One-dimensional Kac model of dense amorphous hard spheres

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Abstract – We introduce a new model of hard spheres under confinement for the study of the glass and jamming transitions. The model is a one-dimensional chain of the $d$-dimensional boxes each of which contains the same number of hard spheres, and the particles in the boxes of the ends of the chain are quenched at their equilibrium positions. We focus on the infinite-dimensional limit ($d \to \infty$) of the model and analytically compute the glass transition densities using the replica liquid theory. From the chain length dependence of the transition densities, we extract the characteristic lengths at the glass transition. The divergence of the lengths are characterized by the two exponents, $-1/4$ for the dynamical transition and $-1$ for the ideal glass transition, which are consistent with those of the $p$-spin mean-field spin glass model. We also show that the model is useful for the study of the growing length scale at the jamming transition.

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Introduction. – When liquids are rapidly cooled well below the melting temperature, the relaxation time and viscosity drastically increase and eventually they freeze into the disordered state. This phenomenon is known as the glass transition \cite{1}. The mechanism of this slowing down and the presence/absence of an underlying genuine phase transition are under active debate \cite{2–4}.

A good way to understand theoretically the glass transition would be to first construct a mean-field theory and then consider finite-dimensional effects. Recently the glass transition of the infinite-dimensional hard spheres has been studied as a mean-field model, and the exact thermodynamic theory of the model is developing \cite{5–8}. The glass transition of the model can be characterized by two relevant densities \cite{5}. The first is the dynamical transition density, $\varphi_d$, below which the phase space is divided into an exponentially large number of metastable states. In the mean-field limit, the dynamics of the system gets frozen at this density as the system is trapped into one of the metastable states. With increasing the density, the number of the metastable states decreases and eventually becomes sub-exponential, at which the system undergoes the thermodynamic transition into the ideal glass state. This transition density $\varphi_K$ is called the Kauzman density.

What types of finite-dimensional effects play a dominant role in the glass transition is not clear yet \cite{3,9}. One promising theoretical scenario which incorporates an effect of fluctuations of finite-dimensional systems is proposed as the random first-order transition (RFOT) theory \cite{10}. This theory assumes that the divergence of the relaxation time at $\varphi_d$ is avoided, and at $\varphi$ between $\varphi_d$ and $\varphi_K$, the liquid state can be seen as a patchwork of the local metastable configurations \cite{11}. The theory predicts that the characteristic size of these domains increases with increasing the density and eventually diverges at $\varphi_K$, where the thermodynamic glass transition occurs.

In practice, this length can be measured through the thermodynamic behavior of liquids under confinement \cite{11}. We prepare an equilibrium configuration of particles and pin only the particles outside of a cavity of the size $L$. One can define and compute the critical cavity size at which the boundary affects the thermodynamics of the system in the cavity, which is referred to as the point-to-set (PS) correlation length. Numerical simulations of realistic liquid models under this confinement have been carried out \cite{12–15}, which confirmed that the PS length indeed grows as the systems slow down. However, computing theoretically the PS length of realistic liquids is still very challenging \cite{16,17}. One of the difficulties is due to the inhomogeneous nature of the confined liquids, which requires the inhomogeneous version of the liquid state theory \cite{18}. The $p$-spin mean-field spin
glass model under confinement has been extensively studied [19,20]. The studies showed that the PS length of the model diverges at the Kauzuman transition point with the power-law behavior with the exponent $-1$ and another length characterizing the local stability of the metastable states diverges at the dynamical transition point with the exponent $-1/4$ [19].

The main purpose of the present letter is to propose a new model of hard spheres under confinement, which can be analyzed using the homogeneous liquid state theory [21]. Focusing on the large-dimensional limit of the model, we compute analytically the PS length using the replica liquid theory.

Since the model proposed is not a spin model but a hard-spheres one, it undergoes another type of phase transition, called the jamming transition, at the higher density [5,22]. This is the transition of the liquid state into the state where hard spheres are packed so closely that the pressure diverges. We additionally show that the model can be used to study the growing lengths at the jamming transition.

**Model.** – Consider a one-dimensional chain of $L + 2$ boxes. Each box is a $d$-dimensional cube of the volume $V$ and contains $N$ hard spheres. We assume that a particle interacts with the other particles in the same box and those in the nearest two boxes. Therefore, the Hamiltonian of the model is

$$H = \sum_{l=1}^{L} \sum_{i<j} v(|x_i^l - x_j^l|) + \sum_{l=0}^{L} \sum_{ij} v(|x_i^l - x_j^{l+1}|),$$

where the $d$-dimensional vector $x_i^l$ denotes the position of the $i$-th particle in the $l$-th box and $v(r)$ is the interaction potential between hard spheres of the diameter $D$, hence $v(r) = \infty$ ($r \leq D$), 0 ($r > D$). We study the model under the condition that the particles in the 0-th and $(L + 1)$-th boxes are quenched at their equilibrium positions. Thus the model is interpreted as the $d$-dimensional hard spheres confined by the amorphous walls. We sketch a typical configuration of our model schematically in fig. 1.

