New Kinds of Phase Transitions: Transformations in disordered Substances

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Abstract

The transitions in disordered substances are discussed briefly: liquid–liquid phase transitions, liquid–glass transition and the transformations of one amorphous form to another amorphous form of the same substances. A description of these transitions in terms of many–particle conditional distribution functions is proposed. The concept of a hidden long range order is proposed, which is connected with the broken symmetry of higher order distribution functions. The appearance of frustration in simple supercooled Lennard–Jones liquid is demonstrated.

It is well known for a long time that there exist sharp phase transitions between different aggregate states and sharp polymorphic phase transitions between different crystalline phases of the same substances. During last two decades a lot of experimental data was obtained on complicated phase diagrams of liquids and amorphous solids, too. Some of these results were presented on the first international conference that took place here in Russia in 2001 \textsuperscript{11} and that can be considered as a formal claim of a new direction of physical investigations – transformations in disordered substances: liquid–liquid transitions and transformations of one amorphous form to another amorphous form of the same substances. The liquid–glass transition, although has longer history, has to be considered in the same context. It is now firmly established by different experimental techniques that sharp liquid–liquid transitions under pressure, formally similar to first–order phase transitions, exist as well as reversible transformations between amorphous states involving changes in local order structures and density. Usually a crystal melts with a conservation of the short–range order (SRO) structure type or into denser liquid with SRO structure similar to that of high pressure crystalline phase.

It should be emphasized that the transitions in liquids are true phase transitions mainly determined by thermodynamic relationships, whereas the transitions in amorphous solids take place far away from equilibrium and are governed by the corresponding kinetics.

A useful microscopic theory of these transitions is not developed yet and only empirical models and computer simulations have been used in practice to date. For example, interesting results were obtained by Stanley through molecular dynamics study basing
on the taking into account the hydrogen bonding in supercooled water \[2\]. It is by the 
demonstration of a simple analytic way of obtaining Stanley results that we begin the 
presentation of our own results on this subject (see, e.g., \[1, 3, 4, 5, 6\] and references 
therein).

From the intuitive point of view liquid-liquid phase transition between low density and 
high density phases may be related to the competition between expanded and compact 
structures. This suggests that the potential should have two equilibrium positions. The 
most obvious form of such potential is:

\[
\Phi(r) = \begin{cases} 
\infty, & r \leq \sigma \\
0, & \sigma < r \leq a \\
-\varepsilon_1, & a < r \leq b \\
0, & b < r \leq c \\
-\varepsilon_2, & c < r \leq d.
\end{cases} 
\]  

(1)

This two–well potential may be considered as a model for the water potential \[2\].

To investigate the possibility of the existence of the second critical point in this case we 
developed the mean-field (van der Waals–like) theory. Using the well-known Bogoliubov 
inequality for the free energy we can write

\[
F \leq F_{HS} + \left< U - U_{HS} \right>_{HS}. 
\]

Here \(F_{HS}\) is the 
free energy of the system of hard spheres with diameter \(\sigma\), and we consider the attractive 
part as a perturbation. Here \(U = \frac{1}{2} \sum_{i \neq j} \Phi(r_{ij})\) and \(U_{HS} = \frac{1}{2} \sum_{i \neq j} \Phi_{HS}(r_{ij})\). The average 
over the hard sphere potential has the form

\[
\left< U - U_{HS} \right>_{HS} = 2\pi \rho N \int_0^\infty \Phi_{atr}(r)g_{HS}(r)r^2 dr, 
\]  

(2)

where \(\Phi_{atr}(r) = \Phi(r) - \Phi_{HS}(r)\), \(g_{HS}(r)\) is the radial distribution function of the hard 
sphere system which we take in the Percus-Yevick approximation \[7\] and for \(F_{HS}\) we use 
the approximate Carnahan-Starling equation \[8\]

\[
\frac{F_{HS}}{k_B T N} = 3 \ln \lambda - 1 + \ln \rho + \frac{4\eta - 3\eta^2}{(1 - \eta)^2}. 
\]  

(3)

Here \(\lambda = h/(2\pi m k_B T)^{1/2}\).

