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Clusters and Short-Range Order in Glasses

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The mean field theory with the replica method for the two-dimensional glasses is proposed. We introduce the order parameter, which identifies the glass phase, by using the topological number of the frozen hedgehog-like soliton based on the gauge-invariant Lagrangian with spontaneous breaking.

1. Introduction

There exists an intriguing development in studies of the structure of liquids and amorphous solids. Based on important ideas by Klemans and Sadoc [1], it has been proposed that the parameter $\rho(r,u)$ in two-dimensional and three-dimensional glasses is specified by rigid-boday rotation, which are related to gauge fields of $SO(3)$ symmetry for S^2 and $SO(4)$ symmetry for S^3, respectively [2-4]. It has been shown by a computer simulation [5] that many anomalous fivefold and sevenfold coordinated disks, which can be viewed as microscopically defined point disclinations are formed in the two-dimensional triangular lattice at high temperature. It is seen that there exist a few dislocation, represented by five fold-seven fold disclination dipoles, even at high temperature.

Because the five fold coodinated disk (the pentagonal disk) is favorable evergetically in comparision with other excited detects, the present author [6-8] stresses that pentagonal disk is one of dominantly exicited solitons in the two-dimensional system at high temperature, and has proposed the theoretical picture for these excited solitons, based on the gauge-invariant Lagrangian with spontaneous breaking.

In the present study, adopting five fold and seven fold coordinated disks as frozen detects, we will propose the mean field theory with the replica method of the two-dimensional glass system and introduce the order parameter, which identifies the glass phase, by using the topological number of the frozen hedgehog-like soliton.

2. A model system for frozen hedgehog-like defects

We will investigate two-dimensional glass by using frozen excited disk, such as the anomalous 5- and 7-coordinated disk. It has been shown that the curvature can be represented by using a component in the other-axis direction, if the two spatial dimensional axes are x and y ones. That is, it is preferable we think of the anomalous disk as the hedgehog-like soliton (defect), taking account of the curvature. We adopt the parameter field $\rho(r,u) \equiv \rho^a$ (a=1, 2, 3), which is similar to that in the Sachdev and Nelson model [4]. It is furthermore assumed that the symmetry of the gauge fields $A_\mu{}^a$, which introduce the curvature of the hedgehog-like soliton, are extended from $SO(3)$ to $SU(2)$.

Now we introduce the Lagrange density as follows,

$$\mathcal{L} = -\frac{1}{4}\left(\partial_\nu A_\mu{}^a - \partial_\mu A_\nu{}^a + g_1 \in_{abc} A_\mu{}^b A_\nu{}^c\right)^2 + \frac{1}{2}\left(\partial_\mu \rho^a - g \in_{abc} A_\mu{}^b \rho^c\right)^2 - \lambda^2 \left(\rho^a \rho^a - v^2\right)^2 . \quad (1)$$

It is thought that the $SU(2)$ triplet fields, $A_\mu{}^a$, are spontaneously broken through the Higgs mechanism similar to the way in which the 6-coordinated symmetry in the triangular lattice is broken around the anomalous 5- and 7-coordinated disks. In other words, in order to introduce the cluster with some radius in this system in the gauge-invariment formula, we must use the Higgs mechanism. If the 5-coordinated disk is formed, we set the symmetry breaking of the triplet field, $\langle 0|\rho^a|0\rangle$, equal to (0, 0, v). On the other hand, if the 7-coordinated disk is formed, we set symmetry breaking, $\langle 0|\rho^a|0\rangle$, equal to (0, 0, $-v$). Then we can introduce the effective Lagrange density:

$$\begin{aligned}\mathcal{L}_{eff} =& -\frac{1}{4}\left(\partial_\nu A_\mu{}^a - \partial_\mu A_\nu{}^a + g_1 \in_{abc} A_\mu{}^b A_\nu{}^c\right)^2 \\ &+ \frac{1}{2}\left(\partial_\mu \rho^a - g \in_{abc} A_\mu{}^b \rho^c\right)^2 \\ &+ \frac{1}{2}m^2\left[\left(A_\mu{}^1\right)^2 + \left(A_\mu{}^2\right)^2\right] \\ &+ m\left[A_\mu{}^1\partial_\mu\rho^2 - A_\mu{}^2\partial_\mu\rho^1\right] \\ &+ gm\left\{\rho^3\left[\left(A_\mu{}^1\right)^2 + \left(A_\mu{}^2\right)^2\right]\right. \\ &\qquad \left. - A_\mu{}^3\left[\rho^1 A_\mu{}^1 + \rho^2 A_\mu{}^2\right]\right\} \\ &- \frac{m_2{}^2}{2}\left(\rho^3\right)^2 - \frac{m_2{}^2}{2m} g\rho^3\left(\rho^a\right)^2 \\ &- \frac{m_2{}^2 g^2}{8m^2}\left(\rho^a\rho^a\right)^2, \end{aligned} \tag{2}$$

where $|m|$ is vg and $|m_2|$ is $2\sqrt{2}\lambda v$. The effective Lagrangian, $\mathcal{L}_{eff}$, represents two massive vector fields, $A_\mu{}^1$ and $A_\mu{}^2$, and one massless vector field, $A_\mu{}^3$. Because these masses are formed through the Higgs mechanism by introducing the 5- and 7-coordinated disks, the gauge fields $A_\mu{}^1$ and $A_\mu{}^2$ are only present around the disks. The inverse, $1/|m|$, of the mass of $A_\mu{}^1$ and $A_\mu{}^2$ reflects the radius of the cluster. Since the $U(1)$ gauge field $A_\mu{}^3$ is massless, it is thought that the gauge field $A_\mu{}^3$ mediates the long-range interaction between two excited disks (the hedgehog-like solitons).

