PHYSICAL REVIEW B VOLUME 36, NUMBER 16 1 DECEMBER 1987

Stable and metastable states in mean-field Potts and structural glasses

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(Received 19 June 1987)

Recent static and dynamical work suggest a close analogy between spin glasses with discontinuous Edwards-Anderson order parameter and structural glasses. The mean-field dynamical spin-glass theory predicts freezing above the usual thermodynamic transition temperature. Here we use the approach of Thouless, Anderson, and Palmer for Potts glasses to show that the dynamical approach locates a thermodynamically metastable glassy state. We also give divergent correlation lengths as both the static and dynamical transition temperatures are approached. We argue that the static transition is analogous to an ideal glass transition temperature in the structural glass problem. We also argue that the static transition temperature can be identified as the temperature at which the configurational entropy vanishes, i.e., the Kauzmann temperature. Dynamical transitions between the metastable states are discussed. We argue that divergent lifetimes occur near the Kauzmann temperature.

I. INTRODUCTION

In the recent literature a close analogy between mean-field theories for spin glasses[1] with discontinuous Edwards-Anderson order parameter, q_{EA}, and mean-field structural glass theories[2] has been noted. Kirkpatrick and Wolynes[3] (KW) argued that the density-functional Hamiltonian for liquids and glasses does not have the reflection symmetry of Ising spin-glass (SG) models. They conjectured that the structural glass problem is more closely related to SG models without reflection symmetry. In the structural glass problem the analog of the Edwards-Anderson order parameter[1] can be identified as the long-time limit of the density correlation function.[2] The structure of the density-functional Hamiltonian suggest that q_{EA} should be discontinuous at the ideal glass-transition temperature T_K. In the course of this paper we give arguments to identify T_K with the Kauzmann temperature.[4,5]

KW therefore conjectured that the structural glass problem should be related to Potts glasses[6–8] (PG's) with more than four components and p-spin-interaction SG models with $p>2$.[9–11] Both of these models are known to exhibit SG transitions with discontinuous q_{EA}. Kirkpatrick and Thirumalai[12] (KT) made this conjecture more precise. They studied the mean-field p-spin-interaction ($p>2$) SG model. Using both a dynamical and static approach they were able to show a close formal analogy between this SG model and mean-field dynamical[13–18] and static density-functional[19] theories for the structural glass. KT identified two distinct transition temperatures. The first was a consequence of the dynamical theory and for reasons discussed below we denote this transition temperature T_A. The static or thermodynamic approach naturally lead to a transition at $T_K<T_A$. A connection was, however, established between the purely dynamical approach and the static approach. This connection involved some rather subtle mathematical points.[20] More recent work[21] on the PG's with $p>4$ found similar behavior. Again, there are two distinct transition temperatures in the mean-field limit with the dynamical transition at T_A, which is greater than the usual thermodynamic transition temperature, which is at T_K.

The main purpose of this paper is to provide a physical interpretation of the results of KT. We also use physical arguments to identify divergent correlation lengths as T_A and T_K are approached. Finally, our results allow us to make some educated speculations on the more difficult structural glass problem where the spatial randomness must be self-generated rather than put in by hand as in SG models.

To be precise we consider the PG model with more than four components ($p>4$). By generalizing the approach of Thouless, Anderson, and Palmer (TAP) approach (Refs. 1, 22, and 23) for the SK spin-glass model to the mean-field PG model, the following conclusions can be drawn. First, the dynamical transition at T_A actually locates a thermodynamically metastable state. In the mean-field limit this metastable state has an infinite lifetime. We argue that this infinite lifetime is a pathology of the mean-field model and that a sharp transition at T_A will not occur in a finite-dimensional short-ranged glass model. Even in a finite-dimensional glass, however, we believe T_A to be physically significant, since for $T<T_A$ well-defined metastable states are possible and transport is at least, in part, activated transport.

In this context it should be noted that the pathologies of mean-field dynamics in usual first-order phase transitions has been studied previously by Binder[25] and others.[26] He also found that dynamical mean-field theories could locate infinitely-long-lived metastable states. Binder argued that these states were physically relevant because in short-ranged models they existed for long times. Infinitely-long-lived metastable states are possible in mean-field discontinuous transitions because, in general, systems which undergo such transitions have metastable states above their equilibrium transition temperatures. Further, nucleation is not possible in the strict mean-field limit because there is no distinction between bulk and surface free energies. Therefore, if in the course of its dynamical evolution a correlation function passes near a local free-energy minimum, then it can become frozen because the activated transport processes which should allow the correlation function to go to its true equilibrium or long-time value cannot take place. This is especially relevant in spin-glass problems because the natural order parameter describing the glass transition is given by the long-time limit of the two-spin time correlation function. As a consequence of this argument we identify T_A as the temperature where activated transport processes become important.

We also use the TAP approach to investigate the thermodynamic transition at T_K. We argue that the transition at T_K is due to an entropy crisis. We identify a configurational entropy in the temperature range $T_K < T < T_A$ and find that it becomes nonextensive at T_K. For $T < T_K$ this configurational entropy becomes the PG complexity[27] and it is of $O(1)$, but singular as $T \rightarrow T_K$. An entropy crisis of this sort was first noted by Simon[4] and emphasized by Kauzmann[5] as a characteristic of structural glass transitions. We therefore conclude that the PG transition at T_K is similar to that found in the Gibbs-DiMarzio[28] picture of the structural glass transition for polymeric systems or in Derrida's random-energy model.[9,10]

The plan of this paper is as follows. In Sec. II the TAP equations for the PG are given. The formal equivalence between the TAP approach and the usual replica approach is established. Section II is concluded with a discussion of two distinct solutions to the TAP equations. In Sec. III the solutions given in Section II are discussed in more detail. The TAP free energies are explicitly given. Correlation lengths near T_A and T_K are proposed. In Sec. IV we present arguments about the activated dynamics between T_A and T_K. In Sec. V we summarize our results and make further remarks on their connection to real glassy systems.

II. TAP APPROACH TO THE PG PROBLEM

Examining the details of KT's calculation[12] suggests that the TAP approach will be useful for understanding the transitions predicted by them. In replica language[1] the transition at T_A seems to involve only self-overlap, $q^{\alpha\alpha}$, where α is a replica index. For the temperature range $T_K < T < T_A$, KT suggest that this is the only type of ordering possible. In this context it is useful (cf. below) to point out that the free energy in the usual replica approach does not explicitly involve $q^{\alpha\alpha}$. In the TAP approach $q^{\alpha\alpha}$ does play a central role and we will explicitly derive an effective Hamiltonian for computing the self-overlap. KT's calculations also show that T_K is the temperature where overlap between distinct replicas can occur. For $T < T_K$ and in the thermodynamic limit, we will find that the TAP approach and the usual replica approach contain the same physics.

The apparent nonequivalence between the TAP and replica methods can be understood on the basis of our eventual conclusion that the dynamical approach naturally picks out a metastable TAP state in the temperature range $T_K < T < T_A$. With this in mind, it is not surprising that the usual replica approach is not appropriate for these temperatures. Our conclusions are also consistent with the fact that we find that the usual replica free energy differs from the component-averaged free energy for $T < T_A$ if the PG is frozen into a metastable state.

An outline of this section is as follows. We first give the TAP equations for the PG. We then sketch the formal argument that the TAP approach contains the usual replica approach. Following this we discuss two distinct solutions to the TAP equations. The first solution involves only replica self-overlap and is appropriate for the temperature range $T_K < T < T_A$. The second solution is at the level of one-replica symmetry breaking[1,29] and it describes the usual thermodynamic transition that occurs at T_K.

