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Infinite Range Interaction Model of a Structural Glass

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In this paper a simple mean-field model for the liquid-glass phase transition is proposed. This is the low density D-dimensional system of N particles interacting via infinite-range oscillating potential. In the framework of the replica approach it is shown that such a system exhibits the phase transition between the high-temperature liquid phase and the low-temperature glass phase. This phase transition is described in terms of the standard one-step replica symmetry breaking scheme.

KEY WORDS: Replicas; mean-field theory; glassy phase; one-step replica symmetry breaking.

1. INTRODUCTION

The problem of the liquid-glass phase transitions attracts permanent interest during last decades (for reviews see, e.g., ref. 1). In the recent years in additional to the traditional experimental and phenomenological investigations a notable progress has been achieved in a first principle statistical mechanical study of the glass phase (see ref. 2 and references therein). Leaving apart a wide scope of non-equilibrium properties of glasses, in a pure statistical mechanical approach one is aiming to investigate the thermodynamical properties of the N-particle system with the two body interparticle interactions described by the Hamiltonian

$$H[\mathbf{x}_i] = \sum_{i,j=1}^{N} U(\mathbf{x}_i - \mathbf{x}_j), \tag{1.1}$$

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where $\mathbf{x}_i$ is the vector in a D-dimensional space which points the position of the ith particle, and $U(\mathbf{x})$ is the interparticle potential (one, of course, can consider more general systems with two or more sorts of particles and different potentials for different particles). In a realistic systems the potential $U(\mathbf{x})$ must be attractive (and sufficiently quickly decaying) at large distances and strongly repulsive at short distances.

In a very simplified form the scheme of calculations is supposed to look as follows. Instead of the plain (and hopeless) integration over all positions of the particles in the partition function

$$Z = \left[\prod_{i=1}^{N} \int d^D \mathbf{x}_i \right] \exp(-\beta H[\mathbf{x}_i]) \tag{1.2}$$

in the systematic approach, first of all, one should find (or rather guess) the space structure and the energy of the (zero-temperature) ground state configuration of the Hamiltonian, and then, using one or another approximation, integrate over the fluctuations around this state. Depending on the value of the temperature one eventually finds that either the proposed non-trivial ground state is stable with respect to the fluctuations (at low enough temperatures), or (at sufficiently high temperatures) the fluctuations destroy proposed ground state and the thermodynamic state of the system is a liquid where all the particles are delocalized.

Indeed, the above scheme works rather well if the low temperature ground state of the system is ordered. In this case we are dealing with the crystal which is characterized by one or another global symmetry breaking, and which can be sufficiently easily described analytically. However, in the study of the disordered glass state, the situation becomes much more complicated, because in this case the low-temperature solid state is characterized by the *random* positions of the particles. This state is characterized by broken translational and rotational symmetries, but unlike of the ordered crystal configurations (having one or another spatial and rotational symmetry), it is very difficult to understand what are the residual symmetries left in the glassy state. All that resembles the problem one is facing in spin-glasses, where the spins are getting frozen in a random state which can not be characterized by any apparent global symmetry breaking(3) (this analogy between spin glasses and the thermodynamics of the glass state was first noticed by Kirkpatrick *et al.*(4)) The only but quite essential difference is that, unlike spin-glasses, here we do not have *quenched disorder* installed in the initial Hamiltonian. Nevertheless, the ideas borrowed from the spin-glass theory, and in particular the use of the replica technique(5) (which, as we know now, has much deeper meaning than just a technical trick to pass over the averaging of the logarithm of the partition function) turned out to be quite fruitful also for structural glasses, as was shown in the series of papers by Mezard and Parisi.$^{(2)}$ It should be noted that at present we know many others examples of the successful applications of the replica approach for glassy-like systems containing no quenched disorder.$^{(6)}$

