

# Data in cluster model of molecules

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The term "cluster model of molecules" was proposed by de Gennes. De Gennes pointed out that the key to the glass state theory is to find the spin interaction between two adjacent hard-sphere molecules (HSMs). This interaction has now been discovered as the de Gennes  $n = 0$  cluster-interaction boson (CI-boson), which is the unit length vector making up the interface of the 2D clusters at the bottom of the potential well. All CI-boson-derived 2D cluster data are divided into seven sections: the discovery process of CI-boson, the definition of new concepts, symbols and labeling methods, the cluster-peculation transition at the Kauzmann temperature, the largest 2D cluster at the glass transition, the 20-fold symmetry of CI-boson, the 20 CI-boson interaction maps of each HSM, and closed-loop hop path for each HSM in the soft matrix. All of these are the geometric data of the  $n = 0$  2D spin system inherent to disorder system itself.

## SM 1. Why is five-HSM / five-cluster / five-local field model ?

### (1) Need to build a soft matrix of the largest cluster along one direction from small to large

Molten polyester can transform entangled random macromolecules into structurally stable fully oriented polyester fibers (the glass transition has been complete) at a super-stretch rate of 30,000% within a few milliseconds under super-high-speed spinning conditions. However, under normal spinning speeds, the resulting fibers are not fully oriented and have unstable structures, and it takes hours or even days to complete the glass transition. The super-high-speed spinning line of polyester melt can link the abnormal viscosity of the entangled polymer melt to the super-tensile hydrodynamic mode and the oriented glass transition within a few milliseconds. One possible explanation is that only the largest 2D cluster (soft matrix) can move. There is a plurality of spatially oriented soft matrices in each localized region of the melt. All soft matrices in the supercooled liquid on the molten super-high speed spinning line are facing the same direction. The normal glass transition involves randomly selecting one direction of the soft matrix in each local area. In the super-high-speed spinning of polyester, within a few milliseconds, the temperature of the molten filament dropped from 300 degrees to room temperature and was stretched by more than 30,000%, which indicates that the formation of the soft matrix is independent of temperature and material deformation.

Experimental data on the cooperative orientation activation energy,  $\Delta E_{co} = 2035 (k_B T)$ , of an on-line measurement of polyester under super-high-speed spinning<sup>57</sup> supports this view. In the experiment,  $1/6 \Delta E_{co} = 339 (k_B T)$  is the energy of the glass transition temperature  $T_g$  ( $\approx 339 K \approx 67^\circ C$ ) of polyester. The coefficient  $1/6$  is derived from the ideal random orientation distribution of macromolecules in the melt. This may mean that the average orientation energy of a soft matrix, whether in the melt or in the glass state should be  $k_B T_g$ , independent of system temperature  $T$ .

On the other hand, whether glass state, glass transition, or molten, the average (directionally coupled electron-pair interface excited state) energy of each soft matrix is Hamiltonian  $H = k_B T_g$  emerging in the local domain, but the direction of all soft matrices in the system is random. Therefore, the average energy  $H$  of the system can be expressed by the disorder energy  $k_B T$  whose "molecular scale" reaches the soft matrix scale, that is,  $H = k_B T_g$ .

**(2) The largest cluster (soft matrix) on the 2D  $x$ - $y$  projection plane is oriented along the  $z$ -axis**

Based on (1), it can be reasonably proposed that the molten  $z$ -component chains of the entangled polymer freezes into a  $\pm z$ -axis oriented glassy structure on the  $x$ - $y$  projection plane.

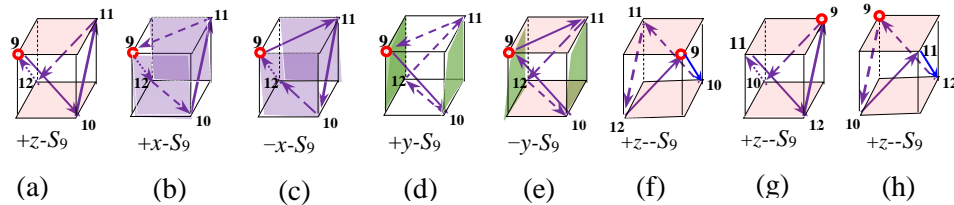
(3) Based on (2), in order to make all HSMs in the 2D lattice oriented along the  $\pm z$ -axis, there must be one or more interface excitation (IE) closed loops on the four sides of each HSM to form a dynamic Ising-spin model, see Fig. 1 and figures S2, S3 and S4.

**(4) The constructed soft matrix must contain about 200 HSMs**

200-HSM is the critical molecular weight of entangled polymer chain obtained through experiments, and requires theoretical support or to verify theory. If it is considered that 200 HSMs are also 200 different spatiotemporal states of a  $z$ -component chain on the molten super-high-speed spinning line, and are statistically equivalent to 200  $z$ -direction chain units on 200 different chains, the projection of these 200  $z$ -direction chain units on the 2D  $x$ - $y$  plane is the largest orientation cluster in the glass state, that is, in the dynamic balance of the generation and disappearance of the soft matrix, the soft matrix must contain an average of 200 HSMs. The five-HSM/five-cluster /five-local field model can meet this requirement. The 3-HSM, 4-HSM or 6-HSM models cannot achieve this goal.