The equation of state is given by \(P = \rho^2 \partial(F/N)/\partial\rho\). In Fig. 1 the two families 
of isotherms are shown for the temperatures close to two critical points \(\beta_1 = \varepsilon_1/k_B T_1\) 
and \(\beta_2 = \varepsilon_1/k_B T_2\). Fig. 1 shows that at low temperatures (\(\beta = \varepsilon_1/k_B T > \beta_1\)) there 
are two van der Waals–like loops in the equation of state which correspond to two fluid-
fluid transitions. In the temperature region \(\beta_2 < \beta < \beta_1\) there is only one loop which 
corresponds to the well known gas-liquid transition, \(\beta_2\) being the gas-liquid critical point 
temperature and \(\beta_1\) – the liquid-liquid critical temperature.

In this example, as at the ordinary critical point, no symmetry of the correlation 
functions is broken at the transition. The order parameter is the difference of densities 
of high and low density phases \(\Delta \rho = \rho_{l1} - \rho_{l2}\). However, it is interesting to describe the 
change of the local structure and the cluster symmetry at the transition.

To describe different kinds of space symmetry breaking we use the formalism of clas-
sical many particle conditional distribution functions

\[
F_{s+1}(r_1 | k_1^0 ... k_s^0) = \frac{F_{s+1}(r_1^0, r_1^0, ... r_s^0)}{F_s(r_1^0, ..., r_s^0)}. 
\]
Figure 1: The isotherms for the double-well potential (1) for different values of $\beta = \varepsilon_1/(k_B T)$. 
Here $F_s(r_1, \ldots, r_s)$ is the usual $s$–particle distribution function \cite{9}. The functions $F_{s+1}(r_1|r_1^0 \ldots r_s^0)$ satisfy the equation

$$\frac{\rho F_{s+1}(r_1|r_1^0 \ldots r_s^0)}{z} = \exp \left\{ -\beta \sum_{k=1}^{s} \Phi(r_1 - r_k^0) + \sum_{k \geq 1} \frac{\rho^k}{k!} \int S_{k+1}(r_1, \ldots, r_{k+1}) \times F_{s+1}(r_1|r_1^0 \ldots r_s^0) \cdots F_{s+1}(r_{k+1}|r_1^0 \ldots r_s^0) \, dr_2 \cdots dr_{k+1} \right\}. \quad (4)$$

Here $z$ is activity, $\rho$ is the mean number density, $S_{k+1}(r_1, \ldots, r_{k+1})$ is the irreducible cluster sum of Mayer functions connecting (at least doubly) $k + 1$ particles, $\beta = 1/k_BT$.

The simplest case is the symmetry breaking of the one–particle function. In the solid phase the local density, proportional to the one-particle distribution function, has the symmetry of a crystal lattice and can be expanded in a Fourier series in reciprocal lattice vectors $G$:

$$\rho (r) = \sum_G \rho_G e^{iGr}, \quad (5)$$

where the Fourier coefficients $\rho_G$ are the order parameters for the transition.

The Taylor expansion of the corresponding free energy functional around the liquid can be written in the following form:

$$\beta \Delta F = \int d\rho \rho(r) \ln \frac{\rho(r)}{\rho_0} - \sum_{k \geq 2} \frac{1}{k!} \int c^{(n)}(r_1, \ldots, r_k) \Delta \rho(r_1) \cdots \Delta \rho(r_k) \, dr_1 \cdots dr_k, \quad (6)$$