To demonstrate the effect of a symmetry breaking in ordered magnetic systems one can introduce a conjugated field coupled to the order parameter, which at the end (after taking the thermodynamic limit) is set to zero. In spin-glasses the same effect can be achieved by introducing several weakly coupled copies (replicas) of the original system. In a similar way, to demonstrate the effect of the freezing into a random glass state in the system of particles described by the Hamiltonian, Eq. (1.1), let us introduce *two identical copies* of the same system described the following Hamiltonian

$$H = \sum_{i,j}^{N} U(\mathbf{x}_i - \mathbf{x}_j) + \sum_{i,j}^{N} U(\mathbf{y}_i - \mathbf{y}_j) + \epsilon \sum_{i}^{N} W(\mathbf{x}_i - \mathbf{y}_i), \tag{1.3}$$

which contains a weak (controlled by the parameter ϵ) attractive potential W between particles $\mathbf{x}$ and $\mathbf{y}$ of the two systems. After taking the thermodynamic limit the parameter ϵ must be set to zero. This trick can result in two types of situations:

(1) After taking the limit $\epsilon \to 0$ the particles of the two systems become independent (uncorrelated). This would indicate that the particles do not have a "memory" of their spatial positions so that they are free to move (non localized in space) and the original system is in the (high-temperature) liquid phase.

(2) After taking the limit $\epsilon \to 0$ the positions of the particles of the two systems remain correlated. This would indicate that the particles become localized in space so that the original system is in the (low-temperature) solid state. The order parameter describing this phase can be defined, e.g., in terms of the correlation function between particles of the two copies of the system.

In fact, like in spin glasses, to obtain more detailed information about this type of phase transition, instead of the two copies it is more convenient to introduce a general n replicas of the original system (see Section 2). It should be also noted that in real calculations the introduction of the supplementary attractive potential between replicas is actually not necessary. It is well known that, e.g., in the case of the paramagnetic-ferromagnetic phase transition, instead of introducing a conjugated field, it is sufficient just *to suppose* the possibility of the global symmetry breaking to prove its existence afterwords. In a similar way, here we are also going *to admit* the possibility of the effective space correlations among particles of different (originally non-coupled) replicas, while the validity of this assumption can be checked *a posteriori.*

Although the above idea is very simple, actual calculations for realistic models turn out to be quite sophisticated (see, e.g., ref. 2). For that reason it would be quite helpful to have here the analog of the mean-field models of spin-glasses, like the SK-model(7) or REM,(8) which despite of their non-physical nature, turned out to be very powerful tool for understanding the nature of the spin-glass state. The first model of this type was proposed by T. R. Kirkpatrick and D. Thirumalai,(9) which has been formulated in terms of somewhat unrealistic density functional Hamiltonian and which, nevertheless, provides a consistent static and dynamic theory of the structural glass transition.

The aim of this paper is to present a very simple mean-field toy model of a structural glass (a distant analog of the SK model of spin-glasses), which is described by the Hamiltonian containing *infinite-range* (non decreasing with the distance) oscillating interactions between particles. Despite its quite unrealistic structure this model exhibits non-trivial liquid-glass phase transition and provide a kind of "toy" illustration of the ideas the general approach. It will be shown that the nature of the "liquid-glass" phase transition in such system is of the so-called one-step replica symmetry breaking type which, in particular, takes place in REM(8) and in many others disordered systems,(10) and it also describes the phase transition in the so-called discontinuous spin-glasses without any quenched disorder.(6) This phase transition is characterized, on one hand, by a finite jump of the order parameter (like at the first-order phase transitions), and, on the other hand, by the continuous free energy function (as it should be at the second-order phase transition).

2. REPLICA CALCULATIONS

The general strategy of the replica calculations for spin-glasses and others disordered systems is well described in all details in a number publications (see, e.g., ref. 3). The adaptation of this technique for systems containing no quenched disorder was proposed in ref. 5, and currently it is widely used for structural glasses(2) as well as for others glass-like systems containing no quenched disorder.(11) For that reason, in this section I am going to remind just the main points of the replica approach (as it can be used for systems with no quenched disorder), while the details the interested reader can find in the referenced cited above.