**(5) In order for the local center  $a_0$ -HSM to establish three independent walking 2D soft matrices on the three projection planes in the  $x$ -,  $y$ - and  $z$ -axes, respectively.**

Based on (1), if it is considered that jumping in a certain direction in the glass transition is the largest cluster soft matrix rather than molecules, in order for the molecules to travel randomly in the melt, it must be possible to respectively construct three independently walking 2D soft matrices,  $\pm z$ - $S_9(a_0)$ ,  $\pm x$ - $S_9(a_0)$ ,  $\pm y$ - $S_9(a_0)$ , of  $a_0$ -HSM along the  $\pm z$ -,  $\pm x$ - and  $\pm y$ -axis<sup>14</sup>. The formation of the  $+z$ - $a_0$ -soft matrix is the 9 closed-loop jumps of the positively charged central particle of  $a_0$ -HSM [ $M^+$ - $P(a_0)$ ] choosing a 4-diagonal path in the  $+z$ -direction on the  $2\Delta d$  cubic lattice / equilateral hexahedron. Only five-HSM model can do this, 3-HSM, 4-HSM or 6-HSM models cannot build a micro-cubic lattice in two-HSM clustered collisions. It also shows that there can be three directions of 2D soft matrix potential energy in 3D space, respectively, balanced with thermal disordered kinetic energy  $k_B T_g$ .



**Figure S1.**  $M^+$ - $P(a_0)$  located at the starting point of the 4-diagonal closed loop (small red circle, point 9), selects 3 different closed loop paths among the 4 vertices (4 trap states) of its  $2\Delta d$  cubic lattice to cycle 9 times forming three soft matrices, **a.**  $+z$ - $S_9$ , **b.**  $+x$ - $S_9$ , **d.**  $+y$ - $S_9$ , which walk independently along the  $+z$ -,  $+x$ - and  $+y$  axes, respectively. There are four ways to form the same  $+z$ - $S_9$ , which are **a**, **f**, **g**, and **h**.

**(6) 200-HSM soft matrix can explain geometrical frustration**

Based on (4), there must be a mechanism to interrupt cluster growth. The largest cluster is also controlled by geometrical frustration. A mechanism including geometric frustration must be found to interrupt the cluster growth. Five-local field model can do this.

**(7) Can be linked to the existing concept of fluctuations in molecular number density**

Each interfacial excitation (IE) closed loop corresponds to a "local phase transition" and results in a sudden change in molecular number density.

**(8) A strict definition can be given for the excluded volume between polymer chain units (HSMs)**

The excluded volume of  $a_0$ -HSM is the volume enclosed by  $a_0$ -HSM and its four adjacent HSMs  $4 \times 16$  sequential overlap-collisions of 0.27%, this volume is not occupied by other HSMs. That is, the excluded volume is actually a molecular interface excited spin in the form of a dynamic equilateral hexahedron, bounded by the oriented  $4 \times 16$  coupled electron pair (CEP) IE states.

**(9) Satisfy the clustered fluctuation symmetry in the random system**

In the soft matrix with  $a_0$  as the center,  $a_0$  collides sequentially with its four adjacent molecules,  $b_0, c_0, d_0$  and  $e_0$ , preferentially form  $V_0(a_0)$  cluster. Then, based on the fluctuating symmetry, clusters centered on  $b_0, c_0, d_0$  and  $e_0$  are sequentially formed:  $V_0(b_0), V_0(c_0), V_0(d_0)$  and  $V_0(e_0)$ . After that,  $V_0(a_0)$  sequentially interacts with  $V_0(b_0), V_0(c_0), V_0(d_0)$  and  $V_0(e_0)$  to form  $V_1(a_0)$  cluster... In the five-local field, the fluctuation symmetry of the five soft matrices is self-similar to the fluctuation symmetry of the five clusters in the  $a_0$  soft matrix, see Figure S3. The advantage is that the energy of rearranging  $a_0$ -soft matrix is  $kT_m^\circ = kT_g^\circ + 4\varepsilon_0$ , when  $V_8(b_0), V_8(c_0), V_8(d_0)$  and  $V_8(e_0)$  appear in fluctuations.  $\varepsilon_0$  is the potential well energy.

**SM 2. Interface excited state and interface excited arrow and  $A$ -local area**

An interface excited (IE) state is actually a  $z$ -axial excited state of the coupled electron pair (CEP) between  $a_0$  and one of its adjacent HSMs ( $b_0, c_0, d_0$  and  $e_0$ ). An IE-arrow (CI-boson refers to a vector with a unit interface scale  $(1 + d_L)$  formed by the appearance of 16  $z$ -axial eigenvalues from one end of the interface to the other to form 2D clusters on the  $x-y$  plane. The key is that the  $\lambda$ -th collision-overlapping IE state of two adjacent HSMs can occur repeatedly  $m$  times, and the overlapping relaxation time is  $\tau_i^\circ$  ( $m = i + 1$ ), which means that the two HSMs overlap only in  $\tau_i^\circ$  time and are each in a random state during two adjacent non-overlapping time intervals. This property will have an important influence on the thermodynamics of the glass transition. When  $a_0$  is clustered with  $b_0, c_0, d_0$  and  $e_0$  in turn, a  $z$ -axis dynamic cubic lattice (HSCL) with  $(1 + d_L)$  sides composed of  $4 \times 16$  IE states surrounding  $a_0$  will be formed. The five HSMs are called the zeroth cluster  $+z-V_0(a_0)$  of  $a_0$ -HSM, and these four IE-arrows are marked as the zeroth  $+z-V_0(a_0)$ -loop of  $a_0$ -HSM, and in the theory of de Gennes  $n = 0$ , the  $+z-V_0(a_0)$ -loop can be defined as the  $+z$ -axis spin of IE states surrounding  $a_0$ , denoted as  $+z-S_1(a_0)$  (Figure 1a). Therefore, when the IE-loop around  $a_0$  appears for the  $i$ -th time, the  $+z-V_0(a_0)$  cluster and  $+z-V_0(a_0)$ -loop and  $+z-S_1(a_0)$  with time  $\tau_i$  are respectively marked as  $+z-V_0(a_0, \tau_i), +z-V_0(a_0, \tau_i)$ -loop and  $+z-S_m(a_0), m = i + 1$ .

