Gauge theory approach to glass transition

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Abstract. This approach combines the gauge field theory of spin-glasses [1, 2, 3, 4] with the critical dynamics methods in order to describe the glass transition. The glass transition is regarded as a phase transition, which is interrupted because of premature critical slowing down, caused by the frustrations. The frustrations induce sources of the gauge field which are additional to the thermal activated spin vortexes. Interaction of this field with the order parameter field leads to the system’s critical slowing at the glass transition temperature, and to the freezing of disordered structure.

1. Introduction
The formulation of the microscopic glass transition theory has remained one of the most intriguing but still unresolved problems of condensed matter physics for a long time. Many systems which manifest this phenomenon regardless of their nature enable us to conclude that this phenomenon does not depend on any microscopic details, but is determined by the symmetry properties of the systems, as in the case of phase transitions. On the other hand this universality allows to conclude that the glass transition is only the result of general dynamical properties of condensed matter. Therefore, the question “Is the glass transition a phase transition, or it is the dynamic effect related with limited diffusion dynamics?” remains to be actual. We have tried to conciliate these positions using the gauge theory technique and critical dynamics.

The key problem of the “phase transition”-like theories is the problem of “order parameter”, $s(\vec{r})$, since the existence criterion of phase transition, $\langle s(0)s(\vec{r})\rangle_{|\vec{r}|=\infty} \neq 0$, does not work in the disordered amorphous phase. The main problem of the “dynamical” glass transition theories is the description of dynamical transition from the ergodic state to the non-ergodic state of the system and physical interpretation of this transition. The first problem can be solved introducing additional degrees of freedom by means of gauge field, which describes the elastic stresses induced by frustrations. Below it will be shown that the glass transition corresponds to the critical point in the gauge field subsystem. The dynamical features of this transition, such as the Vogel-Fulcher-Tamman temperature dependence of the relaxation time and the plateau on the time dependence of the order parameter correlation function, can be revealed by means of functional methods of non-equilibrium dynamics.

2. Two conditions for glass transition
We are of opinion that necessary condition of glass transition is the presence of a thermodynamic phase transition in near region of temperatures. Certainly, it is a virtual phase transition, which is caused by a local ordering but can not occur because of some causes. In case of spin systems...
it could be the paramagnetic to ferromagnetic transition, which is locked by quenched disorder. In the system of atoms it is a virtual phase transition induced by a local ordering to the state with a non-Fedorov crystal group. In this case a full-fledged thermodynamic phase transition is not possible, because all space can not be mapped by the cells with non-Fedorov symmetry.

Another condition for the glass transition is the presence of frustrations in the system. In the first case the frustrations are quenched and sessile because of quenched disorder. In the second case the frustrations are geometrical. They differ from the quenched frustrations because they are movable topological defects (disclinations). In both cases the frustrations depress the phase transition dynamically, and don’t allow system to reach of the long-range ordered state.

3. Model

In more detail the example of the three-dimensional Heisenberg spin-glass model, whose order parameter, \( s \), is considered to be a local magnetization vector with the SO(3) continuous symmetry group, was considered in [5, 6]. One of most elegant method of description of the frustrated systems is given by gauge theory [1, 2, 3, 4]. The static action of a system close to the second order phase transition in general case has the form of

\[
S = \int \left[ \frac{1}{2} (\partial_i s)^2 + U(s) \right] \, dr, \tag{1}
\]

where \( s \) is the some order parameter field, and \( U(s) = \mu^2 s^2 + vs^4 \). The structure of vitreous systems is inhomogeneous in relative orientation of local ordering elements and in density. Congruent connections between the orientations are introduced by means of a gauge field, \( A_\mu^a \)

when ordinary derivative, \( \partial_i s \), is replaced by the covariant derivative, \( D_i s \):

\[
\partial_i s^a \rightarrow D_i s^a = \partial_i s^a + g \varepsilon^{abc} A_i^b s^c. \tag{2}
\]

Besides, the system’s action should contain the term \( \sim (D_i A_\mu^a)^2 \), since we suppose that \( A_\mu^a \) is a continuous function. Therefore, one gets the gauge-symmetric action:

\[
S = \int \left[ \frac{1}{2} (D_i s)^2 + U(s) + \frac{1}{4} F_{\mu \nu} F^{\mu \nu} \right] \, dr, \quad \text{where} \quad F_{\mu \nu} = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g \varepsilon^{abc} A_\mu^b A_\nu^c. \tag{3}
\]

Expansion of the local magnetization field, \( s \), near one of the vacuum states, for instance \( s_0 = (0, 0, i\mu/\sqrt{2v}) \), in small \( \phi = s - i\mu/\sqrt{2v} \) deviations, and use of the gauge transformation properties allow to rewrite the action (3) in the form of the functional of two massive vector bosons, \( A_\mu^\kappa \) \((\kappa = \{1, 2\})\), with the mass \( M_0 = i\mu/\sqrt{2v} \), one massless vector boson, \( A_5^a \), and one scalar field, \( \phi \).