Let us consider a system of N identical particles of the size a confined in a macroscopic box of the size R described by a Hamiltonian $H[\mathbf{x}_i]$ ($i = 1, 2,..., N$). Now, instead of the partition function (1.2) let us introduce the (replica) partition function for n non-coupled copies of the original system (which now consist of Nn particles):

$$Z_n = \frac{1}{(N!)^n} \left[\prod_{i=1}^{N} \prod_{a=1}^{n} \int \frac{d^D \mathbf{x}_i^a}{a^D} \right] \exp\left(-\beta \sum_{a=1}^{n} H[\mathbf{x}_i^a] \right), \tag{2.1}$$

Of course, formally $Z_n = Z^n$. However, physically, this can be correct only if the particles of the system are treated as non-localized in space which is correct only if the thermodynamic state of the system is a liquid. If the system undergoes true thermodynamic phase transition into a disordered glass-like state in which the positions of the particles are localized in space, then the situation becomes much more complicated (in this case the identity $Z_n = Z^n$ is recovered only if in the partition function one makes the summation over *all* the phase space ignoring the presence of infinite barriers of the free energy separating different glass-like disordered states). To take into account the possibility of existence (at low temperatures) of the true thermodynamic glass-like states, in the computation of the above replica partition function, Eq. (2.1), one can *suppose* from the very beginning that the space positions of particles belonging to some replicas are correlated (whether this assumption is correct or not should be then checked *a posteriori*). In other words, this assumption assumes that the particles of some replicas are localized in the same space positions.

In terms of the standard replica formalism$^{(3)}$ the above idea can be formulated in the following way. Let us divide all n replicas into n/m groups each consisting of m replicas, and then let us suppose that the particles belonging to the same group are correlated (so that they create a kind of the "replica molecule"), while particles of different groups are non-correlated (this type of structure is called "one-step replica symmetry breaking"). It is clear that in this case the partition function, Eq. (2.1), reduces to

$$Z_n = [Z_m]^{\frac{n}{m}}, \tag{2.2}$$

and the density of the free energy of the system is then

$$f = -\frac{1}{\beta N n} \ln(Z_n) = -\frac{1}{\beta m N} \ln(Z_m). \tag{2.3}$$

At this point one has to note what is the difference between the replica formalism for the systems with quenched disorder (spin-glasses), and for the present glass-like systems containing no quenched disorder. In the first case, one is facing an additional technical problem (which is absent in the present analysis) of averaging of the free energy (logarithm of the partition function) over parameters describing quenched disorder. For that reason, the parameter n describing the "number of replicas" must be analytically continued to arbitrary non-integer values and eventually set to zero at the end of calculations. Instead of that, here we do not need to average the free energy over quenched disorder, and the replicas were introduced only for physical reasons discussed above. Originally the technical trick with n identical copies of the systems has been introduced to study the localization of particles in random space positions, but eventually we are studying only *one* system, and this indicate that in the present case the parameter n must be set to $n = 1$ at the end.

Coming back to Eq. (2.3), one could conclude that formally the parameter n has simply dropped out from the analysis. Actually this is not quite so, because in Eq. (2.3) we are left with somewhat mysterious parameter m, which by definition is constrained by the condition $m \leqslant n$. Setting $n = 1$ one finds that the parameter m (which now has to be analytically continued for arbitrary non-integer values) is bounded by $m \leqslant 1$ (for further details and physical discussion of the replica parameter m see, refs. 2 and 5).

According to the general strategy of the replica theory the physical free energy of the system is given by the *maximum* of the replica free energy, Eq. (2.3), with respect to the continuous parameter m (bounded by the condition $m \leqslant 1$). As usual in the replica calculations, after the parameter m (which originally was introduced as an integer number) is analytically continued for values smaller than one, the original physical minimum of the free energy turns into a maximum. In the present case the number of independent replica variables is equal to $(m-1)$ (see below), therefore for m smaller than one this number formally becomes negative which effectively changes the minimum of the free energy into the maximum (this situation is quite similar to that of the standard replica calculations in disordered systems(3)).

