RSB}}{N} = -\frac{\beta}{4}\left[1 + (p-1)\left\{(1-m_2)q_2^p + (m_2-m_1)q_1^p\right\} - pq_2^{p-1}\right] - \frac{\ln 2}{\beta} - \frac{1}{\beta m_1} \ln \int Dy \left\{ \int Dw \, \cosh^{m_2}[\zeta(y,w)] \right\}^{m_1/m_2}. \tag{27}$$

We evaluate the 2RSB free energy by solving the above saddle-point equations numerically. There are two more saddle-point equations which can be obtained by varying the free energy with respect to m_1 and m_2. We find, however, that finding a numerical solution of the full set of these coupled saddle-point equations is rather tricky. It is more convenient to solve the two equations (24) and (25) first for given m_1 and m_2 at fixed inverse temperature β. We then evaluate $F_{\rm 2RSB}$ from Eq. (27) and find the values of m_1 and m_2 that maximize the free energy. Since $1 \leqslant m_2 \leqslant m_1 \leqslant n$, we have to have $0 \leqslant m_1 \leqslant m_2 \leqslant 1$ in the limit $n \to 0$.

Before presenting the 2RSB solution, we first look at the trivial limits of these equations. We first note that $q_1 = 0$ is always a solution to Eq. (24), since the integrals become independent of y with $\zeta = \sqrt{\lambda_2} w$. When $q_1 = \lambda_1 = 0$, Eq. (25) for q_2 becomes exactly the same as Eq. (13) for the 1RSB solution if we regard q_2 and m_2 as the 1RSB parameters q and m, respectively. The 2RSB free energy, Eq. (27) also reduces to the one for the 1RSB scheme, Eq. (15). We note that this solution is independent of m_1.

There is another limit where the equations reduce to the 1RSB ones. It is the case where $q_1 = q_2$. We can indeed check this is a solution if we take $\lambda_1 = \lambda_2$ in Eqs. (24) and (25). We find the integrals over w can be done easily as the integrands become independent of w. The right-hand sides of the two equations become identical to each other and also to Eq. (13) for the 1RSB case if we regard $q_1 = q_2$ and m_1 as the 1RSB parameters q and m, respectively. We can also check in this limit that the free energy reduces to the 1RSB one. In this case, the solution is independent of m_2.

The 2RSB solution we look for in this paper therefore corresponds to the case where $0 < q_1 < q_2$. At fixed temperature, we solve Eqs. (24) and (25) numerically for given values of m_1 and m_2. We find that there are two different types of 2RSB solutions, which we denote by type-I and type-II in the following. The type-I solution is characterized by q_1 being much smaller than q_2, and it exists in the entire temperature range below $T^c_{\rm 1RSB}$. At fixed temperature, we calculate the free energy for the type-I solution for various values of m_1 and m_2. For given m_1, we find that the free energy is always a decreasing function of $m_2 (\geqslant m_1)$ so that the maximum free energy for given m_1 is always at $m_2 = m_1$. As we change the value of m_1, we find that the maximum occurs when m_1 is equal to the 1RSB solution $m(T)$ at that temperature. In Fig. 1 we plot the type-I 2RSB solutions, q_1 and q_2 as a function of temperature. In the zero-temperature limit, q_2 approaches 1, while q_1 saturates to a constant value around 0.52.

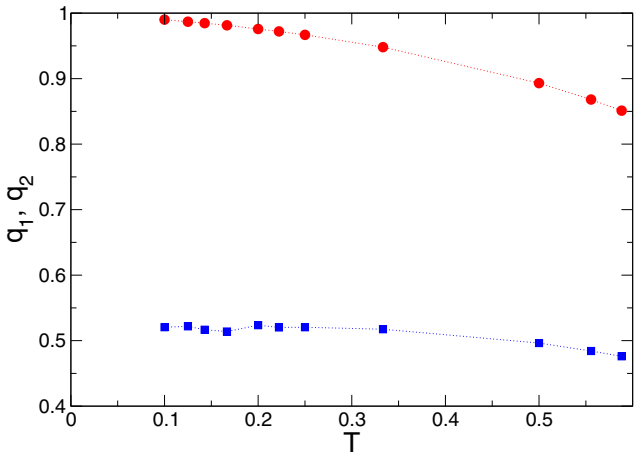

FIG. 1. Type-I 2RSB solutions, q_1 and q_2 as functions of temperature T for $p = 3$. Squares (blue) and circles (red) correspond to q_1 and q_2, respectively.