As is clear from the Hamiltonian, eq. (1), we can treat the model as a $L + 2$ component homogeneous liquid, which enables us to analyze the model using the homogeneous liquid state theory. This is one of the advantages of this model. In particular, the free energy of this model can be evaluated analytically at the large-dimensional limit using the replica liquid theory. In the following sections, we calculate the two relevant densities $\varphi_d$ and $\varphi_K$ for the glass transition as a function of the number of the boxes $L$. By interpreting $L$ as the correlation length, we extract the lengths $\xi_d$ and $\xi_K$ which diverge at $\varphi_d$ and $\varphi_K$, respectively. Additionally, we also apply this method to the jamming transition to discuss the possibility to compute its growing length scales.

**Free energy at large-dimensional limit.** – To compute the free energy of the model, we employ the replica liquid theory assuming the one-step replica symmetry breaking (1RSB) ansatz [5,23,24]. The main idea of the theory is to consider $m$ copies (replicas) of the original system. There is no interaction between the replicas, and therefore the partition function of the replicated system is written as

$$Z_m \equiv \prod_{a=1}^{m} \text{Tr}_{x_a} e^{-\sum_{a=1}^{m} H([x_a])/T},$$

where $H$ is the Hamiltonian of the original system, and $T$ is the temperature. From now on, we set $T = 1$ because the temperature is an irrelevant variable for hard spheres. Within the replica theory, the logarithm of the number of the minima, which is called the configurational entropy, $\Sigma$, can be calculated by the formula [24]

$$\Sigma = -m^2 \frac{\partial}{\partial m} \left( \frac{\log Z_m}{m} \right).$$

If one takes the large-dimensional limit ($d \to \infty$) and the thermodynamic limit ($N \to \infty$, $V \to \infty$, $N/V = \text{const}$), the calculation of the partition function of the replicated system can be greatly simplified because the higher-order terms of the Mayer cluster expansion become negligible, and only the first term needs to be considered [5,21]. The replicated free energy of our model is

$$\log Z_m = \sum_{l=1}^{L} \int d\overline{\mathbf{x}} \rho_1(\overline{\mathbf{x}}) \left( 1 - \log \rho_1(\overline{\mathbf{x}}) \right)$$

$$+ \frac{1}{2} \sum_{l=1}^{L} \int d\overline{\mathbf{x}} d\overline{\mathbf{y}} \rho_1(\overline{\mathbf{x}}) \rho_1(\overline{\mathbf{y}}) f(\overline{\mathbf{x}} - \overline{\mathbf{y}})$$

$$+ \frac{1}{2} \sum_{l=1}^{L-1} \int d\overline{\mathbf{x}} d\overline{\mathbf{y}} \rho_1(\overline{\mathbf{x}}) \rho_{l+1}(\overline{\mathbf{y}}) f(\overline{\mathbf{x}} - \overline{\mathbf{y}})$$

$$+ \int d\overline{\mathbf{x}} d\overline{\mathbf{y}} \rho_1(\overline{\mathbf{x}}) \rho_0(\overline{\mathbf{y}}) f(\overline{\mathbf{x}} - \overline{\mathbf{y}})$$

$$+ \int d\overline{\mathbf{x}} d\overline{\mathbf{y}} \rho_{L-1}(\overline{\mathbf{x}}) \rho_{L+1}(\overline{\mathbf{y}}) f(\overline{\mathbf{x}} - \overline{\mathbf{y}}),$$

where $\overline{\mathbf{x}} = \{x^1, \ldots, x^m\}$ denotes the positions of hard spheres in the replicated space, and $\rho_1(\overline{\mathbf{x}}) = \langle \sum_{a} \prod_{i=1}^{n} \delta(x^a - x_i^L) \rangle$ is the density distribution of the
l-th box. The boundary conditions are included in the last two lines of eq. (4), where \( \rho_0(x) = \sum_i \delta(x - x_i) \) and \( \rho_{L+1}(x) = \sum_i \delta(x - x_{L+1}^{l+1}) \) are the microscopic density distributions of the frozen particles belonging to the 0-th and (L + 1)-th boxes. \( x_i \) and \( x_{L+1}^{l+1} \) are taken from their equilibrium positions. If the system is sufficiently large, the self-averaging properties for the free energy holds:

\[
\log Z_m \approx \log Z_m,
\]

where the overline denotes the average of \( \rho_0(x) \) and \( \rho_{L+1}(x) \). Since the free-energy equation (4) depends linearly on those variables, we have only to replace as \( \rho_0(x) \rightarrow \rho \) and \( \rho_{L+1}(x) \rightarrow \rho \), where \( \rho = N/V \) is the number density of each boxes.