The assumption that the positions $\mathbf{x}_i^a$ of particles in different replicas are correlated can be explicitly represented as follows:

$$\mathbf{x}_i^a = \mathbf{x}_i + \mathbf{u}_i^a, \tag{2.4}$$

where $\mathbf{x}_i$ play the role of the center of mass of the replica "molecule," and $\mathbf{u}_i^a$ are the deviations of the particles from the center of mass. Of course, these deviations are bounded by the condition

$$\sum_{a=1}^{m} \mathbf{u}_i^a = 0 \tag{2.5}$$

and their values have to be small compared to the typical distances $|\mathbf{x}_i - \mathbf{x}_j|$ between the replica molecules. In this way the replica partition function takes the following form:

$$Z_m = \frac{a^{-NmD}}{N!}\left[\prod_{i=1}^{N}\int d^D\mathbf{x}_i\right]\left[\prod_{i=1}^{N}\prod_{a=1}^{m}\int d^D\mathbf{u}_i^a\right]\left[\prod_{i=1}^{N} m^D\delta\left(\sum_{a=1}^{m}\mathbf{u}_i^a\right)\right]$$
$$\times\exp\left(-\beta\sum_{a=1}^{m} H[\mathbf{x}_i+\mathbf{u}_i^a]\right). \tag{2.6}$$

We see that now the problem becomes similar to that of statistical systems with quenched disorder in replica representation: according to Eq. (2.6), $\mathbf{x}_i$'s play the role of disorder parameters, while $\mathbf{u}_i^a$ are the dynamical variables. As usual, after averaging over the disorder parameters $\{\mathbf{x}_i\}$ we will get the partition function Z_m represented in terms of a new replica Hamiltonian $H_m[\mathbf{u}_i^a]$:

$$Z_m = \left[\prod_{i=1}^{N}\prod_{a=1}^{m}\int d^D\mathbf{u}_i^a\right]\exp(-\beta H_m[\mathbf{u}_i^a]), \tag{2.7}$$

where the replica variables $\mathbf{u}_i^a$ could now become effectively coupled.

The standard scenario of the one-step replica symmetry breaking phase transition, observed in various disordered systems,(8, 10) looks as follows. The extremum of the free energy, Eq. (2.3), is defined by the saddle-point equation

$$\partial f(m, \beta)/\partial m = 0. \tag{2.8}$$

If the solution of this equation, $m_*(\beta)$, is smaller than one, then for the physical free energy one finds: $f(\beta) = f(m_*(\beta), \beta)$. This situation corresponds to the solid glassy phase, and it will be shown to take place only at temperatures smaller than a certain critical temperature T_c.

On the other hand, it turns out that in the high-temperature liquid phase, at $T \geqslant T_c$, the formal solution of Eq. (2.8) yields $m_*(\beta) \geqslant 1$, which is not allowed by the constraint $m \leqslant 1$. In this case it can be proved that the maximum of the free energy $f(m, \beta)$ is achieved at $m = 1$, so that the physical free energy of the system is given by $f(\beta) = f(m = 1, \beta)$.

Now let us look how this general scheme works for the concrete mean-field (toy) model of a structural glass which will be introduced in the next section.

3. THE MODEL

The model we consider in this paper consists of N identical particles of the size a confined in a (macroscopic) box of the size R with the density $\rho \equiv N/R^D$, which in the thermodynamic limit ($N \to \infty$, $R \to \infty$) remains finite. This system is described by the Hamiltonian:

$$H = -\frac{1}{\sqrt{N}} \sum_{i<j}^{N} U(|\mathbf{x}_i - \mathbf{x}_j|) \tag{3.1}$$

where

$$U(|\mathbf{x}|) = -\sqrt{2}\cos(|\mathbf{x}|) \tag{3.2}$$

is the *infinite-range* oscillatory interparticle interaction potential. The motivation for this form of the interaction potential is in the following. On one hand, to have true mean-field statistical model one would like to have the interactions between particles to be infinite-range. On the other hand, the structure of the interactions in the model of a glass-like system (containing no quenched disorder) must be such that it would be (in the language of spin-glasses) as frustrated as possible. Forgetting unphysical nature of the interactions (3.2), they satisfy these two demands almost ideally. The interaction potential, Eq. (3.2), yields the alternating concentric space bands of positive and negative energy. For a system of N particles in dimensions greater than $D = 1$ it creates highly complicates "interference" pattern, so that any (random or regular) configuration of such particles appears to be strongly "frustrated," in a sense that no positions of the particles could satisfy all the interactions. As often is done in the studies of glasses, here we are going to ignore the possibility of existence of the exceptional ordered crystal-like ground state configurations (if they do exist, their energy would be of the same order of magnitude as the disordered ones) In other words, we are going to study generic low temperature solid state in this model which is characterized by a random positions of the particles, and according to Eq. (3.1), their energy is extensive in N.

