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Dynamical heterogeneity in terms of gauge theory of glass transition

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HIGHLIGHTS

- We develop the gauge theory of glass transition (GTGT).
- GTGT is applied to describe the dynamic heterogeneity in supercooled liquid.
- The dynamic susceptibility time dependence near the glass transition is obtained.
- The dynamic heterogeneity is driven by two types of relaxation process.

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ABSTRACT

In this paper the phenomenon of dynamic heterogeneity in supercooled liquid systems is considered in terms of the recently proposed gauge theory of glass transition. The physical interpretation of the dynamic scaling is considered. It is shown that the development of the dynamic heterogeneity occurs due to the growth areas in which molecular motion is correlated due to the elastic interaction described by the gauge field. We obtain the analytical expressions for the dependence of the number of dynamically correlated atoms as the function on the system relaxation time, and the time dependence of the dynamic susceptibility near the glass transition. It is shown that the relaxation consists of two processes: α-relaxation process corresponding to the joint motion of the domains disordered with each other, and β-relaxation process corresponding to the motion inside these domains.

1. Introduction

The problem of the theoretical description of the liquid–glass transition is still puzzling theorists. On one hand, this transition has distinctive features of phase transition, such as critical slowing of the system, peak in the temperature dependence of susceptibility, and abrupt change of the heat capacity near the transition. On the other hand, the nonequilibrium dynamics of the process determines the physical properties of the glass system to a considerable degree. For example, it leads to the dependence of the glass transition temperature on the cooling rate. The presence of these features suggests that the theory, which aspires to the full description of the liquid–glass transition, should combine both methods for describing the dynamics of nonequilibrium systems and the elements of the quasi-equilibrium theory of phase transitions. This concept has been implemented in a recently proposed gauge theory of glass transition (GTGT) [1]. The theory is based on the gauge approaches to glass description, which were offered at the end of the last century, [2–8], and is close ideologically to the theory of glass transition by Kivelson [9]. At first sight this theory seems difficult because of the necessity to use the

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field-theoretic technique of gauge fields. However, the results of this theory reveal fairly clear physical mechanisms of the glass transition, and allow us to clearly interpret virtually all experimentally observed properties of the glass transition.

GTGT is based on the methods of non-equilibrium dynamics, which provides a natural way to take into account the dynamic properties of the nonequilibrium vitrescent system. Therefore, it is possible to expect that this theory will allow us to move forward and describe dynamics of the glass transition. However, as of now not all features of the dynamics of glass-forming systems have been described by this theory. In particular, the phenomenon of the dynamic heterogeneity of the supercooled liquids has been scarcely described. The dynamic heterogeneity is difficult to detect by direct experimental methods. It was discovered recently in computer modeling of the glass forming liquids and became one of the most popular topics of discussion among experts in this field. This interest is explained by the fact that the dynamic heterogeneity is considered as the expression of the fundamental mechanisms of the glass transition. Therefore, any adequate theory of glass transition should explain this phenomenon. The purpose of this paper is to discuss the phenomenon of dynamic heterogeneity in terms of GTGT.

2. Model formulation

Following propositions underlie GTGT: 1. It is assumed that the system is in the fluctuation region near the proposed second order phase transition, i.e. fluctuations, which represent spontaneously occurring and collapsing ordered regions, exist and amplify in the system; 2. It is assumed that the system is frustrated. The frustration, on the contrary, blocks the growth of the above-mentioned fluctuations. As shown earlier, the imposition of these conditions results in the freezing of the system in a disordered non-ergodic "solid" state, i.e. in the glass state [1,10].

Because we believe that at a certain temperature T_c in the system without frustration the second order phase transition must occur, we describe the state of the "clean" system using the well-known Hamiltonian of the Ginzburg–Landau theory:

$$\mathcal{H}_0 = \frac{1}{2}\int\left[(\partial_i\mathbf{Q})^2 + \mathbf{Q}^2\left(\mu^2 + \frac{1}{2}v\mathbf{Q}^2\right)\right]\mathrm{d}\mathbf{r}, \tag{1}$$

where $\mathrm{d}\mathbf{r}$ denotes the volume integration, $\mathrm{d}\mathbf{r} = \mathrm{d}r_x\mathrm{d}r_y\mathrm{d}r_z$, $\mu^2 = \alpha(T - T_c)$, α, and v is the system parameter. In the general case one can represent tensor $\mathbf{Q}$ as a position-dependent orthonormal triad of unit vectors $\mathbf{Q}(\mathbf{r}) = [\vec{Q}_1(\mathbf{r}),\ \vec{Q}_2(\mathbf{r}),\ \vec{Q}_3(\mathbf{r})]$ [6], which is associated with the given local ordered structure, for example, with an icosahedron [6].