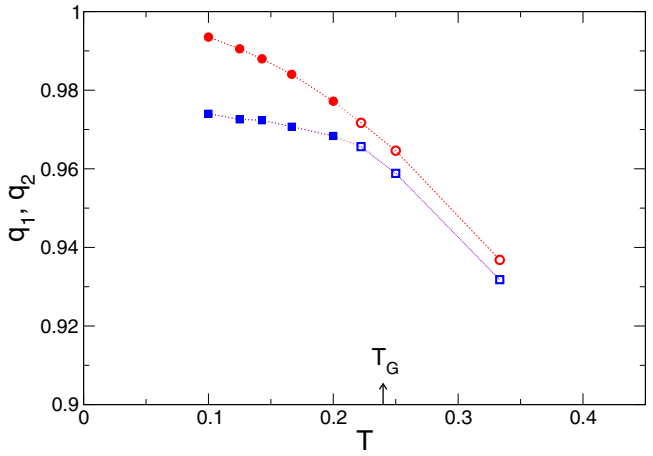

FIG. 2. Type-II 2RSB solutions, q_1 and q_2 as functions of temperature T for $p = 3$. Squares (blue) and circles (red) correspond to q_1 and q_2, respectively. The filled and open symbols correspond to the cases $m(T) < m_1^*(T)$ and $m(T) > m_1^*(T)$ (see Fig. 3). T_G is the Gardner temperature.

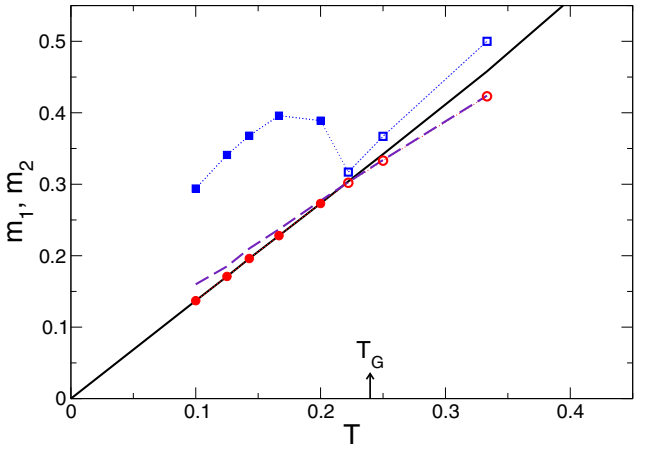

FIG. 3. Type-II 2RSB solutions, m_1 and m_2 as functions of temperature T for $p = 3$. Circles (red) and and squares (blue) correspond to m_1 and m_2, respectively. The solid line is the 1RSB solution $m(T)$. The dashed line is $m_1^*(T)$ above which the type-II 2RSB solution disappears. The filled and open symbols correspond to the cases $m(T) < m_1^*(T)$ and $m(T) > m_1^*(T)$, respectively. T_G is the Gardner temperature.

We can see that the type-I 2RSB solution with $m_1 = m_2$ actually reproduces the 1RSB free energy in the following way. If we put $m_1 = m_2$ in Eq. (25), it becomes

$$q_2 = \frac{\int Dy \int Dw \ \cosh^{m_2}[\zeta(y,w)] \tanh^2[\zeta(y,w)]}{\int Dy \int Dw \ \cosh^{m_2}[\zeta(y,w)]}. \tag{28}$$

If we use the notation

$$\sigma_1 = \sqrt{\lambda_1}, \quad \sigma_2 = \sqrt{\lambda_2 - \lambda_1}, \tag{29}$$

and the vector notation $\vec{\sigma} = (\sigma_1, \sigma_2)$ and $\vec{r} = (y, w)$ for the integration variable y and w, then $\zeta(y, w) = \vec{\sigma} \cdot \vec{r}$, and we can rewrite Eq. (28) as

$$q_2 = \frac{\int D^2\vec{r} \ \cosh^{m_2}(\vec{\sigma} \cdot \vec{r}) \tanh^2(\vec{\sigma} \cdot \vec{r})}{\int D^2\vec{r} \ \cosh^{m_2}(\vec{\sigma} \cdot \vec{r})}, \tag{30}$$

where

$$\int D^2\vec{r} \equiv \int Dy \int Dw = \int \frac{d^2\vec{r}}{2\pi} \, e^{-|\vec{r}|^2/2}. \tag{31}$$