The method of introduction of disorder in the theory is very important and plays a key part. One of the important features of the above model (3) is the existence of soliton solutions, which correspond to the vortexes system. These thermally activated vortexes disordering the spin structure. They are the movable sources of the gauge field, and their system above the glass transition temperature can be considered as a system which remains in thermal equilibrium [3]. But in \( T > T_c \) the gauge field becomes massless and the vortexes vanish. Therefore, in order that a system possess glass properties at \( T < T_c \) we should inject to this system a disorder which gives rise to frustration of its structure at \( T < T_c \). It seems evident that gauge field should be treated as a dynamical one, and full gauge invariance or homogeneity maintained as much as possible. In this case only the sources of gauge fields need be quenched in glass [4]. At \( T > T_c \) these sources are additional to the thermally activated vortexes but as opposed to them do not vanish in the low-temperature state. They can be introduced into the model by means of the sources field, \( J_{\alpha \mu} \):

\[
S = \int \left[ \frac{1}{2} (\partial_\mu \phi)^2 + 2 \mu^2 \phi^2 + \frac{\mu^2}{4v} A_\mu^a A^a_\mu + \frac{1}{4} F_{\mu \nu} F^{\mu \nu} + v \phi^4 + \frac{\mu^2}{2} \phi^2 A_\mu^a A^a_\mu + J_{\alpha \mu} A^a_\mu \right] \, dr. \tag{4}
\]
Since above the $T_c$ the source subsystem is believed to be in thermal equilibrium [3]. Averaging over $J^a_\mu$ leads to redefinition of the partition function:

$$ Z = \int \left[ \int \exp \left( -S - \frac{1}{4} \int I_0^{-1} J^a_\mu^2 d\mathbf{r} \right) D\phi D\mathbf{A}^a_\mu \right], $$ (5)

where $\int \ldots Dx$ is the continual integral. It leads to additional contribution to the $A^a_\mu$ “mass”, which takes the form of

$$ M^2 = -I_0 + \mu^2 g^2 / 4v. $$ (6)

Thus, the frustrations lead to the renormalization of the gauge field mass.

The renormalization of the gauge field mass affects the critical behavior of the system, since it shifts $M^2 = 0$ singularity to the temperature range above the virtual phase transition point, $T_c$. If we assume that $\mu^2 = \alpha k_B (T - T_c)$, where $\alpha$ is some constant, then from (6) we have the critical divergence of the $A^a_\mu$ field correlation radius at $T_g = T_c + 4I_0v/\alpha k_B g^2$ in the disordered solid phase. In [6] it was shown that this leads to critical slowing-downs of the fluctuations. Thus, the disorder-induced frustrations inhibit the growth of the $\phi$ field correlation length, and the system freezes in a disordered state.

4. Analysis of the static spin-glass model

In $T_g$ the gauge field becomes massless, whereas the local magnetization field still has got the “mass”, $\mu$. Analysis of the model close to this point allows to assert that $T_g$ is the nothing else than the glass transition temperature. First of all it is evident from (4) that the linear susceptibility, $\chi_L = \partial \langle \phi \rangle / \partial h \sim \mu^2 = g^2 / 4I_0v$ ($h$ is an external source of the field $\phi$), is finite at $T = T_g$. Similar unsophisticated estimation gives that the correlation length, $r_{cor} \sim \sqrt{g^2 / 4I_0v}$, is finite too. However, nonlinear susceptibility, $\chi_N = \partial^3 \langle \phi \rangle / \partial h^3 = \langle \phi^4 \rangle$ [7] (fig. 1 a), diverges near $T_g$, because of the divergence of the $A$-field loop contribution (fig. 2). This picture is typical for the glass transition.

