Transactions of the Materials Research Society of Japan 25 [4] 983-986 (2000)

Hedgehog-like Clusters and the Glass Transition

I. Kanazawa
Department of Physics, Tokyo Gakugei University, Koganei-shi, Tokyo 184-8501, Japan
FAX: 81-423-297-491, e-mail: kanazawa@u-gakugei.ac.jp

We have proposed the theory of three-dimensional supercooled metallic liquids and glasses, based on the gauge invariant Lagrangian with spontaneous breaking. The mean field theory with the replica method for the three-dimensional glasses is proposed. On the basis of the present theoretical formula, a qualitative picture of the boson peak is discussed.

Key words: cluster, glass transition, soliton, boson peak, replica method

1. INTRODUCTION

Although there are many interesting studies for the dynamics of supercooled liquids and the structural glass transition, a satisfactory theory of the glass transition in supercooled liquid is not yet confirmed so far.

In order to understand the glass transition, we must study the short-range structures of the supercooled liquids and amorphous solids. There exists an important development in studies of the structures of liquids and amorphous solids. Based on important ideas by Kleman and Sadoc [1], it has been proposed that the parameter $\rho(r, u)$ in two-dimensional and three-dimensional metallic glasses is specified by rigid-body rotation, which are related to gauge fields of SO(3) symmetry for S^2 and SO(4) symmetry for S^3, respectively [2-4]. The computer simulation [5] has shown 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. There exist a few dislocations, represented by 5-7 disclination dipoles in this two-dimensional system, even at high temperature.

Because the fivefold coordinated disk (the pentagonal disk) is favorable energetically in comparison with other excited solitons, the present author [6-8] stresses that pentagonal disk is one of dominantly excited 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.

Furthermore, adopting fivefold and sevenfold coordinated disks as the frozen hedgehog-like solitons, we have proposed the mean field theory with the replica method on the two-dimensional glass system [9, 10].

In the present study, we will introduce a theoretical formula based on the gauge invariant Lagrangian with spontaneous breaking, and propose a mean field theory with the replica method for the three-dimensional metallic glass system. On the basis of the present theoretical formula, a qualitative picture of low energy excitation (the boson peak) in glasses and supercooled liquids will be discussed.

2. A MODEL SYSTEM FOR FROZEN HEDGEHOG-LIKE CLUSTERS IN TWO SPATIAL DIMENSIONS

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 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_μ^a, which introduce the curvature of the hedgehog-like soliton, are extended from $SO(3)$ to $SU(2)$. It is thought that the $SU(2)$ triplet fields, A_μ^a, are spotaneously 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-invariant 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:

$$\mathcal{L} = -\frac{1}{4}(\partial_\nu A_\mu^a - \partial_\mu A_\nu^a + g_1 \epsilon_{abc} A_\mu^b A_\nu^c)^2 + \frac{1}{2}(\partial_\mu \rho^a - g\epsilon_{abc} A_\mu^b \rho^c)^2$$

$$
\begin{aligned}
&+\frac{1}{2}m^2\left[(A_\mu^1)^2+(A_\mu^2)^2\right]\\
&+m[A_\mu^1\partial_\mu\rho^2-A_\mu^2\partial_\mu\rho^1]\\
&+gm\left\{\rho^3\left[(A_\mu^1)^2+(A_\mu^2)^2\right]\right.\\
&\quad\left.-A_\mu^3\left[\rho^1A_\mu^1+\rho^2A_\mu^2\right]\right\}\\
&-\frac{m_2^2}{2}(\rho^3)^2-\frac{m_2^2}{2m}g\rho^3(\rho^a)^2\\
&-\frac{m_2^2g^2}{8m^2}(\rho^a\rho^a)^2, \qquad (1)
\end{aligned}
$$

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_μ^1 and A_μ^2, and one massless vector field, A_μ^3. Because these masses are formed through the Higgs mechanism by introducing the 5- and 7-coordimated disk, the gauge fields A_μ^1 and A_μ^2 are only present around the disks. The inverse, $1/|m|$, of the mass of A_μ^1 and A_μ^2 reflects the radius of cluster. Since the $U(1)$ gauge field A_μ^3 is massless, it is thought that the gauge field A_μ^3 mediates the long-range interaction between two excited disks (the hedgehog-like solitons).