In the next step, we introduce the 1RSB Gaussian ansatz [5]:

\[
\rho_I(\pi) = \rho \int dX \prod_{a=1}^{m} \gamma_{A_l}(x_a - X),
\]

where \( \gamma_{A_l}(x) = \exp(-x^2/2A_l)/(2\pi A)^{d/2} \). This ansatz claims that the distribution of the replicated particles is the Gaussian with the variance \( A_l = \sum_{a\neq b,\Bigl(\sum}\langle x_i^a - x_i^b \Bigr)/m(m-1) \). Substituting eq. (6) into eq. (4) and taking the large-dimensional limit [5], one obtains the analytical expression for the free energy:

\[
\frac{\log Z_m}{N} = S_{id} + S_{int},
\]

\[
S_{id} = \sum_{l=1}^{L} \frac{1}{2} \left[ (m-1) \log \frac{\hat{A}_l}{d} + \log \frac{m}{d} + m \right],
\]

\[
S_{int} = -\frac{3L\hat{\varphi}}{2} \left( 1 + \frac{2}{3L} \right) + \frac{\hat{\varphi}}{2} \sum_{l=1}^{L} G_m(\hat{A}_l) + \frac{\hat{\varphi}}{2} \sum_{l=0}^{L} G_m \left( \frac{\hat{A}_l + \hat{A}_{l+1}}{2} \right),
\]

where we introduced the normalized volume fraction \( \hat{\varphi} = 2^d \varphi/d \) and the normalized cage size \( \hat{A}_l = A_l d^2 / D^2 \). \( G_m(\hat{A}) \) is the auxiliary function given by

\[
G_m(\hat{A}) = \int_{-\infty}^{\infty} dy \left[ \Theta \left( \frac{y + \hat{A}}{\sqrt{4A}} \right) \right]^m - \Theta(y),
\]

where \( \Theta(x) = [\text{erf}(x) + 1]/2 \). In eq. (7), the cage size of the 0-th and (L + 1)-th boxes is zero, \( \hat{A}_0 = \hat{A}_{L+1} = 0 \), because of the boundary condition. \( \hat{A}_l \) for other \( l \) is calculated from the saddle point conditions for \( \hat{A}_l \):

\[
\frac{1}{\hat{A}_l} = \frac{2}{(1 - m)d} \frac{\partial S_{int}}{\partial \hat{A}_l} \quad (l = 1, \ldots, L).
\]

Substituting the solution of this set of equations into eq. (7), the free energy of the \( m \) replicated system is obtained.

**Glass transition.** – Here, we evaluate the correlation length of the glass transition. As mentioned before, there are two relevant densities for the glass transition, \( \hat{\varphi}_d \) and \( \hat{\varphi}_K \). Their values can be computed by analyzing the free energy at \( m = 1 \).

First, we examine the behavior of our model near the dynamical transition point, \( \hat{\varphi}_d \), where the exponentially many metastable states emerge on the free energy. In the framework of the replica liquid theory, the order parameter to characterize the metastable states is the cage size, which is given by the solutions of eq. (9) [5]. Their numerical solution for \( A_l \) of the \( L/2 \)-th box, which is the farthest from the boundaries, is shown in fig. 2. For the small densities, the cage size \( A_{L/2} \) is infinity \((1/(1 + A_{L/2}) = 0)\), meaning that the system is ergodic and in the liquid phase. Increasing the density, the cage size jumps discontinuously to a finite value at the dynamical transition point, \( \hat{\varphi}_d \).

From fig. 2, it is clear that \( \hat{\varphi}_d \) increases with increasing \( L \). From this result, we can convert \( \hat{\varphi}_d(L) \) to \( L(\hat{\varphi}) \), the characteristic number of the boxes as a function of the transition density. We define the correlation length by \( \xi_d = L(\hat{\varphi})/2 \) and plot it in fig. 3 [19]. We find that \( \xi_d \) diverges at \( \hat{\varphi}_d \) as \( \xi_d \approx (\hat{\varphi}_d - \hat{\varphi})^{-1/4} \).