A. The TAP equations

The mean-field PG Hamiltonian is[6-8,30]

$$H = -\sum_{a=1}^{p-1} \sum_{\substack{i,j \\ (i<j)}} J_{ij} S_{ia} S_{ja} \ . \tag{2.1}$$

The PG has p components in a $(p-1)$-dimensional vector space. The bonds $\{J_{ij}\}$ are randomly distributed according to

$$P(J_{ij}) = \left[\frac{N}{2\pi J^2} \right]^{1/2} \exp\left[-\frac{(J_{ij})_N^2}{2J^2} \right] , \tag{2.2a}$$

with N the number of lattice sites. To suppress a ferromagnetic transition, one must actually properly fix the average of J_{ij}.[31] We will avoid this problem by always setting the ferromagnetic order parameter equal to zero. The S_{ia} are Potts variables chosen from the set $\{e_a^l\}$ with $(l = 1, 2, \ldots, p)$ (Ref. 32)

$$e_a^l = \left[\frac{p-a}{p+1-a} \right]^{1/2} p^{1/2} \times \begin{cases} 0, & l < a \\ 1, & l = a \\ -1/(p-a), & l > a \ . \end{cases} \tag{2.2b}$$

Some useful identities are

$$\sum_{l=1}^{p} e_a^l e_b^l = p\delta_{ab} \ , \tag{2.3a}$$

$$\sum_{a=1}^{p-1} e_a^l e_a^{l'} = p\delta_{ll'} - 1 \ , \tag{2.3b}$$

$$\sum_{l=1}^{p} e_a^l = 0 \ . \tag{2.3c}$$

Before giving the TAP equations, we note that the usual replica approach leads to a free energy per site given by[6,8]

$$-\beta f = -\frac{\beta F}{N} = \lim_{n \rightarrow 0} (1/n) \max A \ . \tag{2.4}$$

Here, $\beta^{-1}=k_B T$, with k_B Boltzmann's constant and T the temperature, and max denotes maximum. The function A is

$$A=\frac{\mu}{4}(p-1)\left[n-\sum_{\substack{\alpha,\beta\\(\alpha\neq\beta)}}(q^{\alpha\beta})^2\right]+\ln \mathrm{Tr}_{S_a^\alpha=\{e_a^l\}}\exp\left[\frac{\mu}{2}\sum_{\substack{a,\alpha,\beta\\(\alpha\neq\beta)}}S_a^\alpha S_a^\beta q^{\alpha\beta}\right] . \tag{2.5a}$$

Here, $\alpha,\beta,\ldots=1,2,\ldots,n$ denote replica indices,

$$\mu=\beta^2 J^2 , \tag{2.5b}$$

and we have assumed an isotropic PG state,

$$q_{ab}^{\alpha\beta}=\delta_{ab}q^{\alpha\beta} . \tag{2.5c}$$

$q_{ab}^{\alpha\beta}$ is the usual replica order parameter,

$$q_{ab}^{\alpha\beta}=\frac{1}{N}\sum_i m_{ia}^\alpha m_{ib}^\beta , \tag{2.5d}$$

where m_{ia}^α is the magnetization at site i in the replica α. It is relevant to note that the free energy given by Eqs. (2.4) and (2.5) does not explicitly depend on the self-overlap $q^{\alpha\alpha}$.

The TAP equations for the PG follow most simply by generalizing Anderson's argument[23] for the SK spin-glass model. The resulting free energy is

$$\beta F=\frac{1}{p}\sum_{i=1}^{N}\sum_{l=1}^{p}(1+m_{ia}e_a^l)\ln\left[\frac{1+e_b^l m_{ib}}{p}\right]-\sum_{\substack{i,j\\(i<j)}}\beta J_{ij}m_{ia}m_{ja}-\frac{\beta^2}{2}\sum_{\substack{i,j\\(i<j)}}J_{ij}^2(\langle S_{ia}S_{ib}\rangle_T-m_{ia}m_{ib})(\langle S_{ja}S_{jb}\rangle_T-m_{ja}m_{jb}) , \tag{2.6}$$

where repeated vector indices $(a,b,\ldots)$ are to be summed from 1 to $p-1$. Here, m_{ia} is the magnetization at site i in a particular TAP state (we suppress the TAP-state index here). The equal-time site-diagonal spin correlation function in a TAP state is

$$\langle S_{ia}S_{ib}\rangle_T=\delta_{ab}+\frac{1}{p}v_{abc}m_{ic} , \tag{2.7a}$$

with

$$v_{abc\ldots}=\sum_{l=1}^{p}e_a^l e_b^l\cdots . \tag{2.7b}$$

To prove Eq. (2.7a), one needs the sum rules

$$\sum_a\langle S_{ia}S_{ia}\rangle_T=p-1 \tag{2.7c}$$

and

$$\sum_{a,b}v_{abc}\langle S_{ia}S_{ib}\rangle_T=p^2(p-2)m_{ic} . \tag{2.7d}$$

Equation (2.6) clearly reduces to the TAP equation for the SK model $(p=2)$ and, with Eq. (2.7a), Eq. (2.6) can be shown to be equivalent to the result of Lage and Erzan[7] for the general PG's.

The structure of Eq. (2.6) is easy to understand physically. The first term is just the usual mean-field entropy contribution to the PG free energy and the second term is the standard energy contribution to F in a mean-field description. The last term in Eq. (2.6) represents the fact that the spins give a fluctuating mean field on each other. In usual mean-field theories $J_{ij}\sim N^{-1}$ and the last term can be neglected. In mean field SG's, however, J_{ij} scales like $N^{-1/2}$ and this fluctuation contribution is needed for consistency.

The equation of state within the TAP approach follows from

$$\frac{\partial\beta F}{\partial m_{ia}}=0=\frac{1}{p}\sum_{l=1}^{p}e_a^l\ln(1+e_b^l m_{ib})-\beta\sum_j J_{ij}m_{ja}+\beta^2\sum_j J_{ij}^2(\langle S_{ja}S_{jb}\rangle_T-m_{ja}m_{jb})m_{ib}-\frac{\beta^2}{2p}\sum_j J_{ij}^2 v_{abc}(\langle S_{jc}S_{jb}\rangle_T-m_{jc}m_{jb}) . \tag{2.8}$$

We conclude this subsection by noting that, in general, the TAP equations have an extensive number $(\sim e^N)$ of solutions.[1,33] However, almost all of these solutions are unstable with respect to infinitesimal fluctuations. In order to pick out the physically relevant stable and metastable (in the usual sense) states, the TAP solutions should be weighted with their canonical or Boltzmann weight. Of course, in real systems there can be no truly sharp dividing line between metastable and unstable states. However, we can imagine a physical distinction (which becomes sharper as the mean-field limit is approached) between these states. In some sections of this paper we assume that the most important physical transport mechanisms for long times are associated with metastable states that have an infinite lifetime in the mean-field limit.

B. Equivalence between TAP and standard replica approaches

To prove that Eqs. (2.6) and (2.8) are formally equivalent to Eqs. (2.4) and (2.5), we generalize the arguments of De Dominicis and Young[34] (DY) to the PG model. If we denote the TAP states by s, then the partition function is

$$Z=\sum_{s}\exp[-\beta F(m^{s})] \; . \tag{2.9a}$$

With Eq. (2.8), Eq. (2.9a) can be written as

$$Z=\int Dm\left[\prod_{i,a}\delta\left[\frac{\partial\beta F}{\partial m_{ia}}\right]\right]\Delta\{m\}e^{-\beta F\{m\}} \; , \tag{2.9b}$$

where

$$Dm=\prod_{i,a}dm_{ia} \; , \tag{2.9c}$$

and Δ normalizes the δ function,

$$\Delta\{m\}=\left|\mathrm{Det}\left[\frac{\partial^{2}\beta F}{\partial m_{ia}\partial m_{jb}}\right]\right| \; . \tag{2.9d}$$

It is important to note that we weight each TAP state with its canonical weight. As a consequence, the metastable states we find are due to a restricted (around the metastable state) saddle-point evaluation of Eqs. (2.9). Our procedure here differs from the white average calculation of De Dominicis *et al.*[33] The metastable states we find are locally stable and are similar to the metastable states considered in usual first-order phase transitions. These states have infinite lifetimes in the mean-field limit. To distinguish them from other TAP states we will sometimes call them weighted metastable states.