It turns out that all the calculations simplify a lot if one makes the following assumptions. It will be supposed that that the size of the particles a is much smaller than the oscillation period of the potential, Eq. (3.2), (which is of the order of one), and in turn, this oscillation period is much smaller than the typical distance between particles $L = \rho^{-1/D}$:

$$a \ll 1 \ll L \tag{3.3}$$

(in particular, this makes possible to treat the particles as point-like objects).

After splitting of the degrees of freedom $\{\mathbf{x}_i^a\}$ into the center of mass $\{\mathbf{x}_i\}$ and the deviations $\{\mathbf{u}_i^a\}$ (Eqs. (2.4)–(2.5)), for the replica partition function, (2.6), we get:

$$Z_m = \frac{a^{ND(m-1)}}{N!} \prod_{i=1}^{N} \left[\left(\prod_{a=1}^{m} \int d^D \mathbf{u}_i^a \right) m^D \delta \left(\sum_{a=1}^{m} \mathbf{u}_i^a \right) \right] \left[\prod_{i=1}^{N} \int \frac{d^D \mathbf{x}_i}{a^D} \right] \times \exp \left(\frac{\beta}{\sqrt{N}} \sum_{a=1}^{m} \sum_{i<j}^{N} U(|\mathbf{x}_i - \mathbf{x}_j + \mathbf{u}_{ij}^a|) \right) \tag{3.4}$$

where $\mathbf{u}_{ij}^a \equiv \mathbf{u}_i^a - \mathbf{u}_j^a$. Keeping only extensive in N terms (the only relevant ones in the thermodynamic limit $N \to \infty$) for the averaging over $\{\mathbf{x}_i\}$ we obtain:

$$\begin{aligned} &\frac{1}{N!} \left[\prod_{i=1}^{N} \int_{|\mathbf{x}_i|<R} \frac{d^D \mathbf{x}_i}{a^D} \right] \exp \left(\frac{\beta}{\sqrt{N}} \sum_{a=1}^{m} \sum_{i<j}^{N} U(|\mathbf{x}_i - \mathbf{x}_j + \mathbf{u}_{ij}^a|) \right) \\ &\simeq (\text{const}) \left(\frac{L}{a} \right)^{ND} \exp \left(\frac{\beta}{\sqrt{N}} \sum_{a=1}^{m} \sum_{i<j}^{N} \overline{U(|\mathbf{x}_i - \mathbf{x}_j + \mathbf{u}_{ij}^a|)} \right. \\ &\left. + \frac{\beta^2}{2N} \sum_{a,b=1}^{m} \sum_{i<j}^{N} \sum_{k<l}^{N} \overline{U(|\mathbf{x}_i - \mathbf{x}_j + \mathbf{u}_{ij}^a|)\, U(|\mathbf{x}_k - \mathbf{x}_l + \mathbf{u}_{kl}^b|)} \right) \end{aligned} \tag{3.5}$$

where $L = \rho^{-\frac{1}{D}}$, $\rho = N/R^D$, $N! \simeq (N/e)^N$ and

$$\overline{(\cdots)} \equiv \left(\frac{L}{a} \right)^{-ND} \left[\prod_{i=1}^{N} \int d^D \mathbf{x}_i \right] (\cdots). \tag{3.6}$$

One can easily check that due to the infinite-range structure of the interactions (which are of order $N^{-1/2}$) in the Hamiltonian (3.1), the higher order terms of the expansion in Eq. (3.5) are not extensive in N (which is proportional to the volume of the system). For example, taking into account Eqs. (3.7) and (3.8) below, one can easily find that the only non-zero contribution of the 4-th order has the following form:

$$\begin{aligned} N^{-2} \sum_{i<j}^{N} \sum_{a,b,c,d} &\overline{U(|\mathbf{x}_i - \mathbf{x}_j + \mathbf{u}_{ij}^a|)\, U(|\mathbf{x}_i - \mathbf{x}_j + \mathbf{u}_{ij}^b|)} \\ &\times \overline{U(|\mathbf{x}_i - \mathbf{x}_j + \mathbf{u}_{ij}^c|)\, U(|\mathbf{x}_i - \mathbf{x}_j + \mathbf{u}_{ij}^d|)} \end{aligned}$$

which is of order $O(1)$.