Using this theory allows us to determine the temperature dependence of the system heat capacity at $T \rightarrow T_g^+$. $c_p = dU / dT \propto (T - T_g)^{-1/2}$. One can see (fig. 2), that the obtained temperature dependence of the heat capacity near $T_g$ diverges and is not characteristic for glass transition. One can show that this is a result of only the static character of the theory. Below the analysis of the critical dynamics of this system close to $T_g$ allows to make sure in it, and to show that $T_g$ is the glass transition temperature.

5. Analysis of the dynamic spin-glass model

In order to check the another glass transition properties of the model, one can examine the non-equilibrium dynamics of the system near to $T_g$ by means of functional methods of non-equilibrium dynamics [8] near the critical point. It leads to the representation of the partition
Figure 2. The qualitative presentation of the temperature function of the nonlinear susceptibility, \( \chi_N \propto 1/(T - T_g) \gamma \), and linear susceptibility, \( \chi_L \propto 1/(T - T_c) \). The \( \chi_L \) curve is not described by this theory at \( T < T_g \), it is finite in this region. The qualitative picture of the temperature dependence of the heat capacity near \( T_g \), which is obtained from the theory.

function of the system in the form of

\[
Z = \int \exp(-S^*) D\vec{\phi} D\vec{A}_\mu,
\]

with

\[
S^* = \frac{1}{2} \int \left[ \vec{\phi}(t, \mathbf{r}) \mathbf{G}^{-1}(t - t', \mathbf{r} - \mathbf{r}') \vec{\phi}(t', \mathbf{r}') + \vec{A}_\mu^a(t, \mathbf{r}) \mathbf{\Delta}^{-1}_{\mu\nu}(t - t', \mathbf{r} - \mathbf{r}') \vec{A}_\nu^a(t', \mathbf{r}') \right] d\mathbf{r} d\mathbf{r}' dt dt' + \int \left[ g_{\varepsilon}^{abc} (\partial_\mu \vec{A}_\nu^a) A_\mu^b A_\nu^c + g_{\varepsilon}^{abc} (\partial_\mu \vec{A}_\mu^a) \vec{A}_\nu^a \vec{A}_\nu^c + g_{\varepsilon}^{abc} (\partial_\mu \vec{A}_\mu^a) \vec{A}_\nu^a \vec{A}_\nu^c + g_{\varepsilon}^{abc} (\partial_\mu \vec{A}_\mu^a) \vec{A}_\nu^a \vec{A}_\nu^c \right] d\mathbf{r} dt,
\]

where \( \vec{\phi} = \{ \vec{\phi}, \phi \} \), and \( \vec{A}_\mu^a = \{ \vec{A}_\mu^a, A_\mu^a \} \) are vectors, the components of which are named “quantum” and “classical” respectively in the Keldysh representation [8]. \( G^{-1} \) and \( \Delta_{\mu\nu}^{-1} \) are matrices, inverse to the Green functions matrices having the following form:

\[
G = \begin{pmatrix} G^K & G^A \\ G^R & 0 \end{pmatrix}, \quad \Delta_{\mu\nu} = \begin{pmatrix} \Delta^K_{\mu\nu} & \Delta^A_{\mu\nu} \\ \Delta^R_{\mu\nu} & 0 \end{pmatrix},
\]

where

\[
G^{R(A)}(k, \omega) = \frac{1}{k^2 + \mu^2 \pm i\Gamma_\phi \omega}, \quad G^K(k, \omega) = \frac{2\Gamma_\phi}{(k^2 + \mu^2)^2 + \Gamma_\phi^2 \omega^2},
\]
Γ_ ϕ is the kinetic coefficient of the local magnetization,

\[
\Delta_{\mu\nu}^{R(A)}(k, \omega) = \frac{\delta_{\mu\nu}}{k^2 + M^2 \pm i \Gamma_A \omega}, \quad \Delta_{\mu\nu}^{K}(k, \omega) = \frac{2\Gamma_A \delta_{\mu\nu}}{(k^2 + M^2)^2 + \Gamma_A^2 \omega^2},
\]

(11)

Γ_A is the kinetic coefficient of the gauge field.

**Figure 3.** The dependence ⟨ϕϕ⟩_t on ln(t): a) is the contribution of ⟨ϕϕ⟩_0, which is the Debye-relaxation; b) is the contribution of the second term which is given by the cooperative effects; c) is the sum of first and second terms.