To carry out the average over the random bonds in Eq. (2.9b), we introduce an integral representation of the δ function,

$$\prod_{i,a}\delta\left[\frac{\partial\beta F}{\partial m_{ia}}\right]=\int D\left[\frac{\hat{m}}{2\pi}\right]\exp\left[-i\sum_{i,a}\hat{m}_{ia}\frac{\partial\beta F}{\partial m_{ia}}\right] \; , \tag{2.10a}$$

and we introduce Grassman variables (η,η^{*}) to write

$$\Delta\{m\}=\int D\eta\, D\eta^{*}\exp\left[\sum_{\substack{i,j\\a,b}}\eta^{*}_{ia}\frac{\partial^{2}\beta F}{\partial m_{ia}\partial m_{jb}}\eta_{jb}\right] \; . \tag{2.10b}$$

In using Eq. (2.10b) we assume that the absolute value sign in Eq. (2.9d) is not important due to the canonical weight in Eq. (2.9b). Since the average should be performed over $\ln Z$, we introduce n replicas and consider

$$Z^{n}=\int Dm\, D\left[\frac{\hat{m}}{2\pi}\right]D\eta\, D\eta^{*}\exp\left[-i\sum_{i,a,\alpha}\hat{m}^{\alpha}_{ia}\frac{\partial\beta F_{\alpha}}{\partial m^{\alpha}_{ia}}+\sum_{\substack{i,j\\a,b,\alpha}}\eta^{*\alpha}_{ia}\frac{\partial^{2}\beta F_{\alpha}}{\partial m^{\alpha}_{ia}\partial m^{\alpha}_{jb}}\eta^{\alpha}_{jb}-\beta\sum_{\alpha}F_{\alpha}\right] \; , \tag{2.11}$$

with $\alpha=1,2,\ldots,n$ the replica index and $F_{\alpha}=F\{m^{\alpha}\}$.

With Eq. (2.2a) the average, [ ], over the disorder is easily performed. We will evaluate the resulting expression by saddle-point techniques. To this end we introduce the order parameters

$$q^{\alpha\beta}_{ab}\equiv\frac{1}{N}\sum_{i}m^{\alpha}_{ia}m^{\beta}_{ib} \; , \tag{2.12a}$$

$$\hat{q}^{\alpha\beta}_{ab}\equiv\frac{1}{N}\sum_{i}i\hat{m}^{\alpha}_{ia}i\hat{m}^{\beta}_{ib} \; , \tag{2.12b}$$

$$g^{\alpha\beta}_{ab}\equiv\frac{1}{N}\sum_{i}i\hat{m}^{\alpha}_{ia}m^{\beta}_{ib} \; , \tag{2.12c}$$

$$n^{\alpha\beta}_{ab}\equiv\frac{1}{N}\sum_{i}\eta^{*\alpha}_{ia}\eta^{\beta}_{ib} \; . \tag{2.12d}$$

In $[Z^{n}]$ we constrain $x=(q,\hat{q},g,n)$ to have fixed values $\tilde{x}=(\tilde{q},\tilde{\hat{q}},\tilde{g},\tilde{n})$ and then integrate over all possible constrained values. Introducing an integral representation of the constraint and integrating over the Grassman variables, neglecting $1/N$ corrections, yields

$$[Z^{n}]=\int D\tilde{x}\, D\left[\frac{N\lambda}{2\pi}\right]e^{NA} \; . \tag{2.13a}$$

Here,

$$A=C+\ln\int Dm\, D\left[\frac{\hat{m}}{2\pi}\right]e^{L}\mathrm{Det}\left[\sum_{l}\mathbb{1}\frac{e^{l}_{a}e^{l}_{b}}{p(1+e^{l}_{c}m^{\alpha}_{c})}-i\lambda^{\alpha\beta}_{nab}\right] \; , \tag{2.13b}$$

and,

$$L=-\frac{1}{p}\sum_{\alpha,l}\ln\left[\frac{1+e_b^l m_b^\alpha}{p}\right]-\frac{1}{p}\sum_{\alpha,l}e_a^l(m_a^\alpha+i\hat{m}_a^\alpha)\ln(1+e_b^l m_b^\alpha)-i\sum_{\substack{\alpha,\beta\\ a,b}}(\lambda_{qab}^{\alpha\beta}m_a^\alpha m_b^\beta+\lambda_{\hat{q}ab}^{\alpha\beta}i\hat{m}_a^\alpha i\hat{m}_b^\beta+\lambda_{gab}^{\alpha\beta}i\hat{m}_a^\alpha m_b^\beta)\ , \tag{2.13c}$$

where $\mathbb{1}$ is the unit matrix in replica space. Note that Eq. (2.13b) involves only a single-site integration. In Eq. (2.13b), C is given by

$$C=\frac{\mu}{2}\sum_{\substack{\alpha,\beta\\ a,b}}\left[\frac{\tilde{q}_{ab}^{\alpha\beta}\tilde{q}_{ba}^{\beta\alpha}}{2}+\tilde{\hat{q}}_{ab}^{\alpha\beta}\tilde{q}_{ba}^{\beta\alpha}+2\tilde{g}_{ab}^{\alpha\beta}\tilde{q}_{ba}^{\beta\alpha}+\tilde{g}_{ab}^{\alpha\beta}\tilde{g}_{ba}^{\beta\alpha}-\tilde{n}_{ab}^{\alpha\beta}\tilde{n}_{ba}^{\beta\alpha}\right]$$

$$+\mu\sum_{\alpha,a,b}[\tfrac{1}{4}(\delta_{ab}-\tilde{q}_{ab}^{\alpha\alpha})^2-(\delta_{ab}-\tilde{q}_{ab}^{\alpha\alpha})(\tilde{g}_{ab}^{\alpha\alpha}-\tilde{n}_{ab}^{\alpha\alpha})]+i\sum_{\substack{\alpha,\beta\\ a,b}}(\lambda_{qab}^{\alpha\beta}\tilde{q}_{ab}^{\alpha\beta}+\lambda_{\hat{q}ab}^{\alpha\beta}\tilde{\hat{q}}_{ab}^{\alpha\beta}+\lambda_{gab}^{\alpha\beta}\tilde{g}_{ab}^{\alpha\beta}+\lambda_{nab}^{\alpha\beta}\tilde{n}_{ab}^{\alpha\beta})\ . \tag{2.13d}$$

The next step in showing the equivalence between the TAP and replica approaches involves the saddle-point evaluation of Eq. (2.13a). Variation with respect to the λ's yields (from now on we drop the tildes)

$$q_{ab}^{\alpha\beta}=\langle m_a^\alpha m_b^\alpha\rangle,\ \ \hat{q}_{ab}^{\alpha\beta}=\langle i\hat{m}_a^\alpha i\hat{m}_b^\beta\rangle,\ \ g_{ab}^{\alpha\beta}=\langle i\hat{m}_a^\alpha m_b^\beta\rangle\ . \tag{2.14a}$$

Here and below $\langle\ \ \rangle$ denotes an average with a weight given by the integrand of the integral in Eq. (2.13b). Following DY the remaining variations give

$$\lambda_{qab}^{\alpha\beta}=\lambda_{\hat{q}ab}^{\alpha\beta}=\frac{\lambda_{gab}^{\alpha\beta}}{2}=i\frac{\mu}{2}q_{ab}^{\alpha\beta}\ , \tag{2.14b}$$

$$n_{ab}^{\alpha\beta}=g_{ab}^{\alpha\beta}=-\hat{q}_{ab}^{\alpha\beta}=\delta_{\alpha\beta}(\delta_{ab}-q_{ab}^{\alpha\alpha})\ , \tag{2.14c}$$

$$\lambda_{nab}^{\alpha\beta}=0\ . \tag{2.14d}$$

To prove that Eq. (2.14d) is a saddle-point condition, one needs the inverse identity,

$$\left[\frac{1}{p}\sum_l\frac{\mathrm{e}^l\mathrm{e}^l}{(1+e_c^l m_c^\alpha)}\right]_{ab}^{-1}=\delta_{ab}-m_a^\alpha m_b^\alpha+\frac{1}{p}v_{abc}m_c^\alpha\ . \tag{2.14e}$$