where

$$\Delta \rho(r) = \rho(r) - \rho_l$$

is the local density difference between solid and liquid phases. This is the base of the density functional theory of freezing (DFT) \cite{3}. In the frame of this approach tens of melting curves were calculated (see, e.g., the reviews \cite{11}). The full system of equations to be solved in DFT contains the nonlinear integral equation for the function $\rho(r)$, obtained as the extremum condition for the free energy and the equilibrium conditions for the chemical potential and the pressure written in terms of the same functions as in (6). To proceed constructively in the frame of DFT we have to choose an actual form of the free energy functional – a kind of closure or truncating – and we must make an ansatz for the average density of the crystal. The importance of such an ansatz follows from the fact that we are dealing with a theory which is equivalent to Gibbs distribution and one has to break symmetry following the Bogoliubov concept of quasiaverages \cite{12}.

Now let us consider a state of matter which is characterized by the uniform local density, but the broken symmetry of the two–particle distribution function. Such type of order is called the bond orientations order (BOO), where “bond” is the vector joining a particle with its nearest neighbor. This kind of order is well known in theories of two-dimensional melting (hexatic phase) \cite{13, 4}. Near the transition to anisotropic liquid state we have:

$$F_2(r_1|r_1^0) = g(|r_1 - r_1^0|)(1 + f(r_1 - r_1^0)), \quad (7)$$

where $f(r_1 - r_1^0)$ has the symmetry of the local environment of the particle at $r_1^0$ and may be written in the form $f(r_1 - r_1^0) = f(|r_1 - r_1^0|, \Omega)$, $\Omega$ determines the direction of
the vector \( \mathbf{r}_1 - \mathbf{r}_1^0 \). In the case of three dimensions function \( f(r, \Omega) \) may be expanded in a series in spherical harmonics:

\[
f(r, \Omega) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_{lm}(r) Y_{lm}(\Omega).
\] (8)

The microscopic equations for the order parameters \( f_{lm}(r) \) can be obtained from the main equation (4). The linearized equation determines the instability of isotropic liquid against the formation of the state with BOO and has the form [4]:

\[
f_{lm}(r) - \frac{4\pi}{2l + 1} \int \Gamma_l(r, r') g(r') f_{lm}(r') r'^2 \, dr' = 0.
\] (9)

Here \( \Gamma_l(r, r') \) correspond to the isotropic liquid when

\[
\Gamma(r_1, r_1^0, r_2) = \sum_{k \geq 1} \frac{g^k}{(k-1)!} \int S_{k+1}(\mathbf{r}_1 \ldots \mathbf{r}_{k+1}) \times \nabla |\mathbf{r}_3 - \mathbf{r}_1^0| \cdots \nabla |\mathbf{r}_{k+1} - \mathbf{r}_1^0| \, d\mathbf{r}_3 \cdots d\mathbf{r}_{k+1}.
\] (10)

reduces to

\[
\Gamma(r_1, r_1^0, r_2) = \Gamma(r, r', \theta),
\] (11)

\[
\Gamma(r, r', \theta) = \sum_{l=0}^{\infty} \frac{4\pi}{2l + 1} \Gamma_l(r, r') \sum_{m=-l}^{l} Y_{lm}(\Omega_1) Y_{lm}^*(\Omega_2),
\] (12)

The angles \( \Omega_1 \) and \( \Omega_2 \) determine the directions of the vectors \( r \) and \( r' \) and \( r = |\mathbf{r}_1 - \mathbf{r}_1^0|, r' = |\mathbf{r}_2 - \mathbf{r}_2^0|, \theta \) is the angle between vectors \( r \) and \( r' \). It should be notice that the correlation length of the orientational fluctuations \( \xi_{l,m} \to \infty \) when approaching the instability line given by Eq. (9).