The renormalization group analysis of the dynamical model shows that the theory becomes not renormalizable on small time scales, \( t \ll \Gamma_\phi g^2 / 4I_0 v \) [6]. On these scales the fluctuation-dissipation theorem is broken, and one can interpret this as appearing of the dynamical heterogeneity where \( \Gamma_\phi g^2 / 4I_0 v \) is the characteristic scale of time homogeneity. Subject to this heterogeneity one can estimate the temperature dependence of the relaxation time [6]:

\[
\tau_{rel} = \Gamma_\phi \propto \exp \left( \frac{2v g^2 T_g}{\alpha \pi^2 (T - T_g)} \right),
\]

(12)

which corresponds to the well known Vogel-Fulcher-Tammann law. Besides, in the one-loop approximation the ϕ-field correlation function can be represented as the sum of the unperturbed and cooperative parts:

\[
\langle \phi\phi \rangle_t \simeq G^K(t) + \frac{g^4 \mu^2 \ln(L/a_0)}{\Gamma_\phi \pi^2} \int_0^t G^K(t_1) e^{-4I_0 v |t-t_1| / \Gamma_\phi g^2} dt_1.
\]

(13)

This function has the form which is characteristic for glass systems (fig.3) and gives the Edwards-Anderson parameter value in static limit when \( T = T_g \).

One can obtain the qualitative form of the temperature dependence of the heat capacity close to the glass transition:

\[
c_p(T) \propto \frac{\partial}{\partial T} \left[ e^{-CT_g/(T-T_g)} \right] = \frac{e^{-CT_g/(T-T_g)}}{(T - T_g)^{2}} \cdot CT_g,
\]

(14)

where \( C = 2v g^2 / \alpha \pi^2 \). The calculation of heat capacity gives that it has the sharp growth near the glass transition temperature which then drops in \( T_g \), that is characteristic for vitreous
systems. With using the suggested theory it is not difficult to give a simple qualitative explanation of this dependence: At the approaching the system’s temperature to $T_g$, the fluctuations are increase, and consequently, the heat capacity increases too like in the case of second order phase transition; however, the quenched frustrations block this increase over the scales, which exceed some finite scale, which is determined by these frustrations. As a result the heat capacity does not infinitely diverge in $T_g$, but gets a finite maximum in $T_{\text{max}} > T_g$, and then falls (fig. 2).

6. Conclusions
According to the above theory one can offer the following physical picture of the glass transition processes: when the temperature approximates $T_g$, the correlation length of the gauge field diverges, while the correlation length of the order parameter is finite. The infinite correlation of the gauge field means that the relative rotations are correlated at an infinitely large distance. Then the growth of the order parameter field fluctuations becomes impossible, since the spins can not already turn independently of each other. This picture can be described in framework of the quasi-equilibrium static theory as a phase transition in the gauge field subsystem, but very important dynamic features of this transition can be explained only in the dynamic approach.

The statement about that the correlation length of the gauge field grows faster than the correlation length of the order parameter can be explained in the following way: without the frustrations the correlation lengths of both the gauge field and the order parameter field grow equally, because they are components of the same field. In the dual representation the system contains thermally activated vortexes, whose concentration tends to zero when $T \to T^{+}$. The priority growth rate of the correlation length of the gauge field becomes possible when the system contains frustration. The frustration induces vortexes additional to the thermally activated vortexes, as a result in the equilibrium state the vortex concentration is fixed non-zero. The reason for this is that the fluctuations of the gauge field are sure to develop around these sources. In the case of a nonzero concentration of these static sources the fluctuations around them can interflow, which leads to the faster growth of the effective correlation length of the gauge field. With the given source concentration and the appropriate correlation length of the order parameter (or the gauge field without frustrations) it leads to the formation of the percolation cluster which is associated with these sources. Thus, the effective correlation length of the gauge field becomes infinitely large, and the relative rotations at infinitely remote points become correlated and the relaxation time of the system infinitely grows up, but the order parameter correlation length remains to be relatively small. Therefore, the system freezes in a disordered state.

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References
[1] Volovik G E, Dzyaloshinskii I E 1978 Sov. Phys. JETP 48 555
[2] Hertz J A 1978 Phys. Rev. B 18 4875
[3] Rivier N, Duffy D M 1982 J. Physique 43 295
[4] Rivier N 1985 Revista Brasileira de Fisica 15 311
[5] Nusinov Z 2004 Phys. Rev. B 69 014208-1
[6] Vasin M G 2011 J. Stat. Mech. P05009
[7] Binder K, Young A P 1986 Reviews of Modern Physics 58 801
[8] Kamenev A 2005 Nanophysics: Coherence and Transport, edited by H. Bouchiat (Elsevier, Amsterdam)