According to the above definition, Eq. (3.6), one can easily prove (under condition $L \gg 1$):

$$\overline{U(|\mathbf{x}|)} = 0 \tag{3.7}$$

$$\overline{U(|\mathbf{x}_\mathrm{i}|)\, U(|\mathbf{x}_\mathrm{j}|)} \simeq \delta_{ij} \tag{3.8}$$

and

$$\overline{U(|\mathbf{x}_\mathrm{i}|)\, U(|\mathbf{x}_\mathrm{j} + \mathbf{u}|)} \simeq J_0(|\mathbf{u}|)\, \delta_{ij} \tag{3.9}$$

where $J_0(u)$ is the Bessel function. In particular, for $u \ll 1$ we have:

$$J_0(u \ll 1) \simeq 1 - \tfrac{1}{4} u^2. \tag{3.10}$$

Thus, substituting Eq. (3.5) into Eq. (3.4) and supposing that the deviations $|\mathbf{u}_i^a|$ from the center of mass positions are small, using Eqs.(3.7)–(3.10) for the partition function, Eq. (3.4) we obtain:

$$\begin{aligned} Z_m \simeq (\text{const}) \left(\frac{L}{a}\right)^{ND} a^{-ND(m-1)} m^{ND} \prod_{i=1}^{N} \left[\left(\prod_{a=1}^{m} \int d^D \mathbf{u}_i^a \right) \delta\left(\sum_{a=1}^{m} \mathbf{u}_i^a \right) \right] \\ \times \exp\left(\frac{\beta^2}{2N} \sum_{a,b=1}^{m} \sum_{i<j}^{N} \left[1 - \frac{1}{4} (\mathbf{u}_i^a - \mathbf{u}_i^b + \mathbf{u}_j^b - \mathbf{u}_j^a)^2 \right] \right) \end{aligned} \tag{3.11}$$

or

$$\begin{aligned} Z_m \simeq \Bigg[a^{-m} L m \exp\left\{ \frac{(\beta m)^2}{4D} \right\} \left(\prod_{a=1}^{m} \int d^D \mathbf{u}^a \right) \delta\left(\sum_{a=1}^{m} \mathbf{u}^a \right) \\ \times \exp\left\{ -\frac{1}{2} \beta^2 m \sum_{a=1}^{m} (\mathbf{u}^a)^2 \right\} \Bigg]^{ND}. \end{aligned} \tag{3.12}$$

One can easily see, that the assumption that the typical value of the deviations $|\mathbf{u}|$ are small is valid only for $(\beta m) \gg 1$. In this case simple integration yields:

$$Z_m \simeq (\text{const}) \left[a^{-m} L m \exp\left\{ \frac{(\beta m)^2}{4D} \right\} \left(\frac{2\pi}{\beta^2 m} \right)^{\frac{m-1}{2}} m^{-\frac{1}{2}} \right]^{ND}. \tag{3.13}$$

On the other hand the region of integration $|\mathbf{u}| \gg 1$ corresponds to the situation of free non-correlated particles (when no "replica molecules" exists), and in this case, the leading order contribution to the partition function is given by

$$Z_m \simeq \left[\frac{1}{N!}\left(\frac{R^D}{a^D}\right)^N \exp\left\{\frac{1}{4}\beta^2 N\right\}\right]^m \simeq \left[La^{-1}\exp\left\{\frac{\beta^2}{4D}\right\}\right]^{NDm}. \tag{3.14}$$