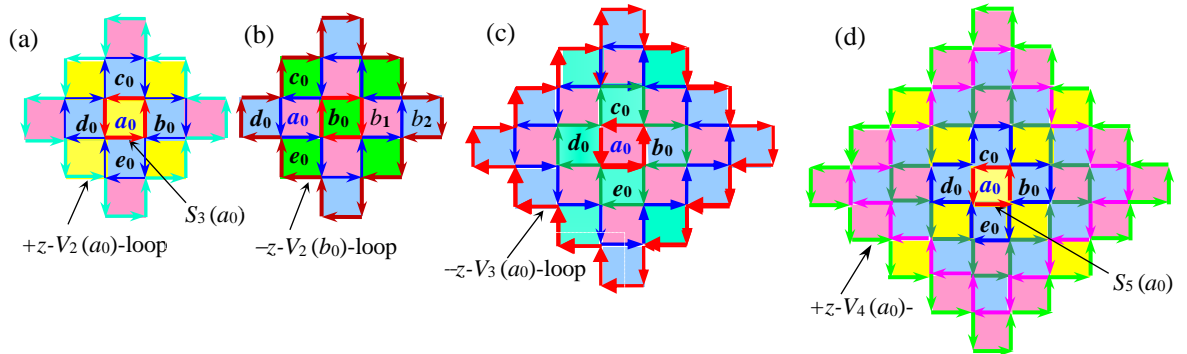
The four adjacent domains of the  $A_0$ -domain,  $B_0$ -,  $C_0$ -,  $D_0$ - and  $E_0$ -domain, all have the same 5-clusters as the  $A_0$ -domain, centered on the  $a_0$ -HSM at the center of the respective domain. For example, in the  $B_0$ -field along the  $\mu_b$ -direction, its five clusters are respectively labeled as  $\mu_b-V_{iB}(a_0), \mu_b-V_{iB}(b_0), \mu_b-V_{iB}(c_0), \mu_b-V_{iB}(d_0)$  and  $\mu_b-V_{iB}(e_0)$ . Note that there are topological connections in the cluster model: The four directions of the four clusters in the  $A_0$ -field,  $\mu_b-V_0(b_0), \mu_c-V_0(c_0), \mu_d-V_0(d_0)$  and  $\mu_e-V_0(e_0)$ , are also the four directions of the four fields,  $B_0$ -,  $C_0$ -,  $D_0$ - and  $E_0$ -field. After averaging five soft matrices with different orientations in 5-local field ( $A_0, B_0, C_0, D_0$  and  $E_0$ ) centered at  $A_0$  of  $a_0$ , the  $z$ -axial  $a_0$ -soft matrix

will contain  $196 + 4$   $\sigma$ -HSMs and five HSCLs "central cavity spaces". The 4  $\sigma$ -HSMs here are the four  $\sigma$ -HSNs in  $V_{0A}(a_1)$  of  $a_1$  on the  $z$ -component chain  $N_z$  in the SM 3.

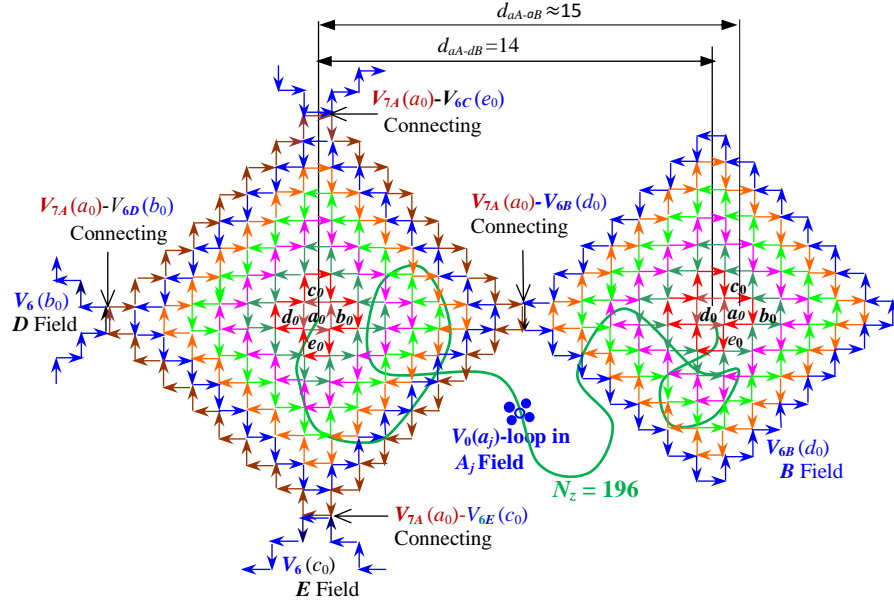
In a referenced  $A_0$ -domain (-field, SM 2), by replica symmetry,  $\mu_b-V_0(b_0)$ ,  $\mu_c-V_0(c_0)$ ,  $\mu_d-V_0(d_0)$  and  $\mu_e-V_0(e_0)$  in four different directions adjacent to  $a_0$  appear in sequence, and project again in sequence to the  $z$ -axial and clustered collide with  $z-V_0(a_0)$  to form a new 2D  $-z-V_1(a_0)$ -cluster [and  $-z-V_1(a_0)$ -loop] and L-J potential  $f_1(\sigma_1/q_1)$ , and  $\sigma_1(a_0)$  has 17  $\sigma$ -HSMs (SM 3). And so on, along the  $q$ -axis of the nine  $z$ -axial L-J potentials, nine 2D  $a_0$ -clusters  $V_i(a_0)$ -cluster, and nine 3D  $a_0$  hard-spheres  $\sigma_i(a_0)$  inverse cascades from small to large, up to the largest 2D  $z-V_8(a_0)$ -cluster (soft matrix).