Since the right-hand side of Eq. (30) depends only on $|\vec{\sigma}|$, it determines the value of $|\vec{\sigma}|$ or

$$q_2 = \left(\frac{2\lambda_2}{p\beta^2}\right)^{1/(p-1)} = \left(\frac{2|\vec{\sigma}|^2}{p\beta^2}\right)^{1/(p-1)} \tag{32}$$

for given $m_1 = m_2$ and β. We note that this equation is exactly the same as the 1RSB one [Eq. (13)] with q_2 and $|\vec{\sigma}|$ playing the role of q and $\sqrt{\lambda}$, respectively, for the 1RSB case. The 2RSB free energy [Eq. (27)] also becomes the 1RSB one [Eq. (15)] when $m_1 = m_2$. Therefore q_2 shown in Fig. 1 is the same as q for the 1RSB scheme. On the other hand, the equation for q_1 [Eq. (24)] becomes decoupled from the rest of the equations for $m_1 = m_2$, and in particular does not appear in the free energy expression. The solution of this equation for q_1 is shown in Fig. 1.

The type-II 2RSB solution is characterized by q_1 being closer to q_2 than the type-I counterpart as shown in Fig. 2. The type-II solution is certainly the relevant solution for temperatures below T_G. At fixed temperature, we again calculate the type-II 2RSB free energy for various values of m_1 and m_2. For given m_1, the maximum free energy occurs at some value of m_2 which is larger than m_1. If we now change m_1, we find that the type-II solution ceases to exist for m_1 larger than some value $m_1^*(T)$. At low temperatures, this limiting value $m_1^*(T)$ is larger than the 1RSB values $m(T)$. We find that the free energy achieves a maximum when m_1 is equal to the 1RSB value $m(T)$ and at some m_2 which is larger than $m_1 = m(T)$. These values of m_1 and m_2 are shown in Fig. 3 as filled symbols. At relatively high temperatures, $m_1^*(T)$ is smaller than $m(T)$; that is, before m_1 reaches the 1RSB value $m(T)$, the solution disappears. Then the maximum free energy just corresponds to $m_1 = m_1^*(T)$ and m_2 being equal to some value larger than $m_1 = m_1^*(T)$. These are shown in Fig. 3 as open symbols. As we can see from Fig. 2 and Fig. 3, the temperature dependence of the parameters is quite different for temperature above and below T_G. The change of behavior actually occurs at a temperature $T \simeq 0.22$ for $p = 3$, which is quite close to but just below T_G. (We suspect that for KRSB as K grows, the change of behavior will approach T_G.) This alteration in behavior is also reflected in the type-II free energy and is shown in Fig. 4. The 2RSB free energy is larger than the 1RSB one for $T < 0.22 \approx T_G$ but becomes smaller than the 1RSB value at temperatures $T > T_G$. It is clear that the type-II solution is just the 2RSB approximation to the state with FRSB, which is expected below T_G [1]. What is perhaps surprising is that this solution has an extension into the temperature region $T > T_G$. Our numerical work fails to find it above a temperature T^{**}. Note that $q_1 \to q_2$ as T grows towards T_{1RSB}^c. If $q_1 = q_2$ the $P(q)$ of 2RSB in Eq. (6) reduces to the 1RSB form of Eq. (5). The iterative procedure used locks onto this 1RSB solution above T^{**} rather than the 2RSB solution.