Defining the new integration variables,

$$i\hat{\mu}_a^\alpha\equiv m_a^\alpha+i\hat{m}_a^\alpha \tag{2.15a}$$

and

$$X_a^\alpha\equiv\frac{1}{p}\sum_l e_a^l\ln(1+e_b^l m_b^\alpha)\ , \tag{2.15b}$$

and using Eqs. (2.14) in Eqs. (2.13) and assuming an isotropic PG phase yields

$$A=\frac{\mu}{4}(p-1)\left[\sum_\alpha(1-2q^{\alpha\alpha})-\sum_{\substack{\alpha,\beta\\(\alpha\neq\beta)}}(q^{\alpha\beta})^2\right]$$

$$+\ln\int DX\,D\left[\frac{\hat{\mu}}{2\pi}\right]\exp\left[\frac{\mu}{2}\sum_{\alpha,\beta,a}i\hat{\mu}_a^\alpha i\hat{\mu}_a^\beta q^{\alpha\beta}-\sum_{\alpha,a}i\hat{\mu}_a^\alpha X_a^\alpha-\frac{1}{p}\sum_{\alpha,l}\ln\left[\frac{1+e_b^l m_b^\alpha}{p}\right]\right]\ , \tag{2.16}$$

with m_b^α implicitly given by Eq. (2.15b). We next prove that Eq. (2.16) is identical to Eq. (2.5a). With the identity

$$\exp\left[-\frac{1}{p}\sum_l\ln\left[\frac{1+e_b^l m_b^\alpha}{p}\right]\right]=\sum_l\exp\left[\sum_a e_a^l X_a^\alpha\right]\ , \tag{2.17}$$

the X integral in Eq. (2.16) forces $i\hat{\mu}_a^\alpha=\{e_a^{l\alpha}\}$. If we use this and Eq. (2.3b), then the self-overlap terms in Eq. (2.16) are seen to cancel and the remaining terms are just Eq. (2.5a).

We remark that two results were obtained in this subsection. We showed that the TAP equations for the PG are consistent with the usual replica approach. More importantly, we have also derived an effective Hamiltonian for computing self-overlap, $q^{\alpha\alpha}$, as well as replica overlap, $q^{\alpha\neq\beta}$.

C. Locally stable solutions of the TAP equation

In this subsection we discuss two distinct locally stable solutions of our previous equations. In our explicit calculations we are interested in PG transitions with $p>4$, where the glass transition is known to be discontinuous.[8] In order to control the discontinuity we choose $p=4+\epsilon$, $\epsilon\ll 1$, so that at the glass transition $q\sim O(\epsilon)$ and an order-parameter expansion is possible. It will be clear that our conclusions are independent of this restriction.

The first solution occurs at a temperature we denote by T_A. At and below T_A there is only self-overlap, $q^{\alpha\alpha}=q$, and no replica overlap $q^{\alpha\neq\beta}=0$. Note that this is the case of maximally broken replica symmetry. We show that T_A coincides with the glass-transition temperature predicted by the dynamical theory.[21] The second solution occurs at a temperature $T_K < T_A$. It coincides with the usual replica-based transition temperature. For this case there is one-replica symmetry breaking (1-RSB). The n replicas are broken into $n/\bar{x}$ clusters of $\bar{x}$ replicas. The replicas within cluster i overlap with weight $q^{\alpha(i)\beta(i)}=q^{\alpha(i)\alpha(i)}=q$, while $q^{\alpha(i)\beta(j)}=0$ for $i\neq j$. The fraction of replicas that overlap is given by $1-\bar{x}$.

To construct an equation of state which is valid for both cases we start with the definition

$$q_{ab}^{\alpha\beta}=q^{\alpha\beta}\delta_{ab}=\langle m_a^\alpha m_b^\beta\rangle \ , \tag{2.18a}$$

with

$$\langle(\ )\rangle=\frac{1}{\Omega}\int D\hat{\mu}\,DX\,e^{L}(\ )\ , \tag{2.18b}$$

where Ω is the normalizing factor,

$$\Omega=\int D\hat{\mu}\,DX\,e^{L}\ , \tag{2.18c}$$

and,

$$L=-\frac{\mu}{2}\sum_{\alpha,\beta,a}\hat{\mu}_a^\alpha\hat{\mu}_a^\beta q^{\alpha\beta}-\sum_{\alpha,a}i\hat{\mu}_a^\alpha X_a^\alpha -\frac{1}{p}\sum_{\alpha,l}\ln\left[\frac{1+e_b^l m_b^\alpha}{p}\right]\ , \tag{2.18d}$$

with $m_a^\alpha(X)$ given by

$$X_a^\alpha\equiv\frac{1}{p}\sum_l e_a^l\ln[1+e_b^l m_b^\alpha(X^\alpha)]\ . \tag{2.18e}$$

Define the self-overlap by

$$q^{\alpha\alpha}=q_1\ , \tag{2.19a}$$

and the replica overlap by

$$q^{\alpha\beta}=\begin{cases}q_0 & \text{if } \alpha\neq\beta \text{ but } \alpha,\beta\in i\text{th cluster}\ ,\\ 0 & \text{otherwise}\ .\end{cases} \tag{2.19b}$$

Using the 1-RSB scheme described above, the equation of state for self-overlap is

$$q_{ab}^{11}=q_1\delta_{ab}=\frac{1}{\bar{\Omega}}\int DH_1DX^1m_a(X^1)m_b(X^1)\exp\left[-\frac{1}{2\mu q_0}\sum_a H_{a1}^2\right]\exp(\mathcal{L}_{11})\left[\int DX_2\exp(\mathcal{L}_{12})\right]^{\bar{x}-1}\ , \tag{2.20a}$$

where

$$\bar{\Omega}=\int DH_2\exp\left[-\frac{1}{2\mu q_0}\sum_a H_{a2}^2\right]\left[\int DX_2\exp(\mathcal{L}_{22})\right]^{\bar{x}}\ , \tag{2.20b}$$

with

$$\mathcal{L}_{ij}=-\frac{1}{2\mu(q_1-q_0)}\sum_a(X_a^j-H_{ai})^2-\frac{1}{p}\sum_l\ln\left[\frac{1+e_b^l m_b(X^j)}{p}\right]\ . \tag{2.20c}$$

The equation of state for two replicas (say 1 and 2) in the same cluster is

$$q_{ab}^{12}=q_0\delta_{ab}=\frac{1}{\bar{\Omega}}\int DH_1DX^1DX^2m_a(X^1)m_b(X^2)\exp\left[-\frac{1}{2\mu q_0}\sum_a H_{a1}^2\right]\exp(\mathcal{L}_{11}+\mathcal{L}_{12})\left[\int DX_3\exp(\mathcal{L}_{13})\right]^{\bar{x}-2}\ . \tag{2.21}$$

Self-consistently, one also finds $q_{ab}^{\alpha(i)\beta(j)}=0$ for $i\neq j$. We note that the Eqs. (2.20) and (2.21) can be derived without replicas by using the cavity approach.[35]

Next, we specialize these equations to the transitions at T_A and T_K described above. If there is only self-overlap, then $q_0=0$ and Eq. (2.20) reduces to

$$q_{ab}^{11}(q_0=0)=q_1\delta_{ab}=\frac{1}{\bar{\Omega}}\int DX^1m_a(X^1)m_b(X^1)e^{\mathcal{I}_1}\ , \tag{2.22a}$$

with

$$\bar{\Omega}=\int DX^1e^{\mathcal{I}_1}\ , \tag{2.22b}$$

where

$$\mathcal{I}_1=-\frac{1}{2\mu q_1}\sum_a(X_a^1)^2-\frac{1}{p}\sum_l\ln\left[\frac{1+e_b^l m_b(X^1)}{p}\right]\ . \tag{2.22c}$$

One also finds $q_{ab}^{12}=0$, as is required for consistency. Note that the $n\to 0$ limit was never used and that the parameter $\bar{x}$ does not appear in this solution.