### SM 3. Clusters and percolation transition and soft matrix

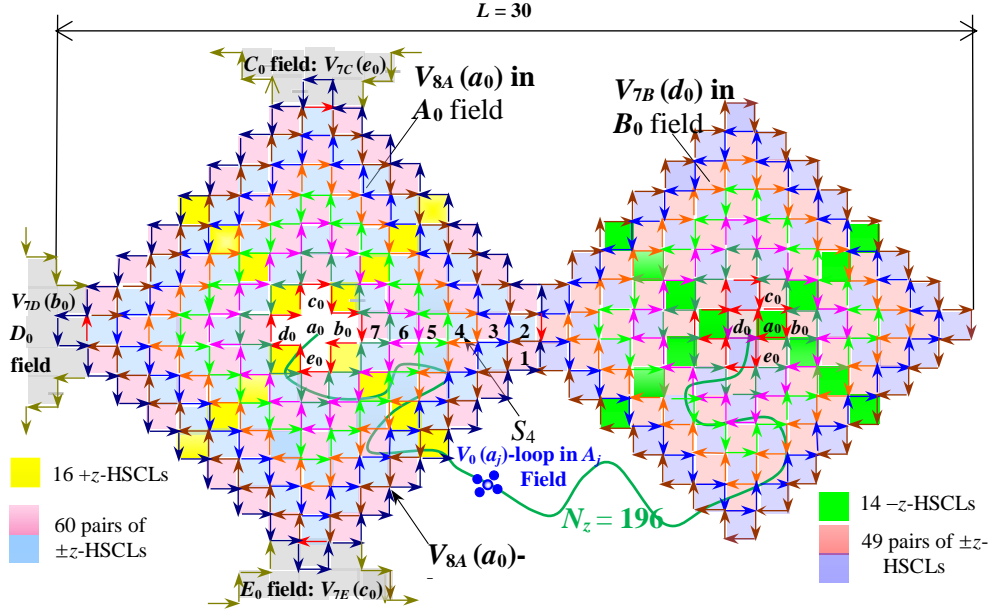
The clustering constant for HSMs:  $\Delta d = 0.05514\dots$ . The "cage" of the HSM is a micro-cubic lattice (equilateral hexahedron) with a side length of  $2\Delta d$ , and the HSM makes 1 to 9 closed-loop jumps along the  $4 \times 16$  singularities on the micro-cubic lattice. Each face of the  $2\Delta d$  micro-cubic lattice in the cluster is an equipotential face, which has a potential energy of  $1/16$  relative to the center of the lattice (the bottom of the potential well). When the  $M^+$ -P of  $a_0$ -HSM starts from point 9 in Fig. 2 along the 4-diagonal closed loop path on the  $2\Delta d$  cubic lattice and returns to point 9, the  $a_0$ -HSM obtains the  $1/16$  potential energy on the  $+z$ -axis, and the  $c_0$ -HSM that circulates synchronously with  $a_0$  obtains the  $1/16$  potential energy on the  $-z$ -axis. Each HSM in the  $V_i$ -loop has a potential energy of  $1/16$  either on the  $+z$ -axis if its IE-loop is along the  $+z$ -axis (marked as  $+z$ -HSM, or  $+z$ -HSCL), or on the  $-z$ -axis if its IE-loop is along the  $-z$ -axis (marked as  $-z$ -HSCL). In Figure. S2, (a) and (b) shows the charge balance between  $V_2(a_0)$  and  $V_2(b_0)$  in the cluster. Dynamic charge balance occurs between 5  $+z$ -HSCLs in  $V_2(a_0)$  and 5  $-z$ -HSCLs in  $V_2(b_0)$ . This property applies to the clustering of all two adjacent clusters.



**Figure S2. Mosaic structure of positive-negative charges in cluster enlargement.** **a.**  $V_2(a_0)$  cluster contains 33 HSMs, 20 of which are edge particles. There are 9  $+z$ -HSNs (red and yellow) and 4  $-z$ -HSNs (blue) in the  $V_2(a_0)$ -loop. After the energy on the  $+z$ -axis and  $-z$ -axis cancel each other out, there are 5  $+z$ -HSNs left (yellow). **b.** There are 5  $-z$ -HSNs left (green) in  $-z-V_2(b_0)$ -loop. **c.**  $V_3(a_0)$  cluster contains 53 HSMs, 28 of which are edge particles. There are 9  $+z$ -HSNs (red) and 16  $-z$ -HSNs (blue and lake green) in the  $V_3(a_0)$ -loop, and there are 7  $-z$ -HSNs left (lake green). **d.**  $V_4(a_0)$  cluster contains 77 HSMs, 36 of which are edge particles. There are 25  $+z$ -HSNs (red and yellow) and 16  $-z$ -HSNs (blue) in the  $V_4(a_0)$ -loop, and there are 9  $+z$ -HSNs left (yellow).