To describe liquid–liquid and liquid–glass transitions we must consider isotropic case with rotationally invariant two–particle distribution function. A possible description of these cases can be given in terms of broken symmetry of higher order distribution functions. At high temperature the nearest neighbors of a molecule can take different relative positions and there is no SRO. At lower temperature SRO appears which can be of different kinds at different densities. The rotation and the translation of the clusters of preferred symmetry give rise to the fact that one-particle and two-particle distribution functions remain isotropic. If a kind of BOO appears the clusters are oriented in similar way and the two-particle distribution function becomes to be anisotropic (as in 2D hexatic phase). However, we can imagine another situation – freezing of the symmetry axes of the clusters in different position. The isotropic phase can be considered as analogous to the paramagnetic phase (of cluster symmetry axes), the BOO phase – to the ferromagnetic phase, and the mentioned freezed phase – to a spin glass phase.

Let us consider for simplicity a 2D system. In the vicinity of the transition one can write (in the superposition approximation for the liquid)

\[
F_3(\mathbf{r}_1, \mathbf{r}_1^0, \mathbf{r}_2^0) = g(|\mathbf{r}_1 - \mathbf{r}_1^0|) g(|\mathbf{r}_1 - \mathbf{r}_2^0|) (1 + f_3(\mathbf{r}_1, \mathbf{r}_1^0, \mathbf{r}_2^0))
\] (13)
In 2D case \( f_3(\mathbf{r}_1|\mathbf{r}_1^0, \mathbf{r}_2^0) \) depends in fact on two distances and two angles

\[
f_3(\mathbf{r}_1|\mathbf{r}_1^0, \mathbf{r}_2^0) = f_3(\mathbf{R}_0, \phi_0; R_1, \Theta_1),
\]

where \( \mathbf{R}_0 = \mathbf{r}_2^0 - \mathbf{r}_1^0 \), \( \mathbf{R}_1 = \mathbf{r}_1 - \mathbf{r}_1^0 \), \( \mathbf{R}_2 = \mathbf{r}_2 - \mathbf{r}_1^0 \) and \( \phi_0 \) is the angle of the vector \( \mathbf{R}_0 \) with the z axis, \( \Theta_1 \) — the angle between \( \mathbf{R}_1 \) and \( \mathbf{R}_0 \) and \( \Theta_2 \) — the angle between \( \mathbf{R}_2 \) and \( \mathbf{R}_0 \).

The linearization of (14) for \( s = 2 \) gives:

\[
f_3(R_0, \phi_0; R_1, \Theta_1) = \int \Gamma'(R_0, \phi_0; \mathbf{r}_2; R_1, \Theta_1) f_3(R_0, \phi_0; R_2, \Theta_2) g(|\mathbf{R}_2 - \mathbf{R}_0|) g(R_2) d\mathbf{r}_2,
\]

where

\[
\Gamma'(R_0, \phi_0; \mathbf{r}_2; R_1, \Theta_1) = \sum_{k \geq 1} \frac{\rho^k}{(k-1)!} \int S_{k+1}(\mathbf{r}_1, ..., \mathbf{r}_{k+1}) g(|\mathbf{r}_3 - \mathbf{r}_1^0|) \times g(|\mathbf{r}_3 - \mathbf{r}_2^0|)...g(|\mathbf{r}_{k+1} - \mathbf{r}_1^0|) g(|\mathbf{r}_{k+1} - \mathbf{r}_2^0|) d\mathbf{r}_3...d\mathbf{r}_{k+1}.
\]

There are two kinds of angles entering the equations and two kinds of order parameters, consequently. One angle (\( \phi_0 \)) fixes the position of one pair of particles of the cluster, and the other (\( \Theta_i \)) — the position of the third particle in the coordinate frame defined by \( \phi_0 \). The order parameter connected with \( \Theta_i \) is the generalization of intracluster hexatic parameter for the case of different coordinate frames. The order parameter connected with \( \phi_0 \) is an analogue of magnetic moment and in glass-like phase one can consider an Edwards-Anderson parameter < \( \cos \phi_0(t) \cos \phi_0(0) \> . In such a way we come to the concept of a “conditional” or “hidden” long range order: if we consider two pairs of particles at infinite distance from one another then there exists a preferable possibility for the relative position of the third particle near each pair. The directions of the bonds in the pairs of particles themselves are subjects to spin-glass-like order. In 3D case the rotation of clusters is given by rotation matrices \( D^{l \leftrightarrow \nu} (\vec{\omega}_0) \) so that we obtain a kind of orientational multipole glass for the clusters. If the intracluster ordering is established then we can consider the system of clusters. The orientational state of this system is defined by the intercluster interaction for different values of temperature and pressure.