At the transition denoted by T_K, one finds

$$q_{ab}^{11}(q_0=q_1)=q_1\delta_{ab}=\frac{1}{\bar{\Omega}'}\int DH_1m_a(H_1)m_b(H_1)e^{\mathcal{I}'_1}\ , \tag{2.23a}$$

with

$$\bar{\Omega}'=\int DH\,e^{\mathcal{I}'_1}\ , \tag{2.23b}$$

where

$$\bar{\mathcal{L}}'_1=-\frac{1}{2\mu q_1}\sum_a H_{a1}^2-\frac{\bar{x}}{p}\sum_l \ln\left[\frac{1+e_b^l m_b(H^1)}{p}\right] . \tag{2.23c}$$

One also finds

$$q^{\alpha(i)\beta(j)}=\begin{cases} q_i & \text{if } i=j \ , \\ 0 & \text{if } i\neq j \ , \end{cases} \tag{2.23d}$$

which is required for consistency. Again, the $n\rightarrow 0$ limit was not needed. Here, $\bar{x}$ appears and we note that Eqs. (2.22) and (2.23) are identical at $\bar{x}=1$. Further, $\bar{x}$ is the break point in the usual description of the PG transition and, at T_K, $\bar{x}=1$.

III. TAP FREE ENERGIES

In this section the two solutions discussed in Sec. II are considered in more detail. In particular, we concentrate on the free energies, component-averaged free energies, and the complexities for these states.

A. Frozen state

The state described by Eqs. (2.22) will be dubbed the frozen state because it is the state into which the dynamical theory seems to freeze. It could also be called the diagonal saddle-point state.[33]

For small q, Eqs. (2.22) yield the equation of state $(q_1=q)$

$$q=\mu q+\frac{\mu q^2}{2}(p-4)-\frac{\mu^3 q^3}{3}(5p-13)+O(q^4) . \tag{3.1a}$$

Equation (3.1a) is most easily derived by taking the q derivative of the right-hand side of Eq. (2.22a) and then integrating the resulting expression. Near T_A we find $1-\mu\sim O(\epsilon^2)$, $q\sim\epsilon$. For small $\epsilon=p-4$, Eq. (3.1a) is consistently

$$0=(\mu-1)q+\frac{\epsilon}{2}q^2-\tfrac{7}{3}q^3 . \tag{3.1b}$$

This equation (for $0<\epsilon\ll 1$) first has a physical nontrivial solution at

$$\left[\frac{k_B T_A}{J}\right]^2\simeq 1+\tfrac{3}{112}\epsilon^2+O(\epsilon^4) . \tag{3.2a}$$

The Edwards-Anderson order parameter at T_A is

$$q(T=T_A)=\frac{3\epsilon}{28}+O(\epsilon^2) . \tag{3.2b}$$

If we take into account that the dynamical theory was for a soft-spin PG model, then we find that Eqs. (3.1) comprise the equation of state found in the dynamical approach to the PG problem.[21] The dynamical theory predicts a glass-transition temperature given by Eq. (3.2a) and an Edwards-Anderson order parameter given by Eq. (3.2b). Also note that Eq. (3.1b) gives $q=q(T=T_A)+O((T_A-T)^{1/2})$.

In this state we need to distinguish between two different types of free energy. There is the free energy calculated with the usual replica approach or by Eq. (2.9a). For the frozen state, $q^{\alpha\neq\beta}=0$, and Eqs. (2.4) and (2.5) yield

$$\beta f=\frac{\beta F}{N}=-\frac{\mu}{4}(p-1)-\ln p . \tag{3.3}$$

This is just the usual paramagnetic-phase free energy. A more physical free energy which can also be readily calculated is the weighted-average—over all TAP components—TAP free energy.[34] Denoting this free energy $\bar{F}$, one has

$$\beta\bar{f}=\frac{\beta\bar{F}}{N}=\frac{\beta}{N}\sum_s F(m_s)P_s . \tag{3.4a}$$

Here, $F(m_s)$ is the free energy in a particular TAP state and is given by Eq. (2.6) and P_s is the canonical probability to be in that state:

$$P_s=\frac{e^{-\beta F(m_s)}}{\sum_s e^{-\beta F(m_s)}}=\frac{1}{Z}e^{-\beta F(m_s)} . \tag{3.4b}$$

F and $\bar{F}$ can be related to one another with Eq. (3.4b). One finds

$$\begin{aligned} F&=\bar{F}+k_B T\sum_s P_s\ln P_s \\ &=\bar{F}-TI\equiv\bar{F}-TS_c \ . \end{aligned} \tag{3.5}$$

Here, $I>0$ is usually[27] called the complexity, but we will argue that for the PG it is more appropriately called the configurational entropy, S_c, for $T_K<T<T_A$. In the SK model I is of $O(1)$ and $F=\bar{F}$ to within $1/N$ correction, so that it is not necessary to distinguish between these two free energies. Physically, I can be related to the additional information needed to specify a particular TAP state. For the physical interpretation of our results, it is crucial that both sides of Eq. (3.5) be evaluated near identical saddle points. Otherwise, it would not be correct to use Eq. (3.5) as an equality. This condition is satisfied due to the equivalence of Eqs. (2.16) and (2.4). Using Eq. (3.5), we will be able to identify the solution degeneracy of the weighted metastable states for $T_K<T<T_A$. The solution degeneracy can also be calculated directly.[36]

$\bar{F}$ can be calculated directly by using the formalism given in Sec. II.[34] An equivalent procedure is as follows. To leading order in N, Eqs. (2.6) and (2.8) are

$$\beta F=\frac{1}{p}\sum_i\sum_l(1+m_{ia}e_a^l)\ln\left[\frac{1+e_b^l m_{ib}}{p}\right]$$

$$-\beta\sum_{\substack{i,j\\(i<j)}}J_{ij}m_{ia}m_{ja}-\frac{N\mu}{4}(p-1)(1-q)^2 \tag{3.6a}$$

and

$$0=\frac{1}{p}\sum_{l=1}^{p}e_a^l\ln(1+e_b^l m_{ib})-\beta\sum_j J_{ij}m_{ja}-\mu m_{ia}(1-q) . \tag{3.6b}$$

Using Eq. (3.6b) to eliminate the multisite term in Eq. (3.6a) yields

$$\beta F=\frac{1}{p}\sum_{i}\sum_{l}\left[1+\frac{m_{ia}e_a^l}{2}\right]\ln\left[\frac{1+e_b^l m_{ib}}{p}\right] -\frac{N}{4}\mu(p-1)(1-q^2)\ . \tag{3.6c}$$

In Sec. II we effectively derived a distribution for the magnetizations on a site i. Averaging over this distribution yields

$$\beta\bar{f}=\frac{\beta\bar{F}}{N}=\frac{1}{p}\sum_{l}\left\langle\left[1+\frac{m_a e_a^l}{2}\right]\ln\left[\frac{1+e_b^l m_b}{p}\right]\right\rangle -\frac{\mu}{4}(p-1)(1-q^2)\ . \tag{3.6d}$$

Before explicitly evaluating $\bar{f}$, to $O(q^4)$, we give two exact identities which are useful in understanding the physics for $T_K < T < T_A$. The first identity is

$$\frac{\partial\beta\bar{f}}{\partial q}=\frac{\mu}{2}(p-1)q-\frac{\mu}{2}\sum_{c}\langle m_c^2\rangle\ , \tag{3.7a}$$

and the second identity is

$$\frac{\partial^2\beta\bar{f}}{\partial q^2}=\frac{\mu}{2}(p-1)(1-\mu)-\frac{\mu^2}{2}(p-1)(p-4)q +\frac{\mu^2}{p}v_{ace}\langle m_a m_c m_e\rangle-\frac{\mu^2}{2}\langle m_a^2 m_b^2\rangle\ . \tag{3.7b}$$

To prove these identities, one needs

$$\langle m_a X_b\rangle=\mu q\delta_{ab} \tag{3.8a}$$

and

$$\langle X_c X_d f\rangle=\mu q\delta_{cd}\langle f\rangle+\delta_{cd}(\mu q)^2\langle f\rangle +\frac{(\mu q)^2}{p}v_{cde}\langle m_e f\rangle-\delta_{cd}(\mu q)^2 -(\mu q)^2\langle m_c m_d\rangle\ , \tag{3.8b}$$

where

$$f\equiv\frac{1}{p}\sum_{l}\ln(1+e_b^l m_b)\ . \tag{3.8c}$$

Equations (3.8) can be obtained by integration by parts. Equation (3.7a) indicates that $\partial\beta\bar{f}/\partial q=0$ yields an equation of state consistent with Eqs. (2.22). This should be contrasted with Eq. (3.3) which does not depend on q.