3. A MODEL SYSTEM FOR FROZEN HEDGEHOG-LIKE CLUSTERS IN THREE SPATIAL DIMENSIONS

We shall introduce a field-theoretical model to treat three-dimensional liquids and glasses by using excited clusters (solitons). It has been proposed that the parameter $\rho(t,r,u)=\rho(t,x,y,z,u)$ in three-dimensional liquids and glasses is specified by the rotation, which is related to the gauge fields of A_μ^a for SO(4) symmetry for S^3 [4]. It has been required that the curvature can be represented by using a component, u, in the other-axis direction, when the three spatial dimensional axis are x, y and z ones. It is preferable that we think of the anomalous density fluctuation in the three-dimensional liquids as the hedgehog-like fluctuation (cluster), taking account of the curvature. We adopt the parameter $\rho(r,u)\equiv\rho^a \quad (a=1,2,3,4)$, which is similar to that in the Sachdev and Nelson model [4]. The SO(4) quadruplet fields, A_μ^a, are spontaneously broken through the Higgs mechanism similar to the way in which the fluid host is broken around the hedgehog-like fluctuation (cluster) [11]. When the hedgehog-like cluster (soliton) is created, we set the symmetry breaking of the quadruplet fields, $\langle 0|\rho|0\rangle$, equal to $(0,0,0,v_4)$.

Now we introduce approximately the Lagrange density as follows,

$$
\begin{aligned}
\mathcal{L} \;=\; &-\frac{1}{4}\left(\partial_\nu A_\mu^a-\partial_\mu A_\nu^a+g_1\epsilon_{abc}A_\mu^bA_\nu^c\right)^2\\
&+\frac{1}{2}\left(\partial_\mu\rho^\beta-g\epsilon_{\beta\alpha\gamma}A_\mu^\alpha\rho^\gamma\right)^2\\
&+c^2\rho^a\rho^a-\lambda(\rho^a\rho^a)^2 \qquad (2)
\end{aligned}
$$

Then we set the symmetry breaking as follows,

$$\rho^a\to(0,0,0,v_4)+\left(\rho^1,\rho^2,\rho^3,\rho^4\right).$$

Thus we can introduce the effective Lagrange density,

$$
\begin{aligned}
\mathcal{L}_{eff} \;=\; &-\frac{1}{4}\left(\partial_\nu A_\mu^a-\partial_\mu A_\nu^a+g\epsilon_{abc}A_\mu^bA_\nu^c\right)^2\\
&+\frac{1}{2}\left(\partial_\mu\rho^\beta-\epsilon_{\beta\alpha\gamma}A_\mu^\alpha\rho^\gamma\right)^2\\
&+\frac{m_1^2}{2}\left[\left(A_\mu^1\right)^2+\left(A_\mu^2\right)^2+\left(A_\mu^3\right)^2\right]\\
&+m_1\left(A_\mu^1\partial_\mu\rho^2-A_\mu^2\partial_\mu\rho^1\right)\\
&+m_1\left(A_\mu^2\partial_\mu\rho^3-A_\mu^3\partial_\mu\rho^2\right)\\
&+m_1\left(A_\mu^3\partial_\mu\rho^1-A_\mu^1\partial_\mu\rho^3\right)\\
&+g_1m_1\left\{\rho^4\left[\left(A_\mu^1\right)^2+\left(A_\mu^2\right)^2+\left(A_\mu^3\right)^2\right]\right.\\
&\left.-A_\mu^4\left[\rho^1A_\mu^1+\rho^2A_\mu^2+\rho^3A_\mu^3\right]\right\}\\
&-\frac{m_1^2}{2}\left(\rho^4\right)^2-\frac{m_2g}{2m_1}\rho^4\left(\rho^a\right)^2\\
&-\frac{m_2^2g^2}{8m_1^2}\left(\rho^a\rho^a\right)^2 \qquad (3)
\end{aligned}
$$

Where m_1 is $v_4\cdot g$ and m_2 is $2\sqrt{2}\lambda\cdot v_4$.

The effective Lagrange density, $\mathcal{L}_{eff}$, represents three massive vector fields A_μ^1, A_μ^2, and A_μ^3, and one massless vector field A_μ^4. Because these masses are created through the Higgs mechanism by introducing the hedgehog-like clusters (solitons), the gauge fields A_μ^1, A_μ^2, and A_μ^3 are only present around the clusters. The inverse, $1/|m|$, of the mass of A_μ^1, A_μ^2, and A_μ^3 reveals approximately the radius of the clusters.