Now let us consider this later situation when the intracluster symmetry is fixed and let us try to estimate the intercluster orientational interaction. If the intercluster interaction had the same sign for all cluster sizes (or all clusters had the same size) one would get the state with simple BOO. However, because of the difference in cluster sizes the orientational interaction for some harmonics may change sign as a function of the cluster size (see Fig. 2). In this case the low temperature state should be amorphous for some harmonics. So the difference of the orientational interaction of the clusters for different cluster sizes may be considered as the reason of some kind of frustration in simple liquids. It should be emphasized that the form of the corresponding component of the orientational interaction is the intrinsic statistical property of the liquid and does not depend on the timescale of the fluctuations in size and symmetry of the cluster. There is no real quenched disorder in the system but only an analog of it which may be treated in a formally same way as the quenched disorder in spin glasses. To analyze qualitatively the orientational freezing in the system we introduce simple lattice model which takes into account the interaction only between clusters with definite symmetry. The model gives the possibility to conclude what harmonics freeze first and what local symmetry prevails immediately below the transition. Let us now describe our results in more detail.
Our starting point is the expression for the free energy of the system as a functional of a pair distribution function \( g_2(r_i, r_0) \) which has the form [4]:

\[
\frac{F}{k_B T} = \int d\mathbf{r} \rho g_2(\mathbf{r}, \mathbf{r}_0) \left[ \ln \left( \lambda^3 \rho g_2(\mathbf{r}, \mathbf{r}_0) \right) - 1 \right] - \\
- \sum_n \frac{\rho^{n+1}}{(n+1)!} \int S_{n+1}(\mathbf{r}_1 \ldots \mathbf{r}_{n+1}) g_2(\mathbf{r}_1, \mathbf{r}_0) \cdots g_2(\mathbf{r}_{n+1}, \mathbf{r}_0) \times \\
\times d\mathbf{r}_1 \cdots d\mathbf{r}_{n+1} d\mathbf{r}_0 - \int \Phi(\mathbf{r} - \mathbf{r}_0) \rho g_2(\mathbf{r}, \mathbf{r}_0) d\mathbf{r} d\mathbf{r}_0.
\] (17)

where the term with logarithm corresponds to the entropy and the other terms — to the interaction energy. Here \( \Phi(\mathbf{r} - \mathbf{r}_0) \) - interparticle potential (for Lennard-Jones potential, \( \Phi_0(r) = 4\varepsilon((\sigma/r)^{12} - (\sigma/r)^{6}) \)), \( \lambda = \hbar/(2\pi mk_B T)^{1/2} \).

We can estimate the change of the energy due to (7). Omitting the entropy term in Eq.17 we obtain up to the second order in \( \delta g(\mathbf{r}, \mathbf{r}_0) \):

\[
\Delta F/k_B T = -\frac{1}{2} \int \Gamma(\mathbf{r}_1, \mathbf{r}_0, \mathbf{r}_2) \delta g(\mathbf{r}_1, \mathbf{r}_0) \delta g(\mathbf{r}_2, \mathbf{r}_0) d\mathbf{r}_1 d\mathbf{r}_2.
\] (18)