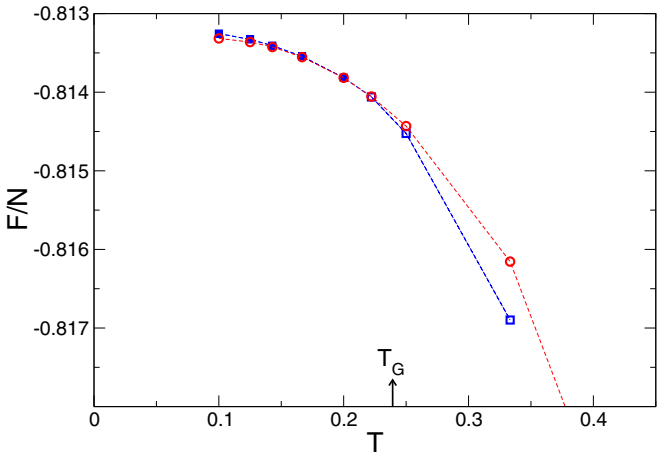

FIG. 4. The free energy per site of the type-II 2RSB solution (squares) vs the 1RSB free energy per site (circles).

We have restricted our studies of the 2RSB state to the physical region where $m_2 \geqslant m_1$ so that the probability associated with the δ function in Eq. (6) at $q = q_1$ remains positive. There are solutions in the unphysical region where $m_2 < m_1$ but they cannot be of physical significance. However, in a different but related context, solutions with negative probabilities have been discussed in the literature [21,22] and related to the properties of metastable states or barriers. The type-I solution is stationary (a maximum) along the line $m_1 = m_2$, but not a true saddle point in the full physical region of the m_1, m_2 space. The type-II solution is a genuine stationary solution in these variables provided $T < T_G$. The ideal solution would be a saddle point rather than one having to be constrained "by hand" to lie in the physical region. However, we expect that this difficulty will go away in the $K \to \infty$ limit when the system is stabilized by finite-size effects or by fluctuations. It is invariably the case that for a system which has FRSB is approximated by KRSB there are unsatisfactory features to be found in that level of approximation.

III. THE CASE OF p EVEN, $p/2$ ODD

The results in Sec. II are for the fully connected p-spin model which provides the mean-field limit for the p-spin model. To go beyond mean-field theory many workers have found it convenient to study a generalization of the p-spin model, the so-called $(M-p)$ models in which one has M different types of Ising spins coupled by short-range (usually nearest-neighbor) p-spin interactions [16,19,23–26]. In this section we introduce a model of this kind which provides a convenient way of discussing fluctuation effects when p is even. We refer to it as the "balanced" $(M-p)$ model as in this model if x and y denote two nearest-neighbor points on a lattice there are always $p/2$ spins on site x and $p/2$ spins on site y. In the usual $(M-p)$ model, the number of spins on either x or y can range from 1 up to $p-1$. The big advantage of the balanced model is that with it there is no need to introduce hard and soft modes, as in Refs. [23,25].

Denote the M different spins which can be placed at site x by $S_i(x)$, $i = 1, 2, \ldots, M$. We shall focus on the case when $p = 6$. Let us define for this case

$$R_{\alpha\beta}(x) \equiv \frac{1}{M^3} \sum_{i_1<i_2<i_3}^{M} S^{\alpha}_{i_1}(x)S^{\beta}_{i_1}(x)S^{\alpha}_{i_2}(x)S^{\beta}_{i_2}(x)S^{\alpha}_{i_3}(x)S^{\beta}_{i_3}(x) \quad (33)$$

$$= \frac{1}{3!M^3} \sum_{\substack{i_1,\,i_2,\,i_3 \\ \text{distinct}}}^{M} S^{\alpha}_{i_1}(x)S^{\beta}_{i_1}(x)S^{\alpha}_{i_2}(x)S^{\beta}_{i_2}(x)S^{\alpha}_{i_3}(x)S^{\beta}_{i_3}(x)$$

$$= \frac{1}{6}\left[\frac{1}{M}\sum_{i}^{M} S^{\alpha}_i(x)S^{\beta}_i(x)\right]^3 - \frac{3M-2}{6M^3}\sum_{i}^{M} S^{\alpha}_i(x)S^{\beta}_i(x)$$

$$\simeq \frac{1}{6}Q^3_{\alpha\beta}(x), \quad (34)$$

where in the large-M limit, the second term, which comes from the diagonal elements, is subleading, and we have defined

$$Q_{\alpha\beta}(x) \equiv \frac{1}{M}\sum_{i}^{M} S^{\alpha}_i(x)S^{\beta}_i(x). \quad (35)$$