Since the gauge field A_μ^4 is massless, it is thought that the gauge field A_μ^4 mediates the long-range interaction between two excited clusters (the hodgelike solitons).

4. THE HEDGEHOG-LIKE CLUSTERS AND THE BOSON PEAK

In glasses and amorphous materials, one observes the thermal conductivity plateau at $\sim$ 10K and the low energy broad peak observed in Raman and neutron scattering [12], the so-called boson peak. It is thought that vibrational states responsible for the boson peak contribute also to the thermal conductivity plateau, because the energy range spanned by the plateau covers that for the boson peak spectra, indicating that acoustic excitations must cease to propagate when their wavelength λ reaches the n m range [13]. That is, acoustic modes may cross over to strongly localized modes satisfying the Ioffe-Regel condition. By a computer simulation of a soft sphere glass, it is found that there are (quasi-) localized modes with effective masses ranging from 10 atomic masses upwards, which is much related to the boson peak [14].

In the present theoretical formula, the effective Lagrangian density $\mathcal{L}_{eff}$ in eq. (2) represents certainly three massive vector fields A^1_μ, A^2_μ, and A^3_μ, which are localized within the radius, $\sim 1/|m|$, around the hedgehog-like clusters. Thus it is suggested that the localized gauge fields A^1_μ, A^2_μ, and A^3_μ around the hedgehog-like clusters (solitions) are much related to the (quasi-) localized modes of the boson peak.

It should be noted that localized modes around the hedgehog-like clusters (solitions) are required naturally through the gause invariant condition in the present theory.

5. THE MODEL FOR THREE-DIMENSIONAL METALLIC GLASSES

Now we can define the topological number q for excited hedgehog-like solitions as follows [15],

$$q = \frac{1}{24\pi^2}\int_{S^3} dS_\mu \epsilon_{\mu\nu\alpha\beta} Tr\left[A^4_\mu A^4_\alpha A^4_\beta\right] \quad , \qquad (4)$$

where S^3 is a sphere, whose radius is much larger than $1/|m|$. If a sphere S^3 surrounds completely one hedgehog-like cluster (solition), whose center position is r_i, its topological number is represented as q_i. When the hedgehog-like solition (monopole-like cluster) is located at the position $r_j = (x_j, y_j, z_j)$ and $|r_i - r_j| > 1/|m|$ is assumed, the gauge field $A^4_\mu(r_i, r_j)$ at the position $r_i = (x_i, y_i, z_i)$ is represented as follows [16, 17],

$$A^4_\mu(r_i, r_j) \propto \frac{q_j}{|r_i - r_j|} \quad .$$

Thus the interaction energy V_{ij} between two hedgehog-like solitions at the position r_i and r_j

$$is \propto \frac{q_i \cdot q_j}{|r_i - r_j|} \quad .$$

When the system is cooled rapidly through the glass transition, many hodgehog-like solitions are frozen randomly.

In this system we can introduce approximately the Hamiltonian as follows,

$$H = \sum_{(ij)} V_{ij} \quad .$$

For the mean field approximate, it is assumed that V_{ij} describes n hedgehog-like solitons interaction, which is mediated by the massless A^4_μ field, in pair (i,j) via infinite-range Gaussian-random interaction for simplifying of discussion,

$$P(V_{ij}) = \frac{1}{(2\pi\langle V^2_{ij}\rangle)^{1/2}}\exp\left(\frac{-V^2_{ij}}{2\langle V^2_{ij}\rangle}\right) \quad . \qquad (5)$$

Now we can evaluate the properties of the three-dimensional metallic glasses from the analogy of the analogy of the Sherrington-Kirkpatrik (SK) formalism [18] by using the Hubbard-Stratorovitch transformation as follows,

$$\begin{aligned}\beta f &= -\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{Nn}\left\{\left\{\exp\left(\frac{\beta^2\widetilde{V}^2 Nn}{4}\right)\cdot\right.\right.\\ &\int\cdots\int\prod_\alpha\sqrt{\frac{N}{2\pi}}dM^\alpha\cdot\\ &\int\cdots\int\prod_{(\alpha,\beta)}\sqrt{\frac{N}{2\pi}}dQ^{\alpha\beta}\cdot\\ &\exp\left(\left(-N\left[\sum_\alpha\frac{1}{2}(M^\alpha)^2\right.\right.\right.\\ &+\sum_{\alpha\beta}\frac{1}{2}(Q^{\alpha\beta})^2\\ &\left.\left.\left.\left.\left.+\ \beta\widetilde{V}\sum_{\alpha\beta}q^\alpha_i q^\beta_i Q^{\alpha\beta}\right]\right)\right) - 1\right\}\right\}, \qquad (6)\end{aligned}$$