Using the approximation for the radial distribution function \( g(r) = \rho^{-1}(n_s/4\pi r_s^2)\delta(r-r_s) \) and the Eq.18 we obtain:

\[
\Delta F(r_s)/k_B T = -\frac{1}{2}\rho^{-2} \left( \frac{n_s}{4\pi} \right)^2 \sum_{l=0}^{\infty} 4\pi f l^2 + 1 \frac{f l^2 + 1}{f l^2 + 1} \sum_{m=-l}^{l} Y_{lm}(\Omega_1) \times \\
\times Y_{lm}^*(\Omega_2) f(r_s, \Omega_1) f(r_s, \Omega_2) d\Omega_1 d\Omega_2 = -\frac{1}{2} \sum_{l=0}^{\infty} J_l(r_s) \sum_{m=-l}^{l} |f_l|^2.
\] (19)

Here \( J_l(r_s) = \rho^{-2} \frac{4\pi}{2l+1} \left( \frac{n_s}{4\pi} \right)^2 \Gamma_l(r_s, r_s) \), \( n_s \) is the number of nearest neighbors of a particle and \( r_s \) is the size of the cluster, which is of the order of the first coordination shell size.

The function \( \Delta F(r_s) \) may be interpreted as the mean-field orientational interaction energy of the system of clusters having the size \( r_s \). To get the full energy of the system one should integrate (19) over the probability of finding the cluster with the size \( r_s \) which is given by the function \( r_s^2 g(r_s) \) in the vicinity of the first maximum.

Using the approximations of [4] for \( \Gamma(\mathbf{r}_1, \mathbf{r}_0, \mathbf{r}_2) \) we obtain the estimation for \( J_l(r_s) \) as a function of \( r_s \). Fig.2 represents \( J_l(r_s) \) for \( l = 4 \) and 6 along with \( r_s^2 g(r_s) \) in the vicinity of its first peak. It is seen that \( J_l(r_s) \) changes sign. This result enables us to suppose that there is a kind of frustration (which is analogous to that in spin glasses) appearing as a result of variations in the sizes of clusters according to \( g(r) \) and that it is possible to study the transition in the system of interacting clusters on the base of simple model lattice Hamiltonian:

\[
H = -\frac{1}{2} \sum_{<i \neq j>} \sum_{l=0}^{\infty} J^l_{ij} \sum_{m=-l}^{l} U_{lm}(\Omega_i) U^*_{lm}(\Omega_j).
\] (20)

The functions \( U_{lm}(\Omega_i) \) are the lattice harmonics for the point groups corresponding to the cluster symmetry. This Hamiltonian describes correctly BOO of clusters. In this case
the energy calculated from Eq. (20) in the mean-field approximation (taking into account that \( \langle U_{lm}(\Omega_i) \rangle = f_{lm} \)) coincides with the intercluster energy (19) under appropriate choice of \( J_{ij}^l \). We will use the Hamiltonian (20) to study the system of interacting clusters with various sizes.

To simplify the problem we neglect in Hamiltonian (20) all the terms except ones corresponding to the unit representation of the point group. Furthermore, we consider only the cases \( l = 4 \) and \( l = 6 \) which represent the cases of cubic and icosahedral symmetries. This Ising-like model may be called a “minimal” model:

\[
H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \hat{U}_i \hat{U}_j. \tag{21}
\]

Functions \( \hat{U} \equiv U(\varphi, \theta) \) are the combinations of spherical harmonics. We will consider separately symmetries of “simple” cube \( (l = 4, m = 0, \pm 4) \), cube \( (l = 6, m = 0, \pm 4) \) and icosahedron \( (l = 6, m = 0, \pm 5) \) correspondingly [14, 16]. For example, for \( l = 4 \) one has:

\[
\hat{U} \equiv U(\varphi, \theta) = \sqrt{\frac{7}{12}} \left\{ Y_{40}(\varphi, \theta) + \sqrt{\frac{5}{14}} (Y_{41}(\varphi, \theta) + Y_{44}(-\varphi, \theta)) \right\} \tag{22}
\]