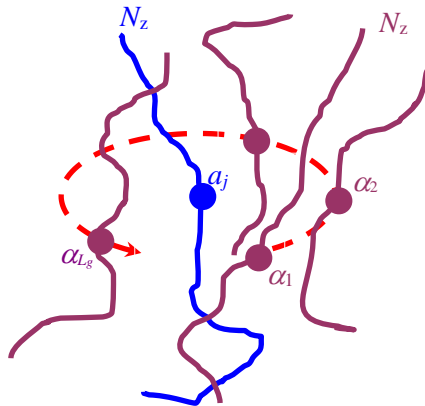


**Figure S3 The image of the percolation transition connected by  $V_{7A}(a_0)$ -loop and  $V_{6B}(d_0)$ -loop.** When  $V_{7A}(a_0)$ -loop appears, the  $V_{7A}(a_0)$ -loop formed by 60 IE arrows is connected to the  $V_{6B}(d_0)$ -loop formed by 52 IE arrows. Two of the IE arrows merge into one arrow at the connected interface and reduce the two edge particles between the two clusters  $V_{7A}(a_0)$  and  $V_{6B}(d_0)$ , thereby reducing the lattice Hamiltonian.  $V_7(a_0)$  cluster contains 173 HSMs, 60 of which are edge particles. There are 64  $-z$ -HSCLs and 49  $+z$ -HSCLs in the  $V_7(a_0)$ -loop, and there are 15  $-z$ -HSMs left.  $V_6(a_0)$  cluster contains 137 HSMs, 52 of which are edge particles. There are 49  $+z$ -HSCLs and 36  $-z$ -HSCLs in the  $V_6(a_0)$ -loop, and there are 13  $+z$ -HSCLs left. The critical length of polymer chain entanglement is 200 HSMs. The 196 HSMs (green curve) in the  $A_j$ -field are represented as  $a_0, a_1, a_2, \dots, a_j, \dots$  and  $a_{195}$ , and the field of the  $a_j$ -th HSM forming the  $a_j$ -soft matrix is denoted as  $A_j$ -field. The other 4 HSMs (blue) out of the 200 HSMs are the four HSMs that form  $+z-V_0(a_j, \tau)$ . Since the background temperature is  $T_k$ ,  $+z-V_0(a_j, \tau)$  is now  $+z-V_0(a_j, \tau)$ . The  $z$ -component chain  $N_z$  is a random chain in  $z$ -space (2D  $x$ - $y$  projection plane) with one end  $a_0$  is located at  $a_0$  in the  $A_0$ -field (domain), and the other end  $a_{195}$  is located at  $d_0$  in the  $B_0$ -field. Due to random distribution,  $196 = 14^2 = (d_{aA-dB})^2$ ,  $d_{aA-dB}$  is the mean square end distance of random statistics chain. Note: For the chain  $N_z$  of a specific local area in the solid state, the distance between the two endpoints of the chain  $N_z$  can be a random number, such as 12 or 17, etc., but for the statistical average of an infinite number of local regions, the statistical chain  $N_z$  is equivalent to an ideal free chain with a mean squared end-to-end distance of 14.



**Figure S4. The image of the  $V_{8A}(a_0)$ -soft matrix-loop and  $V_{7B}(d_0)$ -cluster-loop.** The lattice Hamiltonian to generate the soft matrix is the average energy of 60 IEs (56 dark blue arrows plus 4 reverse red arrows) with a relaxation time of  $\tau_8$ . When four clusters  $V_{8A}(b_0)$ ,  $V_{8A}(c_0)$ ,  $V_{8A}(d_0)$  and  $V_{8A}(e_0)$  appear sequentially,  $V_{8A}(a_0)$  disappears, and the four sides (four arrows) of the IE-spin of  $a_0$  disappear and the vacancy space of 5-HSM appears.  $V_8(a_0)$  cluster contains 200 HSMs, 60 of which are edge particles. There are 136 HSCLs, 76  $+z$ -HSCLs and 60  $-z$ -HSMs in the  $V_8(a_0)$ -loop. When the  $V_{8A}(a_0)$  soft matrix appears, there are unbalanced 16  $+z$ -HSCLs (yellow) in the  $V_{8A}(a_0)$ -IE-loop. Each  $+z$ -HSCL has 1/16 potential energy, and 16  $+z$ -HSCLs in the  $V_8(a_0)$ -loop. At this time, the average position of all negative charges, the midpoint position of all  $z$ -axis repulsive electron pairs, is at the bottom of the potential well (set the potential to 0); And the average position of all positive charges is the equipotential point of 1/16 of the start and end points of each  $M^+$ -P in the 16 yellow  $+z$ -axis HSCLs in the soft matrix along its 4-diagonal closed-loop jump. At the glass transition temperature  $T_g$ , the  $+z-V_0(a_j, \tau_7)$  of the  $A_j$ -field can now also be in the  $+z-V_0(a_j, \tau_8)$ -soft matrix state in the mean field representation. That is, the statistical chain of  $(196 + 4)$  HSMs in the  $z$ -space is a self-avoiding random walk ( $n_z$ -steps) chain satisfying de Gennes  $n = 0$ , and the satisfying way is to sequentially appear a soft matrix composed of  $(196+4)$  HSMs,

#### SM 4. Theoretical derivation of anomalous viscosity of entangled polymer melts



**Figure S5.** The  $N$   $z$ -axial soft matrices appearing in sequence share the generation energy  $k_B T_g^\circ$  of a  $z$ -axis soft matrix.. Due to the inverse cascading, the energies of the CEP IE states in the  $a_j$ -soft matrix all evolve into the  $V_8$ -IE-loop energy  $k_B T_g^\circ$  of the soft matrix. And  $V_8$ -IE-loop energy  $k_B T_g^\circ$  can be equivalent to a "loop-flow" composed of  $\alpha_{Lg}$  ( $= k_B T_g^\circ / \varepsilon_0$ ) equivalent particles ( $\alpha_1, \alpha_2, \alpha_3 \dots \alpha_{Lg}$ ).