The Hamiltonian for the balanced $(M-p)$ model for $p = 6$ is

$$H = -\frac{1}{2}\sum_{x\neq y}\sum_{i_1<i_2<i_3}^{M}\sum_{j_1<j_2<j_3}^{M} J^{(i,j)}_{(x,y)}\, S_{i_1}(x)S_{i_2}(x)S_{i_3}(x)S_{j_1}(y)S_{j_2}(y)S_{j_3}(y), \quad (36)$$

and each $J^{(i,j)}_{(x,y)}$ is chosen independently from a Gaussian distribution of variance J^2/M^{p-1} and it couples only sites x and y, which are nearest neighbors. The replicated partition function for the even p balanced model basically looks like

$$\overline{Z^n} \sim \mathrm{Tr}\exp\left[\frac{1}{2}\sum_{x,y}K(x,y)\sum_{\alpha<\beta}R_{\alpha\beta}(x)R_{\alpha\beta}(y)\right] \sim \int\prod_{\substack{x \\ \alpha<\beta}} d\phi_{\alpha\beta}(x)\ \exp\left[-\frac{1}{2}\sum_{x,y}\sum_{\alpha<\beta}\phi_{\alpha\beta}(x)K^{-1}(x,y)\phi_{\alpha\beta}(y)\right]$$

$$\times\,\mathrm{Tr}\exp\left[\sum_{x}\sum_{\alpha<\beta}\phi_{\alpha\beta}(x)R_{\alpha\beta}(x)\right], \quad (37)$$

where $K(x, y)$ is zero if x and y are not nearest neighbors. Reference [25] distinguishes the case of p even and $p/2$ even (such as $p = 4$) and the situation when p is even and $p/2$ is odd (such as $p = 6$). In the case of $p = 4$ the field theory in $\phi_{\alpha\beta}$ has terms like $w_2\phi^3_{\alpha\beta}$ with w_2 nonzero, which can be obtained by tracing out $R_{\alpha\beta}$. For the case $p = 6$ coefficients like w_2 are all zero. In other words, the field theory in terms of $\phi_{\alpha\beta}$ for $p = 6$ is manifestly time-reversal invariant and rather like that of the zero field Ising spin glass model. For $p = 4$ the field theory is more like that of the Ising spin glass model in a field.

A. The fully connected limit of the balanced model

For the fully connected $p = 6$ balanced model each $J^{(i,j)}_{(x,y)}$ is chosen independently from the Gaussian distribution with zero mean and the variance

$$\frac{J^2}{NM^{p-1}} = \frac{J^2}{NM^5}$$

for $p = 6$. We shall now show that when M is large the fully connected balanced model reduces to the $p = 6$ model in Eq. (8).

The replicated and bond-averaged partition function is

$$\overline{Z^n} = e^{nNC}\mathrm{Tr}\exp\left[\frac{\beta^2J^2M}{4N}\sum_{x\neq y}\sum_{\alpha\neq\beta}R_{\alpha\beta}(x)R_{\alpha\beta}(y)\right], \quad (38)$$

where C is a constant coming from the diagonal replica terms and $R_{\alpha\beta}(x)$ is a shorthand notation for the collection of spins given in Eq. (33). This can be rewritten using the integral representation (via $\Lambda_{\alpha\beta}$) of the δ function constraint enforcing $R_{\alpha\beta} = \frac{1}{N}\sum_x R_{\alpha\beta}(x)$ or

$$NMR_{\alpha\beta} = \frac{1}{M^2}\sum_x\sum_{i_1<i_2<i_3}^{M} S^\alpha_{i_1}(x)S^\beta_{i_1}(x)S^\alpha_{i_2}(x)S^\beta_{i_2}(x)S^\alpha_{i_3}(x)S^\beta_{i_3}(x) \quad (39)$$

as

$$\overline{Z^n} = e^{nNC}\int\prod_{\alpha<\beta}dR_{\alpha\beta}\int\prod_{\alpha<\beta}d\Lambda_{\alpha\beta}\ \exp\left[\frac{\beta^2J^2NM}{4}\sum_{\alpha\neq\beta}R^2_{\alpha\beta}\right. \quad (40)$$

$$\left. - NM\sum_{\alpha<\beta}\Lambda_{\alpha\beta}R_{\alpha\beta} + N\ln\mathrm{Tr}_S\ e^{A(\Lambda)}\right], \quad (41)$$