The interactions \( J_{ij} \) are chosen in such a way that the MF approximation gives exact solution (infinite-range interactions). It is easily seen that in the minimal model (21) without disorder in the framework of the MF approximation there is a first order phase transition to the state with BOO (compare to [14, 15]). From Fig.2 it is clear that, as the first qualitative step, \( J_{ij}^l \) may be chosen as random interactions with Gaussian probability distribution

\[
P(J_{ij}) = \frac{1}{\sqrt{2\pi J}} \exp \left[ -\frac{(J_{ij} - J_0)^2}{2J^2} \right] \tag{23}
\]
where $J = \tilde{J}/\sqrt{N}$, $J_0 = \tilde{J}_0/N$ can be related to the microscopic parameters. We approximate $r^2g(r)$ by a gaussian exponential near the position of the first maximum $r_0$. So $r^2g(r) \sim \exp[-(r - r_0)^2/2\sigma]$. The approximation for the functions $\Gamma_i$ is then linear: $\Gamma_i \approx \alpha_i + \beta_i(r - r_0)$. That is: $J_0 = \alpha, J = \beta\sqrt{\sigma}$.

The free energy of the system can be obtained using replica approach (see, e.g., [23]). In the replica-symmetric (RS) approximation we have [17]:

$$F = -NkT\left\{ -\left(\frac{J_0}{kT}\right) \frac{m^2}{2} + t^2q^2/4 - t^2p^2/4 + \int_{-\infty}^{\infty} dz \sqrt{\frac{2}{\pi\sigma}} \exp\left[-\frac{z^2}{2}\right] \ln \text{Tr} \left[ \exp \left( \hat{\theta} \right) \right] \right\},$$

(24)

where the trace in this case is defined as follows: $\text{Tr}(\ldots) \equiv \int_0^{2\pi} d\varphi \int_0^\pi d\cos(\theta)(\ldots)$. Here $t = \tilde{J}/k_BT$ and

$$\hat{\theta} = \left[zt\sqrt{q} + m \left(\frac{J_0}{kT}\right)\right] \hat{U} + t^2\frac{p - q}{2} \hat{U}^2.$$

The order parameters are: $m$ is the regular order parameter (an analog of magnetic moment in spin glasses), $q$ is the glass order parameter and $p$ is an auxiliary order parameter. The extremum conditions for the free energy (24) give the following equations for these order parameters:

$$m = \langle \hat{U} \rangle, \quad p = \langle \hat{U}^2 \rangle, \quad q = \langle \hat{U} \rangle^2,$$

(25)

where $\langle \ldots \rangle = \text{Tr}(\ldots e^{\hat{\theta}})/\text{Tr}e^{\hat{\theta}}$ and $\langle \ldots \rangle = \int_{-\infty}^{\infty} \sqrt{\frac{2}{\pi\sigma}} \exp\left[-\frac{z^2}{2}\right][\ldots]$. We find from these equations the temperature dependence of the order parameters. The RS solution is stable unless the replicon mode energy $\lambda_{\text{repl}}$ is nonzero [18, 17]. For our model we have

$$\lambda_{\text{repl}} = 1 - t^2 \langle \langle \hat{U}^2 \rangle \rangle^2,$$

(26)

where $\langle \langle \ldots \rangle \rangle$ denotes the irreducible correlator. We find the temperature $T_{g_{\text{A-T}}}$ that corresponds to $\lambda_{\text{repl}} = 0$. To obtain the actual glass transition temperature one has to study the dynamics of the system. In this paper we limit ourselves by the static approach. As is usually believed [19, 20] and correctly shown in [21] the dynamical $T_g$ can be obtained in the frame of the static approach as the temperature $T_m$ of the marginal instability of the one-step RS breaking solution. We have calculated $T_m$ and found that within the accuracy of calculations $T_m$ and $T_{g_{\text{A-T}}}$ coincide. We expect that as in spin glasses below $T_{g_{\text{A-T}}}$ the liquid dynamics is characterized by long relaxation times and other phenomena characteristic to glass transitions. So there is the glass transition in the simple cube case with $T_{g_{\text{A-T}}} \approx 0.39$; in the other cases, icosahedron and cube, there is no glass transition but just a first order transition to BOO state at temperatures about 0.45, 0.42 correspondingly at $\rho\sigma^3 = 0.973$. The last two temperatures of BOO transitions are in agreement with the results of molecular dynamics simulations of Ref. [22]. It should be noted that all these temperatures are well below the melting temperature $T = 0.703$ at this density [22, 15].