The rough original proof of this section is shown in Ref.12, which is now partially corrected and more accurate. Taking inspiration from SM 1 (1), we can derive the theory of glass state from the theoretical derivation of the abnormal viscosity of the 3.4 power law of entangled polymer melts. The author's research method differs from that of most scholars. First, he correctly guessed the expression for the anomalous viscosity that matched the experiment very well. For flexible chains, equation (1) derives  $\eta \sim N^{3.4}$ , and for non-flexible chains, equation (1) also matches the existing experimental data .

$$\eta \sim N^9 (1-T_g / T_m) \quad (1)$$

Due to the exponential relationship, the reliability of equation (1), which is highly consistent with the experiment, is high. The pattern of molecular collective jumping and the theory of glass state should be included in equation (1) , so the theoretical proof of equation (1) is an effective way to explore the nature of glass state.

De Genre's snake model gives an expression for the anomalous viscosity of the entangled polymer melt

$$\eta \sim N^3 \quad (2)$$

One possible explanation for the ultra-high-speed spinning mechanism is that the only soft matrices in all local regions in the melt that can beat are in the  $z$ -axial direction. Because the hydrodynamic mode is characterized by the total number of degrees of freedom (DoF) of the system. Thus, the chain length  $N$  in equation (2) is replaced by the total number of DoF  $N^*$  required for  $N$  chain particles to spread freely.

$$N^* = N_z^* \cdot N_x^* \cdot N_y^* = (N_z^*)^3 \quad (3)$$

Equation (2) is rewritten as

$$\eta \sim (N_z^*)^9 \quad (4)$$

The glass state theory to be sought is thus contained in the rigorous proof of equations (3) and (5).

$$N_z^* \sim N^{(1-T_g / T_m)} \quad (5)$$

In the glass transition, all  $N$  soft matrices that are excited and to be excited in each local area jump  $n_z$  steps along the same direction (as in the  $z$ -axis) in sequence. The  $z$ -axis repulsive electron pairs in the  $N V_8$ -IE-loops form a dynamic "wall" of length  $N$  whose energy, expressed in terms of temperature  $T$ , is the same as the wall energy of  $a_0$ - $V_8$ -loop, both are  $k_B T_g$ .

Each equivalent particle has a unit DoF energy  $\epsilon_0$  and is located on its own equivalent chain of chain length  $N_z$  ( $z$ -component chain of chain  $N$ ). The probability that a  $V_8(a_j)$ -loop of  $a_j$  occupies the  $N$  associated  $V_8$ -loops on chain  $N_z$  is  $1/N$ . Since the energy of  $N$  related  $V_8$ -loops on chain  $N_z$  is still numerically  $k_B T_g$  ( $= k_B T_g^\circ$ ), the  $L_g$  equivalent particle can be equivalent to the association of  $N$   $V_8$ -loops, as long as each equivalent particle is regarded as having a  $V_8(a_j)$ -loop and the probability of occupying  $N$   $V_8$ -loops is also  $1 / N$ .

Statistically, the occurrence probability  $\hat{p}_+$  of the  $V_8(a_0)$ -soft matrix is equal to the probability of simultaneous occurrence of  $L_g$  equivalent particles in the  $V_8(a_0)$ -loop:

$$\hat{p}_+ = (1/N_z)^{k_B T_g / \epsilon_0} \quad (6)$$

Like the generation energy of  $V_8(a_0)$ -soft matrix, the  $O(a_0)$  cavity in its center is also shared by all chain HSMs on the  $N_z$  chain. Let the occupied share of  $a_0$  in the  $O(a_0)$  cavity be  $n_z$ , similar to Eq. (6), the probability  $\hat{p}_-$  of the disappearance of  $V_8(a_0)$ -soft matrix is

$$\hat{p}_- = (n_z)^{k_B T_m / \epsilon_0} \quad (7)$$

From  $\hat{p}_+ = \hat{p}_-$  and  $(1/N_z)^{T_g} = (n_z)^{T_m}$

$$n_z = (N_z)^{-T_g / T_m} \quad (8)$$

For the flexible chains  $T_g / T_m = 5/8$ , take  $N = 200$  in Eq. (8) to adapt to the small molecule system, and obtain

$$n_z \leq 0.036 \quad (8)$$

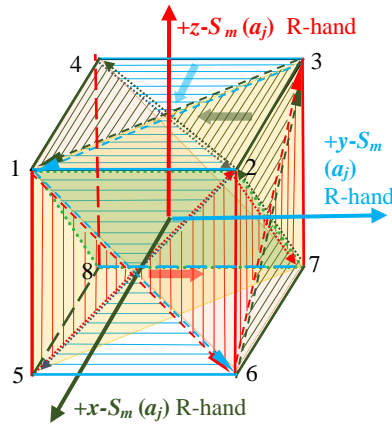
$n_z$  is also the step-size and the number of DoF for  $a_0$  to walk. Therefore, the number of DoF  $N_z^*$  required to "move the entire  $n_z$  steps" of the chain  $N_z$  along the  $+z$  axis is

$$N_z^* = N \cdot n_z = (N)^{(1 - T_g / T_m)} \quad (10)$$

This is Eq. (5). Equation (10) shows that the  $z$ -axis IE energy in all  $N$   $z$ -axis  $V_8$ -loops in each local region, from the glass state to the molten state, is correlated with the loss of potential energy in the  $A$ - $q_L$  interval (Fig. 2) in the  $z$ -axis L-J potential, and maintains the value  $k_B T_g^*$  ( $= k_B T_g$ ) shared by the  $N$  soft matrices that appear sequentially. In particular, at the glass transition temperature  $T_g$ , on average, only one soft matrix is excited in each local region, and the energy of the disappearing soft matrix is lacking, so there is almost no isolated wave beating of the soft matrix. Further, the lower the temperature is  $T_g$ , the less soft matrices describe the collective beating of molecules, and the greater the viscosity.