where

$$A(\Lambda) = \sum_{\alpha<\beta}\frac{\Lambda_{\alpha\beta}}{M^2}\sum_{i_1<i_2<i_3}^{M} S^\alpha_{i_1}S^\beta_{i_1}S^\alpha_{i_2}S^\beta_{i_2}S^\alpha_{i_3}S^\beta_{i_3} \quad (42)$$

and we have neglected the diagonal terms in sites which are subleading in the large-N limit. In the large-N limit, the integral is dominated by the saddle-point values. Varying with respect to $R_{\alpha\beta}$, we have

$$\Lambda_{\alpha\beta} = \beta^2J^2R_{\alpha\beta}. \quad (43)$$

The replicated partition function can now be written as

$$\overline{Z^n} = e^{nNC}\int\prod_{\alpha<\beta}dR_{\alpha\beta}$$

$$\times\exp\left(-\frac{\beta^2J^2NM}{2}\sum_{\alpha<\beta}R^2_{\alpha\beta} + N\ln\mathrm{Tr}_S\ e^{A(R)}\right). \quad (44)$$

From Eq. (42), we have

$$A(R) = \beta^2J^2M\sum_{\alpha<\beta}\frac{R_{\alpha\beta}}{M^3}\sum_{i_1<i_2<i_3}^{M} S^\alpha_{i_1}S^\beta_{i_1}S^\alpha_{i_2}S^\beta_{i_2}S^\alpha_{i_3}S^\beta_{i_3}$$

$$= \beta^2J^2M\sum_{\alpha<\beta}\frac{R_{\alpha\beta}}{3!M^3}\sum_{\substack{i_1,\,i_2,\,i_3\\ \text{distinct}}}^{M} S^\alpha_{i_1}S^\beta_{i_1}S^\alpha_{i_2}S^\beta_{i_2}S^\alpha_{i_3}S^\beta_{i_3}$$

$$\simeq \frac{\beta^2J^2M}{6}\sum_{\alpha<\beta}R_{\alpha\beta}\left(\frac{1}{M}\sum_i^M S^\alpha_iS^\beta_i\right)^3, \quad (45)$$

where we have neglected the subleading terms in the large-M limit. We again insert the δ function constraint using $\lambda_{\alpha\beta}$ to enforce

$$q_{\alpha\beta} = \frac{1}{M}\sum_i^M S^\alpha_iS^\beta_i, \quad (46)$$

and then we have

$$\overline{Z^n} = e^{nNC}\int\prod_{\alpha<\beta}dR_{\alpha\beta}\int\prod_{\alpha<\beta}dq_{\alpha\beta}\int\prod_{\alpha<\beta}d\lambda_{\alpha\beta}$$

$$\times\exp\left(-\frac{\beta^2J^2NM}{2}\sum_{\alpha<\beta}R^2_{\alpha\beta} + \frac{\beta^2J^2NM}{6}\sum_{\alpha<\beta}R_{\alpha\beta}q^3_{\alpha\beta}\right.$$

$$\left. - NM\sum_{\alpha<\beta}\lambda_{\alpha\beta}q_{\alpha\beta} + NM\ln\mathrm{Tr}\ e^{\tilde{A}(\lambda)}\right), \quad (47)$$

where

$$\tilde{A}(\lambda) = \sum_{\alpha<\beta}\lambda_{\alpha\beta}S^\alpha S^\beta. \quad (48)$$

The saddle-point equation for $R_{\alpha\beta}$ gives

$$R_{\alpha\beta} = \tfrac{1}{6}q^3_{\alpha\beta}, \quad (49)$$

and we have

$$\overline{Z^n} = e^{nNC}\int\prod_{\alpha<\beta}dq_{\alpha\beta}\int\prod_{\alpha<\beta}d\lambda_{\alpha\beta}\ \exp[NMG(q,\lambda)], \quad (50)$$

where

$$G(q,\lambda) = \frac{\beta^2J^2}{72}\sum_{\alpha<\beta}q^6_{\alpha\beta} - \sum_{\alpha<\beta}\lambda_{\alpha\beta}q_{\alpha\beta} + \ln\mathrm{Tr}\ e^{\tilde{A}(\lambda)}. \quad (51)$$