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References

[1] V.V. Brazhkin, S.V. Buldyrev, V.N. Ryzhov, and H. E. Stanley [eds], New Kinds of Phase Transitions: Transformations in Disordered Substances [Proc. NATO Advanced Research Workshop, Volga River] (Kluwer, Dordrecht), 2002.
[2] O. Mishima and H. E. Stanley, Nature 396, 329 (1998).
[3] V. N. Ryzhov and E. E. Tareyeva, Phys. Lett. A 75, 88 (1979).
[4] V. N. Ryzhov and E. E. Tareyeva, Theor. Math. Phys. 73, 463 (1987); J. Phys. C: Solid State Phys. 21,819 (1988). Phys. Rev. B 51,8789 (1995); JETP 81, 1115 (1995).
[5] E.E. Tareyeva and V.N. Ryzhov, Particles & Nuclei 31, part 7B, 184 (2000).
[6] N.M. Chchelkatchev, V.N.Ryzhov, T.I.Schelkacheva, E.E.Tareyeva, Phys.Lett. A 329, 244 (2004).
[7] W. R. Smith and W. Henderson, Mol. Phys. 19, 411 (1970).
[8] J.A. Barker and D. Henderson, Rev. Mod. Phys. 48, 587 (1976).
[9] N.N.Bogoliubov, Problems of dynamical theory in statistical physics (Moscou, Gostehisdat, 1946).
[10] T.V.Ramakrishnan, M.Youssouff, Phys. Rev. B 19, 2775 (1979); A. D. J. Haymet and D. W. Oxtoby, J. Chem. Phys. 74, 2559 (1981).
[11] Y. Singh, Phys. Rep. 207, 351 (1991); M. Baus, J. Phys.: Condens. Matter 1, 3131 (1989); H. Löwen, Phys.Rep. 237, 249 (1994).
[12] N.N.Bogoliubov, JINR Preprint R-1451, Dubna, 1963; Phys.Abh.S.U., 6, 1, 113, 229 (1962).
[13] D.R. Nelson and B.I. Halperin, Phys. Rev. B 19, 2457 (1979).
[14] A.D.J. Haymet, Phys. Rev. B 27, 1725 (1983).
[15] D.R. Nelson, “Defects and geometry in condensed matter physics”, Cambridge University Press, 2002.
[16] C.J. Bradley, A.P. Cracnell, The mathematical theory of symmetry in solids, (Clarendon, Oxford), 1972.
[17] N.V. Gribova, V.N. Ryzhov, T.I. Schelkacheva, E.E. Tareyeva. Phys. Letters A, 315, 467 (2003).
[18] J.R.L. Almeida and D.J. Thouless, J.Phys. A: Math. Gen. 11, 983 (1978).
[19] L.F. Cugliandolo, Dynamics of glassy systems, arXiv: cond-mat/0210312.
[20] T.R. Kirkpatrick and D. Thirumalai, Phys. Rev. Lett. 58, 2091 (1987).
[21] A. Baldassari, L.F. Cugliandolo, J. Kurchan, and G. Parisi, J. Phys. A: Math. Gen. 28, 1831 (1995).
[22] P.J. Steinhardt, D.R. Nelson, and M. Ronchetti, Phys. Rev. B 28, 784 (1983).
[23] D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. 32, 1972 (1975); S. Kirkpatrick, D. Sherrington, Phys. Rev. B17, 4384 (1978).