If we evaluate the averages in Eq. (3.7b) to $O(q^2)$, then, by integration over q, the free energy, $\bar{f}$, to $O(q^4)$, can be easily obtained,

$$\beta\bar{f}=-\ln p-\frac{\mu}{4}(p-1)+\frac{\mu}{4}(p-1)(1-\mu)q^2 -\frac{\mu^2}{12}(p-1)(p-4)q^3+\frac{\mu^4 q^4}{24}(p-1)(5p-13) +O(q^5)\ . \tag{3.9}$$

Note that Eqs. (3.1), (3.7), and (3.9) are all consistent.

With Eq. (3.9) we can interpret the frozen state predicted by the dynamical theory in the temperature range $T_K < T < T_A$. We write Eq. (3.9) as

$$\beta\bar{f}=-\ln p-\frac{\mu}{4}(p-1)+\delta(\beta\bar{f})\ . \tag{3.10}$$

The first two terms in Eq. (3.10) are just the paramagnetic-phase (PM) free energy given by Eq. (3.3), and $\delta(\beta\bar{f})$ is the free energy required for the self-overlap ordering for $T < T_A$. With Eqs. (3.9) and (3.1), $\delta(\beta\bar{f})$ can be evaluated, and one finds that, for $T' < T < T_A$, $\delta(\beta\bar{f}) > 0$. This implies that in this temperature range the frozen state is thermodynamically metastable. At T', $\delta(\beta\bar{f})=0$, and in the next subsection this temperature is shown to be equal to T_K, the temperature where replica overlap can occur. Also note from Eqs. (3.10), (3.3), and (3.5) that $\delta(\beta\bar{f})$ is equal to the configurational entropy. $T'=T_K$ is also the temperature where the configurational entropy becomes zero. A continuation of the frozen phase to $T < T'$ would lead to an unphysical, negative value of S_c.

We conclude this subsection by calculating the PG susceptibility[1] and identifying a divergent correlation length near T_A^-. Defining the susceptibility matrix by

$$\beta\chi_{ab}^{ij}=\langle S_{ia}S_{jb}\rangle_T-m_{ia}m_{jb}\ , \tag{3.11a}$$

the PG susceptibility is given by

$$\chi_{\text{PG}}=\frac{1}{N}\sum_{\substack{i,j\\a,b}}\chi_{ab}^{ij}\chi_{ba}^{ji}\ . \tag{3.11b}$$

Following the technique developed by Bray and Moore[37] for the SK spin-glass model yields

$$\chi_{\text{PG}}=\frac{\beta^2(p-1)}{\mu}\frac{p-1-\Delta}{\Delta}\ , \tag{3.11c}$$

where

$$\Delta=\frac{\mu}{2}\frac{\partial^2\beta\bar{f}}{\partial q^2}\ , \tag{3.11d}$$

with the second-derivative term in Eq. (3.11d) given by Eq. (3.7b). Now, if we use that T_A is defined by when [cf. Eq. (3.7a)] $\partial\beta\bar{f}/\partial q=0$ first has a nontrivial solution, then it is clear that T_A actually denotes a spinodal point or a limit of metastability.[24-26] It then follows, in general, that $\Delta(T\to T_A^-)\to 0$ and that $\chi_{\text{PG}}(T\to T_A^-)$ diverges. This can be explicitly confirmed with the solution given by Eqs. (3.2). Further, for small ϵ, Eqs. (3.2) yield $\Delta(T\to T_A^-)\sim(T_A-T)^{1/2}$. If we assume a square-gradient term in the effective q Hamiltonian, then this, in turn, indicates a divergent correlation length near T_A given by

$$\xi_A(T\to T_A^-)\sim|T-T_A|^{-1/4}\ . \tag{3.11e}$$

The exponent $\frac{1}{4}$ is usual[25] for a correlation length near a mean-field spinodal.

Finally, we mention that our conclusion that the frozen state is only thermodynamically metastable is consistent with the general results of van Hemmen.[38] van Hemmen's arguments indicate that the configurational entropy (cf. below) given by Eqs. (3.3), (3.5), and (3.10) can only be extensive if the self-overlap or frozen state is metastable.

B. The PG state

We call the true thermodynamic phase for $T<T_K$ the PG state. This phase has been discussed before in the literature.[8,21] Here we make some connections between this state and the frozen state and between the usual replica approach and the TAP approach. We also define a divergent correlation length near T_K.

For the PG state, which is the equilibrium state for $T<T_K$, F and $\bar{F}$ can be shown to be equal except for N^{-1} terms. With 1-RSB, Eqs. (2.4) and (2.5), or the generalization of Eq. (3.6d), give the free energy

$$\beta f=-\ln p-\frac{\mu}{4}(p-1)-\frac{\mu}{4}(p-1)(1-\mu)(1-\bar{x})q^2+\frac{\mu^2}{12}(p-1)(p-4)(1-\bar{x})q^3-\frac{\mu^2}{6}(p-1)(1-\bar{x})^2q^3$$
$$-\frac{\mu^4q^4}{24}(p-1)(1-\bar{x})(5p-13)+(1-\bar{x})0[q^5,(1-\bar{x})q^4]\ . \qquad (3.12)$$

Equation (3.12) is valid to $O(\epsilon^4)$ with $q\sim O(\epsilon)$, $\mu\simeq 1+O(\epsilon^2)$, and for $T_K\simeq T$, and we show that $1-\bar{x}\simeq 1-T/T_K$. The equation of state follows from $\partial\beta f/\partial q=0$, or by expanding Eqs. (2.23) in powers of q,

$$0=(\mu-1)q+\frac{\epsilon}{2}q^2-\tfrac{7}{3}q^3-(1-\bar{x})q^2+O(\epsilon^4,\epsilon^3(1-\bar{x}))\ . \qquad (3.13a)$$

Here we have assumed that $1-\bar{x}\neq 0$. Note that near T_K we will find $1-\bar{x}\rightarrow 0$ and Eq. (3.13a) reduces to Eq. (3.1b). This was noted before in Section II. The equation for $\bar{x}$ follows from $\partial\beta f/\partial\bar{x}=0$,

$$1-\bar{x}\simeq\frac{3}{q^3}\left[\frac{\epsilon}{12}q^3-\tfrac{1}{4}(1-\mu)q^2-\tfrac{7}{24}q^4\right]\ , \qquad (3.13b)$$

with $0<\bar{x}<1$. Note that the right-hand side (rhs) of Eq. (3.13b) is $\sim-\delta(\beta\bar{f})$ in Eq. (3.10), and that Eq. (3.13b) first has a physical solution at $1-\bar{x}\sim-\delta(\beta\bar{f})=0$. Denoting this transition temperature by T_K, one finds

$$\left[\frac{k_BT_K}{J}\right]^2\simeq 1+\frac{\epsilon^2}{42}+O(\epsilon^4)\ . \qquad (3.14a)$$

The order parameter at T_K is

$$q(T=T_K)=\frac{\epsilon}{7}+O(\epsilon^2)\ . \qquad (3.14b)$$

Note that $T_K<T_A$ here, and to all orders in ϵ this must be the case. This follows since by definition T_A occurs when Eq. (3.13a), at $\bar{x}=1$, or Eq. (3.1b) first has a solution at any order in ϵ. T_K occurs when both Eqs. (3.13) (and their generalization to higher order in ϵ) are satisfied.