Thus, in the thermodynamic limit ($N \to \infty$) the free energy density, Eq. (2.3), is dominated by the contribution (3.13) for $\beta m \gg 1$, and it is dominated by the contribution (3.14) for $\beta m \ll 1$:

$$f(\beta, m) = \begin{cases} \frac{D}{\beta}\ln a - \frac{1}{4}\beta m - \frac{D}{\beta m}\ln L - D\frac{1}{2\beta m}\ln m & \\ \quad + D\frac{m-1}{2\beta m}\ln\beta + D\frac{m-1}{2\beta m}\ln(\beta m); & \text{for} \quad \beta m \gg 1 \\ \frac{D}{\beta}\ln a - \frac{1}{4}\beta - \frac{D}{\beta}\ln L; & \text{for} \quad \beta m \ll 1. \end{cases} \tag{3.15}$$

One can easily prove that this function of the parameter m has a unique *maximum* at $m = m_*(\beta)$, which at $L \gg 1$ can be obtained explicitly:

$$m_*(\beta) \simeq \frac{1}{\beta}\sqrt{4D\ln L} + O(\ln\ln L). \tag{3.16}$$

Since the function $f(\beta, m)$ is defined only at the interval $0 \leqslant m \leqslant 1$, in the case $m_*(\beta) > 1$ the maximum of f is achieved at $m = 1$. Thus, the maximum of the function $f(\beta, m)$ $(0 \leqslant m \leqslant 1)$ takes place at

$$m_*(\beta) = \begin{cases} \frac{\beta_c}{\beta}; & \text{for} \quad \beta > \beta_c \\ 1; & \text{for} \quad \beta \leqslant \beta_c \end{cases} \tag{3.17}$$

where

$$\beta_c \simeq \sqrt{4D\ln L} + O(\ln\ln L). \tag{3.18}$$

Correspondingly, for the physical free energy of the system, $f(\beta) = f(\beta, m_*)$, (with the accuracy $O(\frac{\ln\ln L}{\sqrt{\ln L}})$ we obtain the following result:

$$f(\beta) \simeq \begin{cases} f_0(\beta) - \frac{1}{2}\beta_c; & \text{for} \quad \beta > \beta_c \\ f_0(\beta) - \frac{1}{4}\beta - \frac{\beta_c^2}{4\beta}; & \text{for} \quad \beta \leqslant \beta_c \end{cases} \tag{3.19}$$

where

$$f_0(\beta) = \frac{D}{\beta}\ln a. \tag{3.20}$$

It should be noted that, as usual for the systems with continuous symmetry (in the model under consideration the coordinates of the particles are described by the continuous parameters), the absolute value of the free energy (as well as the absolute value of the entropy) depends on the choice of the measure of integration. In our case this measure is defined by the size of the particles a, (which is just an arbitrary parameter) and which provides the trivial contribution $f_0(\beta)$ to the free energy. The physically interesting peace of the free energy is the difference between its absolute value and this trivial contribution. In terms of this difference, $\tilde{f}(\beta) \equiv f(\beta) - f_0(\beta)$, the above result demonstrate the typical scenario of the so-called one-step replica symmetry breaking phase transition observed in the Random Energy Model of spin glasses$^{(8)}$ as well as in many others disordered systems:$^{(10)}$ (1) both the free energy and the entropy are continuous at the phase transition point; (2) $\tilde{f}(\beta)$ at $\beta \geqslant \beta_c$ becomes a constant, and the corresponding entropy $\tilde{S}(\beta)$ becomes zero. The last point tells that (like in REM) below T_c the system "localizes" exactly in one of the disordered states in the cofigurational space.

It should be noted that the result (3.19) represents only the leading contribution in terms of the big parameter $\ln L$. Of course, the next order terms describing in particular the thermal fluctuations of the particles near their random space positions, would make the the situation slightly more complicated, and in particular entropy of the glassy phase will become non-zero.