When the temperature continues to increase, the positively charged central particle of  $a_0$ -HSM,  $M^+-P(a_0)$ , jumps 9 closed loops along the clustered path of  $9 \rightarrow 12 \rightarrow 10 \rightarrow 11 \rightarrow 9$  in figure S1 (b) to obtain the  $x$ -axial soft matrix of  $a_0$ , written as  $x$ - $V_8(a_0)$ . In order for the  $x$ - $V_8(a_0)$  to jump freely along  $x$ -direction,  $a_0$  must consume  $N_z^*$  more DoF. Similarly, in order for  $x$ - $V_8(a_1)$  to jump freely in the  $x$ -direction,  $a_1$  must also consume more  $N_z^*$  DoF. Thus, in order for  $N$   $x$ -axis soft matrices to jump freely in the  $x$ -direction, the chain  $N$  seems to consume  $N \cdot N_z^*$  DoF. However, as with the  $N_z$  component chain, the generation of the  $N$   $x$ -axis soft matrix in the  $N_x$  component chain is also associated with the disappearance of the  $A$ - $q_L$  interval potential of the L-J potential in the  $x$ -axial, and the number of DoF required for the  $N_x$  chain to freely jump  $n_x$  steps in the  $x$ -axial is  $N_x^*$ , that is, the number of DoF required for the  $N$ -chain to spread freely in  $z$ - $x$  2D space is  $N_x^* \cdot N_z^*$ . This leads to the number of DoF required for a chain of length  $N$  to spread freely in 3D space,  $N^* = N_x^* \cdot N_z^* \cdot N_y^*$ . This is Eq. (3).

## SM 5. Cluster structure of molecules in liquid state

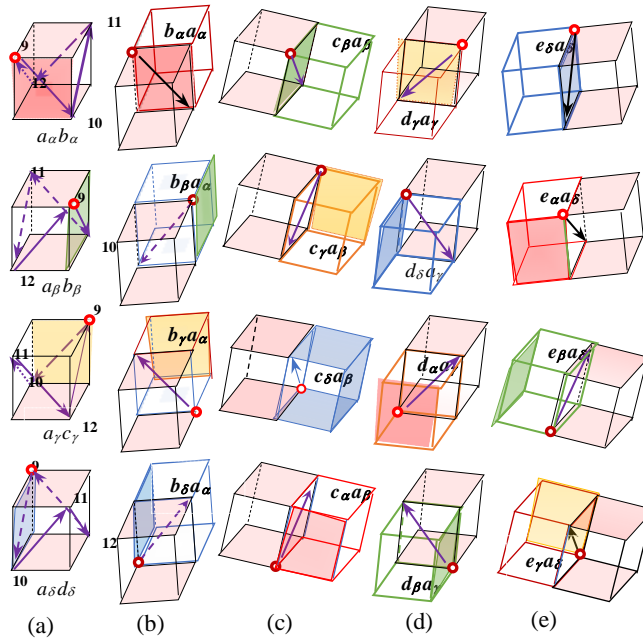


**Figure S6. Exclusion volume diagram of mean field hard-sphere molecules in melt (liquid).** Each of the 2D interface excited spins can have both left and right hands, indicated by the direction of the arrow of the relative axis.

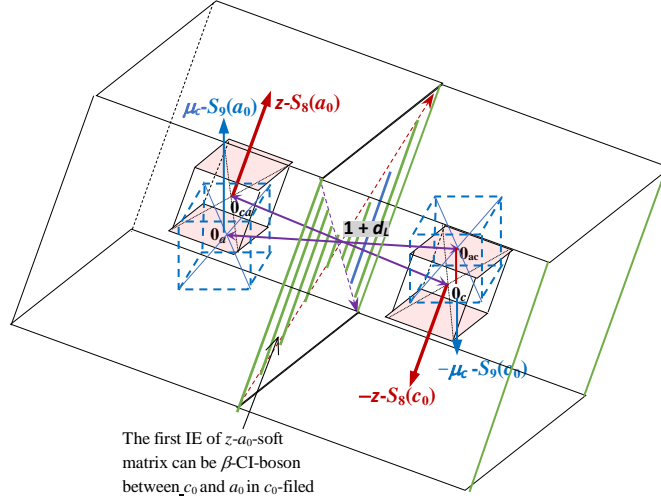
In the liquid state, in addition to the various crystal structures of molecules described by quantum mechanics, there can be various dynamic equilateral hexahedral space-time structures composed of changes in quenching disordered eigenvalues caused by changes in temperature, pressure, and impurities. The 5-HSM central HSM in the liquid state has  $6 \times 16$  spatial angle-linel states, which can form three axial 2D spins.

### SM 6. 20-fold symmetry of CI-boson starting position in the glass state

symbol  $a_\alpha b_\alpha$  in Figure S6 indicates that  $b_0$  is projected to  $a_0$ -field and the CI-boson between  $a_0$  and  $b_0$  is  $\alpha$ , which is also one state in the 20-fold symmetry of the CI-boson interaction between  $a_0$ -HSM and its four neighboring HSMs. That is, at any temperature of the entire solid-liquid  $\leftrightarrow$  transition, each HSM has 20 different spatial positions to construct the first CI-boson, or each HSM has 20 different CI-boson interaction states, which is an inherent geometric property of disordered molecular systems, called the 20-fold symmetry of the glass state.