With Eqs. (3.13) the free energy in the PG state near T_K is

$$\beta f\simeq-\ln p-\frac{\mu}{4}(p-1)+\tfrac{1}{6}(p-1)(1-\bar{x})^2q^3\ , \qquad (3.15)$$

with $1-\bar{x}\sim 1-T/T_K$. Several features of this free energy should be noted. First, although $q^{\alpha\neq\beta}$ jumps discontinuously at T_K, the free energy given by Eq. (3.15) predicts no latent heat and a discontinuous specific heat.[8] A physical interpretation of this will be given below. Secondly, note that f in the PG state is greater than the continuation of the PM-state free energy. This is usual in SG's.[1] Technically, it arises because the space of order parameters $\{q^{\alpha\neq\beta}\}$ is of dimension $(n/2)(n-1)$, which is negative as $n\rightarrow 0$. As a consequence, the dominant saddle point in the evaluation of the partition function is a local maximum. This should be contrasted with the frozen state discussed in the first part of this section. The space of order parameters $\{q^{\alpha\alpha}\}$ is of positive dimension and the true equilibrium state is a minimum with respect to the variation of these parameters.

To gain further insight into this phase transition, we examine the complexity given by Eq. (3.5),[27]

$$I=-k_B\sum_s P_s\ln P_s\ . \qquad (3.16)$$

In SG's it is known that the average number of states with weight P between P and $P+dP$ is $f(P)dP$, with[1,39]

$$f(P)=\frac{P^{(-1-\bar{x})}(1-P)^{\bar{x}-1}}{\Gamma(1-\bar{x})\Gamma(\bar{x})}\ . \qquad (3.17a)$$

The complexity is then[1]

$$\frac{I}{k_B}=-\int_0^1 dp\, f(P)P\ln P=\psi(1)-\psi(1-\bar{x})\ , \qquad (3.17b)$$

with ψ the digamma function. Near $T\simeq T_K$, or $\bar{x}\simeq 1$, one finds that I is singular,

$$\frac{I}{k_B}\simeq\frac{1}{1-\bar{x}}\simeq\frac{1}{1-T/T_K}\ . \qquad (3.17c)$$

This, in turn, implies that the effective number of relevant states, K^*, is exponentially large near T_K,

$$K^*(T<T_K)=\exp(I/k_B)\simeq\exp\left[\frac{T_K}{T_K-T}\right]\ . \qquad (3.17d)$$

Equation (3.17d) indicates that near T_K the number of possible states into which the system can freeze is exponentially large. This is probably why there is no latent heat at T_K. There are so many states to freeze into, that the system is in a statistical sense equally disordered at T_K^+ and T_K^-.

We can also use Eq. (3.17d) to identify a divergent correlation length, ξ_K, near T_K, and to identify T_K as a "Kauzmann" temperature for the PG. The argument is as follows. In the mean-field limit the system appears to freeze into a thermodynamically metastable state at T_A. We conjecture that in a finite-dimensional PG, the PG will not freeze at T_A, but instead T_A will denote a temperature where nontrivial locally stable metastable states are first possible and the long-time dynamics is determined by activated transport processes. With this, we can use Eq. (3.5) to define a configurational entropy for $T < T_A$. From Eqs. (3.5) and (3.10), S_c near T_K is proportional to

$$S_c(T \to T_K^+) \sim Nk_B \left[\frac{T}{T_K} - 1 \right] . \tag{3.18a}$$

The number of states into which the system can make activated transitions is then extensive and is proportional to

$$K^*(T \to T_K^+) = \exp\left[\frac{S_c}{k_B} \right] \simeq \exp\left[N \left[\frac{T}{T_K} - 1 \right] \right] . \tag{3.18b}$$

At T_K the number of possible states becomes nonextensive and the system undergoes an ideal-glass transition. This scenario is similar to the structural glass-transition picture of Gibbs and Di Marzio[28] and T_K is the Kauzmann temperature.

A divergent correlation length can be identified by using $N \sim V \sim L^d =$ the volume of systems. On the T_K^+ side of the transition, we can then equate Eqs. (3.17d) and (3.18b) to define a length scale below which the system behaves as though it were frozen. Defining ξ_K in this way yields

$$\xi_K \sim | T/T_K - 1 |^{-2/d} . \tag{3.19}$$

This agrees with the scaling ansatz of Gross, Kanter, and Sompolinsky.[8]

IV. "DROPLETS" AND ACTIVATED TRANSITIONS IN THE POTTS GLASS

The existence of infinitely many metastable states for the infinite-ranged Potts glass between T_A and T_K suggests some interesting dynamical consequences for the more realistic finite-ranged Potts system. A complete analysis of the dynamics of the finite-ranged model has several complications. The most important complication is the diversity of states below T_A. This diversity will probably be important in giving the nonexponential relaxations characteristic of glasses and viscous fluids.[1,2] In addition, the finite-range model will exhibit critical fluctuation effects, at least near T_A, but perhaps below this temperature as well. Because of these dual complexities we will limit ourselves to a qualitative and somewhat speculative discussion of activated dynamics in a very-long-ranged Potts glass. A formal analysis along these lines would require an extension of instanton techniques to random systems. Although some work along those lines exists,[40,41] it does not seem directly applicable here. The role of droplets and activated transitions in the ordered phase of Ising spin glasses has recently been emphasized by Huse and Fisher.[42] The differing mean-field-theory structure of the Potts glass leads us to a rather different discussion, although there may eventually be many points in common.

The dynamics in between T_A and T_K resembles that of nucleation for ordinary first-order transitions. There are several differences, however. First there are many order parameters: The magnetization at each lattice site is given by a probability distribution. There can be transitions between the paramagnetic state, $m = 0$, and any ordered state, or between the ordered states. Another difference from usual first-order transitions is that the dynamical theory[12,21] suggests that one is initially forced to be in one of the ordered states despite their higher free energy. The free energy of the totality of the metastable states contains a configurational entropy and is, in fact, equal to the free energy of the paramagnetic solution.

In the analogy to first-order transitions, T_A acts like a spinodal temperature.[24–26] In the infinite-range model the nucleation barriers are infinite below this temperature. Thus the metastable states have an infinite lifetime and would, in fact, be "experimentally" observed. Therefore, for the infinite-range system, T_A is a dynamical transition[12,21] from ergodic to nonergodic behavior. For a long- but finite-range model the barriers below T_A are finite. The divergent susceptibility at T_A [$\chi_{\rm PG} \sim (T - T_A)^{-1/2}$] implies that the barriers vanish at T_A. The interface between two different metastable states should diverge as $\xi_A \sim (T_A - T)^{-1/4}$. Nucleation clusters near T_A will be quite noncompact. In fact, the spinodal cannot be a sharp line for these short-range models, and no strict divergences would occur because it is meaningless to talk of barriers less than $k_B T$ since there would be no separation of time scales. We note that Hall and Wolynes[43] have already argued that, in three-dimensional structural glasses at the point where aperiodic solutions of the density-functional equations begin to exist, the barriers are only of size $k_B T$ since the distance between minima of a structural glass is of the order of the thermal vibrations in a single minimum. This is in accord with our interpretation of T_A as a quasispinodal in the Potts glass.

The slowing down of density fluctuations in dense liquids as predicted by mode-coupling theory[13–18] near "T_A" is also connected with this pseudospinodal behavior.[3] A local stability analysis (in the "glass" phase) of the dynamical nonlinear integral equation describing the structural "glass" transition[13–18] has the same form as the dynamical equations describing a mean-field spinodal of an ordinary first-order phase transition as studied by Binder.[25] On the liquid side of the transition the dynamical glass theories are complicated by non-Markovian effects. The transition in both cases is smoothed out by activated transport.