where we set $k_B = 1$, $\beta = 1/T$, and $\widetilde{V} = \sqrt{N\langle V^2_{ij}\rangle}$ 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 simplity βf in the method of steepest descent and replica symmetry condition as follows,

$$\begin{aligned}\beta f &= -\frac{1}{4}(\beta\widetilde{V})^2(1-G)^2\\ &-\frac{1}{\sqrt{2\pi}}\int\exp\left(-\frac{1}{2}z^2\right)\cdot\\ &\log\left\{z\cosh\beta\widetilde{V}\sqrt{G}z\right\}dz \quad , \qquad (7)\end{aligned}$$

where $G \equiv \langle q^\alpha_i q^\beta_i\rangle = Q^{\alpha\beta}$, $\langle q^\alpha_i q^\beta_i\rangle$ represents the canonical average with weight of

$$\exp\left(-\beta\widetilde{V}\sum_{(\alpha\beta)} q^\alpha_i q^\beta_i Q^{\alpha\beta}\right) \quad .$$

We can estimate G self-consistently from $\partial f/\partial G = 0$ as follows,

$$G = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\left(-\frac{1}{2}z^2\right)\tanh^2(\beta\widetilde{V}\sqrt{G}z)dz \quad . \qquad (8)$$

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

More exactly we must treat this system in the replica symmetry breaking condition. We can define the order parameter $\widetilde{G} \equiv \int_0^1 dx Q(x)$, where $Q(x)$ is Parisi order parameter and is derived from $Q^{\alpha\beta}$, in Parisi's theoretical formula [19, 20]. In the temperature region below $\widetilde{V}/k_B$,we got the phase of the order parameter $G \neq 0$ and $\langle q_i^\alpha \rangle = 0$, which corresponds to the glass phase.

6. CONCLUSION

The order parameter $G(\widetilde{G})$ is introduced by using the topological number of the frozen hodgehog-like soliton in the three-dimensional system. On the basis of the present theoretical formula, a qualitative picture of the boson peak is proposed. In the mean field theory with the replica method, the phase of the order parameter $G(\widetilde{G}) \neq 0$, which corresponds to the glass phase, is obtained in the temperature region below $\tilde{V}/k_B$.

References

[1] M. Kleman and J. F. Sadoc, J. Phys. (Paris) 40, LS67 (1979).

[2] D. R. Nelson, Phys. Rev. Lett. 50 (1983) 982.

[3] J. P. Sethna, Phys. Rev. Lett. 50 (1983) 2198.

[4] S. Sachdev and D. R. Nelson, Phys. Rev. 1332, 1480 (1985).

[5] D. R. Nelson, Phys. Rev. B28 (1983) 5515.

[6] I. Kanazawa, J. Non-Crist. Solids, 150, 271 (1992).

[7] I. Kanazawa, Phys. Lett. A176, 246 (1993).

[8] I. Kanazawa, Physica C 235-240, 2645 (1994).

[9] I. Kanazawa, Prog. Theor. Phys. Suppl, 126, 397 (1997).

[10] I. Kanazawa, Phys. Rev. E, to be published.

[11] I. Kanazawa, Radiat. Phys. Chem, in press.

[12] U. Buchenau, H. M. Zhou, N. Nucker, K. S. Gilroy and W. A. Phillips, Phys. Rev. Lett, 60 (1988) 1368.

[13] J. Graebner, B. Golding and L. C. Allen, Phys. Rev. B34, 5696 (1985).

[14] B. B. Laird and H. R. Schober, Phys. Rev. Lett. 66, 636 (1991).

[15] R. Rajaraman, Soliton and Instantons (Elsevier Science Pub., 1989).

[16] A. M. Polyakov, Gauge Fields and Strings (Harwood Academic Pub., 1987).

[17] E. Fradkin, Field Theories of Condensed Matter Systems (Addison-Wesley, 1991).

[18] D. Sherrington and S. Kirkpatrik, Phys. Rev. Lett. 35, 1792 (1975).

[19] G. Parisi, Phys. Lett. A73, 203 (1979).

[20] B. Daplanter, J. of Phys. A14, 283 (1981).

(Received December 17, 1999; Accepted August 16, 2000)