This is the standard expression for the fully connected six-spin model if we change $J^2 \to 36J^2$; compare Eq. (8). [The

first term is $(\beta^2 J^2/2)\sum_{\alpha<\beta} q_{\alpha\beta}^p$ for the p-spin model.] The saddle-point equations are

$$\lambda_{\alpha\beta} = \frac{\beta^2 J^2}{12} q_{\alpha\beta}^5, \tag{52}$$

$$q_{\alpha\beta} = \langle S^\alpha S^\beta \rangle_{\tilde{A}}. \tag{53}$$

B. Instability of the 1RSB state against thermal fluctuations of time-reversed droplets for p even, $p/2$ odd

In Ref. [17] one of us argued that the 1RSB state in the $M-p$ model is unstable against thermal fluctuations and so cannot exist outside the mean-field limit. The argument was based on calculating the interface free energy obtained by reversing the signs of $J_{(x,y)}^{(i,j)}$ for the couplings across a $d-1$ dimensional hyperplane. A system like the balanced $(M-p)$ model with $p=6$ has the features for which the calculation of Ref. [17] is valid. For odd values of p and for p even with $p/2$ even (such as $p=4$) (i.e., for situations where $w_2 \neq 0$) the arguments of this reference need modifying. We suspect that there are fluctuations which will also destabilize their 1RSB state, but it is only for the case of p even, $p/2$ odd such as $p=6$ that we can explicitly identify the destabilizing fluctuations as time-reversed droplets and do the calculations which show that in the 1RSB state these droplets cost very little energy so that thermal excitation of them will destroy the 1RSB order.

The key observation is that for $p=6$ the field theory has $w_2=0$, i.e., it has the same features as the Ising spin glass in zero applied field. This is not the case for $p=4$ which has w_2 nonzero. For it flipping the sign of the bonds across a $d-1$-dimensional hyperplane induces complicated changes to the state whereas for $p=6$ the field $\phi_{\alpha\beta}$ merely has a sign change, just as for the Ising case studied in Ref. [27] which were carried over into Ref. [17]. We will not repeat the details of the calculation here. The essence of the calculation is that the interface free energy will be vanishingly small in any state which is *not marginal*. In the 1RSB state (or KRSB state with K finite) there are no massless modes. We deduce from this that it is only in the mean-field limit that the 1RSB state can be stable for $p=6$. In any finite dimension it will be unstable. In its place we believe that there is a discontinuous transition to a state with FRSB. In states with FRSB there are marginal modes which stabilize the system against destruction by time-reversed thermal fluctuations.

IV. DISCUSSION

We know of no simulations of $(M-p)$ models with $p=6$. There are, however, simulations of models of $(M-p)$ models with $p=4$ in Ref. [19]. When $p=4$ there is time-reversal invariance just as for $p=6$, so its $P(q)$ in the 1RSB state will have support over the full range $-1<q<1$. For models with time-reversal invariance Eq. (5) $P(q)$ at mean-field level becomes (with $q_0=0$)

$$P(q) = m\delta(q) + (1-m)/2\delta(q-q_1) + (1-m)/2\delta(q+q_1). \tag{54}$$

Note that here q relates to the overlap of two copies of the system as in Eq. (2). The δ functions in the simulations of Ref. [19] were smeared out, although it is not clear whether this was due to finite-size effects in the system or arising because the system is just not in the 1RSB state.

There are other simulational studies on the $p=4$ model in three dimensions which reveal striking differences with the results which might have been expected based on studies of the fully connected p-spin model. Franz and Parisi [20] found for both $M=3$ and $M=4$ that as the temperature is reduced in the high-temperature paramagnetic phase there was a growing (possibly diverging) length scale and susceptibility. In both the RS and 1RSB phases the length scales can be calculated, and at least at the level of Gaussian fluctuations about the mean-field solution no divergence as $T \to T_{\rm 1RSB}^c$ [16] arises. (The study of the length scales in the p-spin type of model at Gaussian level is not straightforward [16,28,29], because one has to consider fluctuations in the size of the blocks in the 1RSB matrix. It may also be further complicated by the need to allow for the degeneracy of the free energy of states with KRSB as found in this paper.) At Gaussian level the length scales are determined by the eigenvalues of the Hessian matrix: For the RS and 1RSB states there are no null eigenvalues and therefore no long length scales [16].