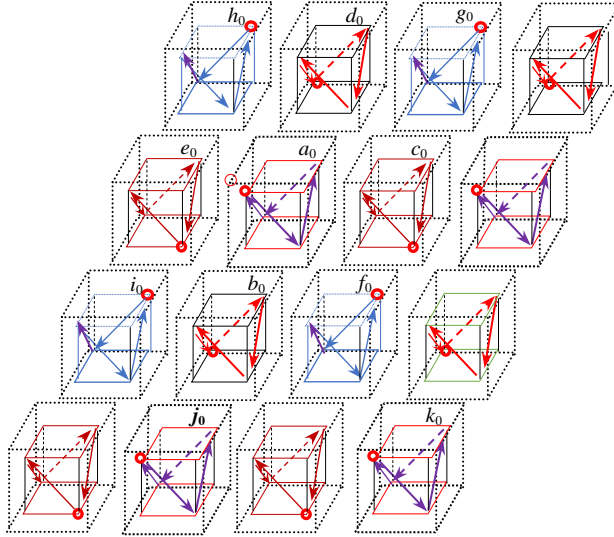


**Figure S6.** An  $a_0$ -soft matrix can be reduced to the positive charge center particle  $M^+$ -P of  $a_0$ -HSM completing nine closed-loops on the 4-diagonal of the 2D cubic lattice (the starting point of the cycle is marked with a small red circle), which is equivalent to four closed-loops of four CI-bosons appearing nine times. **a.** In the  $V_0(a_0)$ -loop, there are 4 options for where the first IE boson appears (four colored interfaces). The formation of the  $a_0$ -soft matrix requires its four adjacent  $V_0$ -loops. **b.** The four interfaces of  $\mu_b$ -axial- $V_0(b_0)$ -loop. **c.** The four interfaces of  $\mu_c$ -axial- $V_0(c_0)$ -loop. **d.** The four interfaces of  $\mu_d$ -axial- $V_0(d_0)$ -loop. **e.** The four interfaces of  $\mu_e$ -axial- $V_0(e_0)$ -loop. So there are 20 choices for the position of the first CI-boson in the glass state to obtain the same z-axis  $a_0$ -soft matrix. The symbol  $a_\alpha b_\alpha$  means  $b_0$  is projected to  $a_0$ -field and the CI-boson between  $a_0$  and  $b_0$  is  $\alpha$ , which is the first state in the 20-fold symmetry.



**Figure S7. Symmetry of orientation fluctuation of MIES.** In  $z$ - $S_9(a_0)$  and  $z$ - $S_8(c_0)$  projected from  $c_0$  to  $a_0$ -field (two blue dashed  $2\Delta d$  cubic lattices), the distance between the two vibrational equilibrium centers  $0_a$  and  $0_{az}$  is  $1 + d_L$ . Similarly, in the projection from  $a_0$  to  $c_0$ -field, the distance  $0_{ca}$  and  $0_c$  between the two centers of vibration equilibrium is still  $1 + d_L$ . When the first CI-boson in the path forming the  $a_0$ -soft matrix is the  $\beta$ -CI-boson between  $c_0$  and  $a_0$  in the  $c_0$ -field, the site of  $M^+$ -P( $a_0$ ) is marked with a small red circle and the  $a_0$  state is marked as  $c_\beta a_\beta$  (Figure S6c).

### SM 7. Correlation of closed-loop hop paths for all HSMs in the soft matrix



**Figure S8. Distribution of four closed-loop paths (four colors) in a soft matrix.** The starting position (phase) of each  $M^+$ -P in the soft matrix when it performs a 4-diagonal closed loop jump on its  $2\Delta d$  micro-cubic lattice. Once the  $M^+$ -P ( $a_0$ ) has determined its 4-diagonal path, the 4 diagonal closed-loop paths of all  $M^+$ -Ps in the soft matrix have been confirmed. A phase difference of  $2\pi i$  is allowed between two  $M^+$ -Ps with the same starting position, and  $i$  is the  $i$  in the  $V_i$  cluster where the  $M^+$ -P is located. For example,  $j_0$  belongs to the  $V_1$  cluster [3], and its starting phase lags behind  $a_0$  ( $V_0$  cluster)  $2\pi$ , and  $k_0$  belongs to the  $V_2$  cluster, its phase lags behind  $a_0$   $4\pi$ . Each HSM in the polymer soft matrix has 3 concentric HSCLs<sup>14</sup>. The dotted cubic lattice in the figure is a cubic lattice of  $H^+$ -P (the positively charged particle of hydrogen atom) that jumps synchronously with  $M^+$ -P.

Figures S6 and S7 show only the spatial geometry of the CI-boson interaction states of HSM. When considering the temporal nature of an CI-boson that can be repeated at the same spatial location, an  $+z$ -axial  $a_0$ -soft matrix centered on  $a_0$ -HSM has four equivalent representations in different scenarios. They are:  $+z$ - $V_8(a_0)$ -cluster,  $+z$ - $V_8(a_0)$ -loop,  $+z$ - $S_9(a_0)$  and  $+z$ - $V_0(a_0, \tau_8)$ . The fourth representation refers to the completion of 9 closed loops by four CI-bosons at the four interfaces of the  $+z$ -axis of the  $(1 + d_L)$  cubic lattice of  $a_0$ -HSM, with a relaxation time of  $\tau_8$