To complete the qualitative study of the above phase transition one has to introduce the proper order parameter. The order parameter which describes the correlations of the particles inside the replica "molecules" in the glassy phase can be defined in the standard way:

$$Q = \langle (\mathbf{u}^a - \mathbf{u}^b)^2 \rangle \tag{3.21}$$

where $a \neq b$. Since all the replicas are equivalent we can also define Q as follows:

$$Q = \frac{1}{m(m-1)} \sum_{a,b}^{m} \langle (\mathbf{u}^a - \mathbf{u}^b)^2 \rangle. \tag{3.22}$$

Using the constraint, Eq. (2.5), we get:

$$Q = \frac{2Dm}{(m-1)} \langle (u_\alpha^a)^2 \rangle \tag{3.23}$$

where the replica number a and the space vector component α are arbitrary. Note that the above definition of the order parameter is valid only for the glassy phase at $m < 1$. In the liquid phase ($m \equiv 1$) the positions of the particles are not correlated by definition.

Proceeding similarly to the calculation of the replica partition function, one finds:

$$\langle (u_\alpha^a)^2 \rangle = \frac{\left[\prod_{a=1}^m \int d^D\mathbf{u}^a\right](u_\alpha^a)^2\, \delta(\sum_{a=1}^m \mathbf{u}^a) \exp(-\frac{1}{2}\beta^2 m \sum_{a=1}^m (\mathbf{u}^a)^2)}{\left[\prod_{a=1}^m \int d^D\mathbf{u}^a\right] \delta(\sum_{a=1}^m \mathbf{u}^a) \exp(-\frac{1}{2}\beta^2 m \sum_{a=1}^m (\mathbf{u}^a)^2)}. \tag{3.24}$$

Straightforward calculations yield:

$$\langle (u_\alpha^a)^2 \rangle = \frac{m-1}{(\beta m)^2}. \tag{3.25}$$

Correspondingly for the order parameter, Eq. (3.23), we get:

$$Q = \frac{2D}{\beta(\beta m)}. \tag{3.26}$$

Substituting here the saddle-point value of $m = m_*(\beta)$ obtained above, Eq. (3.16), we eventually find:

$$Q \simeq \frac{2D}{\beta\sqrt{4D \ln L}} = \frac{2D}{\beta\beta_c}. \tag{3.27}$$

We see that in the whole low-temperature region at $\beta > \beta_c \simeq \sqrt{4D \ln L} \gg 1$ the value of the order parameter Q (as well as the value of the typical deviation $\langle (u_\alpha^a)^2 \rangle$) remains small, which justify the approximation made in calculation of the replica partition function, Eq. (3.12), as well as the whole original idea of splitting the degrees of freedom into the centers of masses of the replica "molecules" and the *small* deviations $\mathbf{u}^a$, Eqs. (2.4)–(2.5).

4. DISCUSSION

Physically the order parameter Q describes the typical value of the space fluctuations of the localized particles around their random equilibrium positions. It is interesting to note that the value of this order parameter remains finite in the whole low-temperature (glassy) phase including the phase transition point. In particular, according to Eq. (3.27) at $\beta = \beta_c$ we have:

$$Q_c \simeq \frac{1}{2 \ln L} \tag{4.1}$$

and $Q(T \to 0) \to 0$. Note also that in the high-temperature phase this order parameter is not defined: in terms of replicas it can be defined only for $m \neq 1$ while at $\beta < \beta_c$, $m_*(\beta) \equiv 1$, and in physical terms it describes the fluctuation of the localized particles which are just absent at $\beta < \beta_c$.

Thus, here we face the typical scenario of the phase transition with one-step replica symmetry breaking well known after the random energy model of spin glasses.(8) On one hand, in terms of the free energy this is the phase transition of the second order (the free energy function is continuous at T_c and it has a singularity only in the second derivative over the temperature, see Eq. (3.19)), while on the other hand, the order parameter which characterizes the low-temperature phase has a finite value right at T_c (which corresponds to the first-order phase transitions).

Of course, from the physical point of view, due to long-range structure of the interactions between particles, the present model could be considered as not more than a "toy" model of the structural glass. On the other hand, the big advantage of this extremely simple model is that the mean-field approach for it is exact, and it provides the non-trivial solution which makes possible to test on the qualitative level the general ideas of the replica approach for the structural glasses. Besides, the model exhibits rather peculiar type of the liquid-glass phase transition, which seems to be interesting in itself.

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