Campellone *et al.* [19] suggested that the difference between their results and the mean-field picture was due to nonperturbative contributions which had produced in $P(q)$ features usually associated with that of full replica symmetry breaking (FRSB) but did not provide any details of how this might arise. We have argued that fluctuations around the mean-field solution will convert the order below $T_{\rm 1RSB}^c$ from 1RSB to FRSB in finite dimension, but we too are unable to provide a quantitative treatment.

If the discontinuous transition at $T_{\rm 1RSB}^c$ is to a state which has FRSB, a number of questions arise. One concerns the existence of the Gardner transition [1,11] which is a continuous transition from within the 1RSB state to a state with FRSB. As we are claiming that there is already FRSB present for $T < T_{\rm 1RSB}^c$, it becomes a moot point as to whether in such a situation there will still be a Gardner transition.

The field theory of the balanced $(M-p)$ models is in the variable ϕ_{ab}. This field theory has quite different physics for the cases $p=4$ and $p=6$ where in the latter case $w_2=0$. The Gardner transition is to a state similar to that expected from the Ising model in a field [1]. It is difficult to see how that would happen in finite dimensions for the $p=6$ balanced model.

Another question concerns suspicions that FRSB may not actually exist in dimensions $d<6$ [30–32]. That might be the reason why within the Migdal-Kadanoff RG procedure applied to the $M-p$ spin model with $p=3$ and $M=2$ and $M=3$ in dimensions $d=3$ and $d=4$ we failed to see *any* phase transition [23,26] as the temperature was reduced. There was, however, evidence of an "avoided" transition as the correlation length grew considerably, just as was reported in the direct simulations of Refs. [19,20]. An avoided transition is one at which the correlation length grows but not to infinity as the temperature is reduced. The p-spin type of model seems in low dimensions, i.e., $d=3$ or $d=4$, to have similarities with the Ising spin glass in an external field. Thus the effect of fluctuations around the mean-field solution

might be to remove the discontinuous transition completely in low dimensions, though that might occur for $d > 6$ where we expect FRSB to survive.

Since p-spin models are of interest only by virtue of their possible relevance to structural glasses and RFOT theory, we shall comment on possible implications of this avoided transition for them. The length scale in the high-temperature phase in structural glasses is that of the point-to-set length scale $\xi_{\rm PTS}$ [33,34] and according to the RFOT [2–6] $\xi_{\rm PTS}$ diverges at the Kauzmann temperature T_K [8], the temperature at which the configurational entropy per particle s_c is supposed to vanish. Below T_K the glass is hypothesized to enter the so-called "ideal glass state" [2,3,6] where the configurational entropy s_c is zero. The growth of $\xi_{\rm PTS}$ is driven by the "rarefraction" of states as $T \to T_K$. (Some suspect [35,36] that s_c never actually vanishes.) Now, as the temperature is reduced below the glass transition temperature T_g, $\xi_{\rm PTS}$ increases [37,38]. In the vicinity of T_g, $\xi_{\rm PTS}$ is actually small, only a few molecular diameters [34,37,38]. As a consequence of new simulational methods (the swap algorithm [9,38]) it has now become possible to study $\xi_{\rm PTS}$ at temperatures well below T_g where indeed it becomes somewhat longer. According to RFOT theory it diverges as $T \to T_K$, but if the discontinuous transition is removed by fluctuations around the mean-field solution and the transition is avoided, the correlation length will not actually diverge, just as was seen in the Migdal-Kadanoff RG procedure [23,26].

A recent attempt to explain the growing length scale can be found in Refs. [39,40]. This work too focusses on the effect of fluctuations on the mean-field solution. One of their scenarios was that the growing length scale was in the same universality class of the Ising spin glass in a field (a scenario favored by us [24]), but their chief scenario was that there was a genuine RFOT like transition at T_K.

Our work in this paper suggests that the discontinuous transition from the RS paramagnetic state to a state with 1RSB, which was first derived in the fully connected model, might be modified even in very high dimensions, or just by finite-size effects alone, to a discontinuous transition to a state with FRSB. As the dimensionality is lowered further, possibly below six dimensions, these same fluctuations might also remove the state with FRSB completely. But our main message is that the nature of the ideal glass state might not be as simple as that envisaged on the basis of it being a state whose order parameter is that predicted by 1RSB, and that much further work remains to be done.

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