Considerably below T_A, activated dynamics is dominant. A single TAP state's lifetime is determined by nucleation of a cluster of sufficient size within which may be found *any* of the different TAP states. Naively, we would argue that this cluster would be compact because there is no divergent susceptibility below T_A according to mean-field theory. This differs from the usual mean-field Ising glass,[1] which is critical for all temperatures at which TAP solutions exist. The mean-field theory thus indicates that the surface tension σ is finite. (This is a delicate point where the randomness may play a role: some of the TAP states may match more perfectly than others with the state under consideration. They would have lower surface (perhaps vanishing) tensions and barriers.[23]) This observation may be related to the fact that the Potts glass is less frustrated than the Ising glass.[44] This point is also consistent with the fact that the frozen state, where there is no replica overlap, is not frustrated in the usual sense.[23]

The nucleation picture gives an estimate for a typical lifetime of the TAP state. Here we concentrate on transitions between different "ordered" TAP states. We note, however, that the transition to the paramagnetic state is in some sense equivalent to all the possible transitions to the different TAP states because the difference between the paramagnetic-state free energy and the component-averaged free energy is just the configurational entropy of all the weighted metastable states. Since different TAP states have roughly the same free energy per unit volume, the nucleation cluster forms because of the configurational entropy arising from the fact that *any* of the TAP states may be in the cluster, leading to escape from the original TAP state. Thus, for a cluster of radius R there is a volume free energy of the form $F_{\text{bulk}} \sim Ts_c R^d/d$, where s_c is the configurational entropy per unit volume and d is the spatial dimensionality. The surface free energy is $\sim \sigma R^{d-1}$ according to mean-field theory (but could scale as a lower power of R if there is more frustration than indicated by mean-field theory). A Cahn-Hilliard argument[45] gives a nucleation cluster of size $R^* \sim (d-1)\sigma/Ts_c$ and an activation free energy of $\sim Ts_c R^{*d} \sim (T-T_K)^{1-d}$. Thus the rate of transitions per unit volume is proportional to

$$\exp\{-\sigma[(d-1)\sigma/Ts_c]^{d-1}\} \ .$$

Also note that in the present theory the driving force of the cluster is entropic.[46]

A divergent activation energy is one of the characteristics of glassy behavior. Adams and Gibbs[47] obtained such a divergence based on the Gibbs–Di Marzio entropy crisis by a different argument. We note that a relaxation time $\tau \sim \exp[A/(T-T_K)^2]$ is consistent with the behavior of three-dimensional structural glasses.[43] Indeed, it may be used to fit transport as well as the Vogel-Fulcher law.[2]

The dynamic picture near T_K only makes sense if the drops are large compared with the correlation length ξ_K. Since ξ_K diverges like $(T-T_K)^{-2/d}$, the picture should break down for $d<2$ and be marginal in two dimensions.

An unusual aspect of using the many-state nucleation analogy for activated dynamics is that the growth of a nucleation cluster should be very slow. Once a critical cluster is formed, it must have a *particular* TAP state in it. Thus there is no free-energy driving force for growth. This might support an argument that the relevant time scale is not determined by the maximum of the droplet free energy but by the radius at which the droplet free energy crosses zero. This would give essentially the same scaling form, however. Multiple nucleation events may thus be important in the complete dynamics in the temperature region $T_K < T < T_A$. We conclude by noting that the nucleation picture may also be complicated by the lack of time-scale separation caused by the unusual growth mechanism.

V. DISCUSSION

The Potts glass has many of the features that are connected with glassy phenomena in general and the liquid-glass transition in particular. One motivation for this analogy has been the connections[3,12] between the aperiodic crystal-liquid transition starting from theories of freezing[19] and the mode-coupling dynamic theories,[13–18] both of which are based on translational order parameters. Similarly qualitative analogies between plastic crystals and their glass transitions[48] also bring to mind this connection. Theories of the low-temperature properties of glasses have also indicated a relationship between disordered quadupolar systems (which have the same properties as the Potts system) and orientational glasses.[49] Another route to the connection is through a liquid-glass transition associated with bond-orientational order.[50]

In this paper we have sought to explore and interpret more fully the nature of the transitions in the Potts glass in the mean-field limit. A major finding is that there are a great number of points of contact with the theory of first-order transitions.[45] Two temperatures—T_A and T_K—appear in the theory.[12,21] The first is associated with the appearance of well-defined free-energy minima, the latter with their ultimate thermodynamic stability.

The phenomena at T_A indicate a change of transport mechanism. Such a change cannot be a sharp phase transition in a finite-range system, but there may well be vestiges in the details of correlation functions. For example, in the long-range limit one expects noticeable plateaus in time correlation function to appear near T_A and perhaps pseudospinodal behavior,[25,51] e.g., the fast part of the decay of the correlations should get slower as one approaches T_A from below. In the naive static theories[19] of the structural glass transition, which are based on density-functional theory or a self-consistent phonon description, T_A is the limit of stability of the glassy state. We expect that it is the transition at T_A which is located by some[14,15] of the dynamical theories[13–18] of the structural glass transition. These theories use self-consistent perturbation expansions to generate nonlinear equations describing dynamical correlation functions in dense simple liquids. In general, there are two sources of the nonlinearities in these equations. The first source is of purely dynamical origin and arises even if the underlying free energy is quadratic. The second source of nonlinearities is from a nontrivial free energy which in some[14,15] of these theories is implicitly given by density-functional theory.[3] It is important to note that the final one-loop results have the same structure, even if only the first source of nonlinearities is taken into account.[16] However, the more complete theories[14,15] are needed to make connections[3] with static theories[19] of the glass transition.

Recently, higher-order dynamical theories[52,53] have claimed to avoid the transition at T_A. For the case[16,52] where only a quadratic free energy is used, this seems reasonable because there is no underlying spinodal point in the mean-field limit. For the case where there is a mean-field spinodal point, this is a bit perplexing since this theory[53] does not contain activated transitions which seem to be the natural source of rounding of the transition. Still, because the barriers vanish at T_A there could be a remnant of these phenomena in a perturbative calculation.

The transition at T_K is truly thermodynamic and should be robust. This transition, first found by Gross *et al.*,[8] we now see is connected with a configurational entropy crisis like that of structural glasses. This entropy crisis is somewhat more subtle than in other models such as the Gibbs–Di Marzio model[28] since there is still a great deal of disorder in the glassy phase. Also, further instabilities may be encountered at lower temperatures[8,11] that may be associated with secondary relaxations.[2] The similarity of the PG to the random-energy model[9,10] also is consistent with the entropy crisis.

A very crude droplet argument gives a dramatic Vogel-Fulcher–like slowing down as the transition at T_K is approached. Thus it may be very difficult to get very close to the transition in the laboratory, and in practical experiments the glass transition will appear kinetic in origin.

More dynamic studies of plastic crystals which may be closer to the Potts system microscopically would be valuable here. Angell[54] has emphasized the distinction between "strong" and "fragile" systems both for plastic crystals and liquid-glass transitions. The mean-field theory may be a useful guide here.

The transition at T_K is quite unusual and is associated with a diverging length. Certainly the relevance of scaling and renormalization-group ideas needs to be examined at this transition, although the inability to approach close to the transition may make mean-field theories more accurate. Arguments based on a combination of mean-field ideas and renormalization-group ideas may also be helpful in understanding the role of the laboratory time scale in determining glassy phenomena. Studies of glass transitions in confined geometries[55] or in molecular clusters[56] might also be of some interest in observing the effects of this length scale.

ACKNOWLEDGMENTS

One of us (T.R.K.) would like to thank D. Thirumalai for useful discussions on many aspects of this work. We are also pleased to acknowledge discussions with Y. Fu, U. Mohanty, J. R. Schrieffer, and J. P. Sethna. This work was supported by the National Science Foundation through Grants No. DMR-86-07605, No. CHE-84-18619, and No. PHY-82-17853, supplemented by funds from the National Aeronautics and Space Administration. P.G.W. also acknowledges support from the J. S. Guggenheim Foundation and T.R.K. acknowledges support from the Presidential Young Investigator Program.

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