3. The model for two-dimensional metallic glasses

Now we can define the topological number q for excited hedgehog-like solitons as follows,

$$q = \frac{1}{2\pi}\int_\Sigma ds_{\mu\nu}\left(\partial_\mu A_\nu{}^3 - \partial_\nu A_\mu{}^3\right),$$

where Σ is a sphere, whose radius is larger than $1/|m|$. If a sphere Σ surrounds completely one 5-coordinated disk, whose center position is r_i, the value of q_i is $+1$. If a sphere Σ surrounds completely one 7-coordinated disk, whose center position is r_i, the value of q_i is -1. when cooled rapidly through the glass transition, many hedgehog-like solitons are frozen randomly in the two-dimensional system. In this system we can introduce approximately the Hamiltonian as follows,

$$H = \sum_{(ij)} V_{ij} q_i q_j. \tag{3}$$

For the mean-field approximate, it is assumed that V_{ij} describes N hedgehog-like solitons ($q_i = \pm 1$) interaction, which mediated by the massless $A_\mu{}^3$ field, in pairs (ij) via infinite-range Gaussian-random interactions:

$$P(V_{ij}) = \frac{1}{\left(2\pi\langle V_{ij}{}^2\rangle\right)^{1/2}} \exp\left(\frac{-V_{ij}{}^2}{2\langle V_{ij}{}^2\rangle}\right). \tag{4}$$

We ignore the possibility of a mean V_{ij} for simplity of discussion. Here it should be noted that the Hamiltonian in eq. (3) is adequate in the temperature region below the glass transition temperature T_g, because hedgehog-like solitons must be frozen. In this condition, we can evaluate the properties of the two-dimensional metallic glasses from the anology of the Sherrington-Kirkpatrik (SK) formalism [9] by using the replica method [10].

Thus the free energy for one frozen hedgehog-like soliton is represented by using the Hubbard-Stratorovitch transformation as follows,

$$\begin{aligned}\beta f =& -\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{Nn}\left\langle\!\!\left\langle \exp\left(\beta^2\tilde{V}^2 Nn/4\right)\right.\right. \\ &\int\cdots\int\prod_\alpha\sqrt{\frac{N}{2\pi}}dM^\alpha \\ &\int\cdots\int\prod_{(\alpha\beta)}\sqrt{\frac{N}{2\pi}}dQ^{\alpha\beta} \\ &\exp\left(\!\!\left(-N\left[\sum_\alpha\frac{1}{2}(M^\alpha)^2 + \sum_{\alpha\beta}\frac{1}{2}(Q^{\alpha\beta})^2\right.\right.\right. \\ &\left.\left.\left.\left.\left. + \beta\tilde{V}\sum_{\alpha\beta} q_i{}^\alpha q_i{}^\beta Q^{\alpha\beta}\right]\right)\!\!\right) - 1\right\rangle\!\!\right\rangle, \end{aligned} \tag{5}$$

where we set $k_B = 1$, $\beta = 1/T$, and $\tilde{V} = \sqrt{N}\langle V_{ij}\rangle$

which is the Gaussian average of V_{ij} in eq. (4). α and β are replica indices. M^{α} and $Q^{\alpha\beta}$ are integral variables for the Hubbard-Stratorovitch transformation.

Then, we can simplify βf in the method of steepest descent and replica symmetry condition as follows,

$$\beta f = -\frac{1}{4}\left(\beta\tilde{V}\right)^2 (1-G)^2 - \frac{1}{\sqrt{2\pi}} \int e^{-(1/2)z^2} \log\left(z \cosh \beta\tilde{V}\sqrt{G}z\right) dz, \quad (6)$$

where $G \equiv \langle q_i{}^{\alpha} q_i{}^{\beta} \rangle = Q^{\alpha\beta}$, $\langle q_i{}^{\alpha} q_i{}^{\beta} \rangle$ represents the canonical average with weight of $\exp\left(-\beta\tilde{V}\sum_{(\alpha\beta)} q_i{}^{\alpha} q_i{}^{\beta} Q^{\alpha\beta}\right)$. Then we can estimate G self-consistently from $\partial f/\partial G = 0$ as follows,

$$G = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-(1/2)z^2} \tanh^2\left(\beta\tilde{V}\sqrt{G}z\right) dz. \quad (7)$$

In the temperature region below $T_C = \tilde{V}/k_B$, we can obtain the phase of $G \equiv \langle q_i{}^{\alpha} q_i{}^{\beta}\rangle = Q^{\alpha\beta} \neq 0$ and $\langle q_i{}^{\alpha}\rangle = 0$. It is thought that this phase corresponds to the two-dimensional glass.

So far we don't know the relationship between $T_C = \tilde{V}/k_B$ and the glass-formation temperature T_g. If it is assumed that T_C is comparable with T_g, the present theory for the two-dimensional glass is meaningful only in the temperature region of $T < T_C$.

From eq. (6) and (7), we can introduce the temperature linear-like specific heat in the temperature region of $T < T_C$. More exactly we must treat eq. (5) in the replica symmetry breaking condition. We can define the order parameter $\bar{G} \equiv \int_0^1 dx Q(x)$, where $Q(x)$ is Parisi order parameter and is dirived from $Q^{\alpha\beta}$, in Parisi's theoretical formula [11,12]. In the temperature region below $\tilde{V}/k_B$, we got the phase of the order parameter $\bar{G} \neq 0$, which corresponds to the glass phase.

4. Conclusion

The order parameter $G(\bar{G})$ is introduced by using the topological number of the frozen hedgehog-like soliton in the two dimensional system. In the mean field theory with the replica method, the phase of the order parameter $G(\bar{G}) \neq 0$, which corresponds to the glass phase, is obtained in the temperature region below $\tilde{V}/k_B$.

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