The differentia of the glasses is the frustration. The frustration availability implies invariance of the system Hamiltonian with respect to local transformations, although this is not enough for the frustration of the system yet. An illustrative example is demonstrated in Fig. 1, which shows the geometrical frustration, characteristic of the dense packing of the particles with a spherically symmetric interaction potential. In this case the local ordered state corresponds to tetrahedral packing, therefore the tensor of the local orientational order parameter is invariant with respect to the local rotations of the icosahedron symmetry group, $Y \subset \mathrm{O}(3)$. It turns out that the Hamiltonian (1) is not invariant under such transformation, the derivative in first term hampers this. Therefore, in order to keep the gauge invariance of the continuous model, one has to move from the ordinary differentiation with respect to the spatial coordinates to the covariant differentiation: $\partial_i Q_{lk} \to D_i Q_{lk} = \partial_i Q_{lk} + g\varepsilon_{iab}A_{la}Q_{kb}$, where ε_{iab} is the rotation matrices, g is the topological charge, and A_{la} is the gauge field which controls the rotations of $\mathbf{Q}$ in space. If $y(\mathbf{r})$ is the matrices of the symmetry group Y, $\mathbf{Q}(\mathbf{r}) \to y(\mathbf{r})\mathbf{Q}(\mathbf{r})$, then $\varepsilon_{iab}A_{la}(\mathbf{r}) = \mathbf{A}(\mathbf{r}) = y(\mathbf{r})\mathbf{A}(\mathbf{r})y^{-1}(\mathbf{r}) - (\nabla y(\mathbf{r}))y^{-1}(\mathbf{r})$. In this case the Hamiltonian has the following gauge symmetric form [8,10,11]:

$$\mathcal{H}_0 \to \mathcal{H}_{sym} = \frac{1}{2}\int\left[(\vec{D}\mathbf{Q})^2 + \mu^2\left(\mathbf{Q}^2 + \frac{1}{2}v\mathbf{Q}^4\right) + \frac{1}{2}\mathbf{F}^2\right]\mathrm{d}\mathbf{r},$$

where $F_{a\mu\nu} = \partial_\mu A_{a\nu} - \partial_\nu A_{a\mu} + g\varepsilon_{abc}A_{b\mu}A_{c\nu}$. It is well known that the problem of the minimization of this Hamiltonian has got the singular solutions (vortexes) which correspond to the disclinations in the ordered atomic structure. The presence of these disclinations destroys the gauge invariance and can be described with sources $\mathbf{J}$ of the gauge field ($\mathcal{H}_{sym} \to \mathcal{H}'$):

$$\mathcal{H}' = \frac{1}{2}\int\left[(\vec{D}\mathbf{Q})^2 + \mu^2\left(\mathbf{Q}^2 + \frac{1}{2}v\mathbf{Q}^4\right) + \frac{1}{2}\mathbf{F}^2 + \mathbf{JA}\right]\mathrm{d}\mathbf{r}, \tag{2}$$

where $E_{cor} = \int \mathbf{JA}\mathrm{d}\mathbf{r}$ is the total energy of the disclinations cores. This value should be minimal for an equilibrium system, therefore $E_{cor} \to 0$ for the ideal systems with order parameter tensor having a crystallographic symmetry. $E_{cor} \neq 0$ in the case of systems contaminated by impurities. Also $E_{cor} \neq 0$ when space cannot be continually filled by the atomic structure with given symmetry of the order parameter tensor because of the topological reasons. In these cases the disclinations are always present in the structure.

As it was noted above, the availability of the gauge symmetry is not enough for the frustration of the system. The system is not frustrated until the gauge field is a smooth function. Frustration corresponds to the presence a singularity of the gauge field, i.e. its source, which presents as the disclination in the atomic structure. The disclinations disorder the structure, and, in general, are mobile when the system is in the liquid state. According to N. Rivier's arguments [5,7] it is natural to assume that at $T > T_c$, when the system is in the equilibrium liquid phase, the subsystem of the vortices is also in thermal equilibrium,