Next, we evaluate the correlation length near the Kauzman density by calculating the configurational entropy, \( \Sigma \), which is obtained by plugging the free energy into eq. (3). The final expression in the large-dimensional limit becomes

\[
\Sigma(m, \varphi, L) = \frac{d}{2} \log d - \frac{3\hat{\varphi}}{2} \left( 1 + \frac{2}{3L} \right) + O(d),
\]

up to the order of \( O(d \log d) \). From this expression, it is clear that \( \Sigma \) vanishes at

\[
\hat{\varphi}_K(L) = \frac{d \log d}{3(1 + 2/3L)}.
\]

Following the same argument as for \( \xi_d \), the growing length around the Kauzman density is

\[
\xi_K = \xi_GCP = \frac{L}{2} = \frac{\hat{\varphi}}{3(\hat{\varphi}_K - \hat{\varphi})},
\]

where \( \hat{\varphi}_K = d \log d / 3 \) is the Kauzman density of the bulk system \((L \rightarrow \infty)\).
Fig. 3: (Colour on-line) The correlation lengths near the \( \varphi_d \) and \( \varphi_{th} \). The filled circles stand for \( \xi_d \) as a function of \( \varepsilon = (\varphi_d - \varphi)/\varphi_d \). The filled squares stand for \( \xi_{th} \) as a function of \( \varepsilon = (\varphi_{th} - \varphi)/\varphi_{th} \).

**Jamming transition.** — Hard spheres also undergo the jamming transition when the system is compressed quickly or making the pressure infinity [22]. The infinite-dimensional hard spheres serve as a mean-field model of the jamming transition as well and are studied extensively using the replica liquid theory. The theory showed that the jamming transition is also characterized by the two relevant densities [5]. The jamming state obtained by compressing the ideal glass state up to the infinite pressure is referred to as the glass close packing, and its density is denoted as \( \varphi_{GCP} \). If the jammed state is prepared by a fast compression of low-density hard spheres, the pressure becomes infinity at a much lower density than \( \varphi_{GCP} \) [25]. The lowest density of the jammed states \( \varphi_{th} \) is called the threshold density.

In this section, we show that the growing length scales at the jamming transition can be computed from the analysis of the jamming transition of the present model. We essentially follow the strategy developed in the previous section. Using the replica liquid theory with the 1RSB ansatz, we compute \( \varphi_{th} \) and \( \varphi_{GCP} \) of the model as a function of the number of the boxes, \( L \), which naturally gives rise to the two characteristic lengths \( \xi_{th}(\varphi) \) and \( \xi_{GCP}(\varphi) \). Note that recent studies showed that the full RSB ansatz is needed for the fully exact computation near the jamming transition [7,8]. However, such a computation for the present model seems quite involved. Here, we wish to stick to the 1RSB ansatz and demonstrate that the replica theory analysis of the model provides the analytical expressions of the growing length scales at the jamming transition.

In the replica liquid theory, the divergence of the pressure corresponds to taking the \( m \to 0 \) limit, because \( m \) is inversely proportional to the pressure [5]. Thus, \( \varphi_{th} \) can be calculated by taking the \( m \to 0 \) limit in the self-consistent equation for the order parameter, eq. (9). Since the cage size, \( A_l \), vanishes at the \( m \to 0 \) limit, we set \( A_l = m a_l \) [5]. This is substituted into eq. (9) before the \( m \to 0 \) limit is taken. We numerically solve the equation and find that the behavior of \( \alpha_{L/2} \) is qualitatively the same as that of \( \alpha_{L/2} = 1/4 \) for the glass transition (fig. 2). At low densities, \( \alpha_{L/2} = \infty \) is the only solution of eq. (9). This means that there are no jammed states at those densities. At higher densities, the solution of eq. (9) becomes finite. This transition density is the lowest density, \( \varphi_{th} \), of the jammed states. As in the case of the glass transition, the characteristic length \( \xi_{th}(\varphi) \) is computed from the \( L \) dependence of \( \varphi_{th} \). This length \( \xi_{th} \) is also plotted in fig. 3. We find the power-law divergence \( \xi_{th} \approx (\varphi_{th} - \varphi)^{-1/4} \). Likewise, we analyze the correlation length near \( \varphi_{GCP} \). The logarithm of the number of the jammed states is calculated by the \( m \to 0 \) limit of the configurational entropy, eq. (10) and \( \varphi_{GCP} \) is defined as the density where the configurational entropy becomes zero. From eq. (10), it is clear that the behavior of \( \varphi_{GCP} \) should be the same as those of \( \varphi_{th} \) because eq. (10) is independent from \( m \). Thus, we obtain the critical behavior of the diverging length near \( \varphi_{GCP} \) as \( \xi_{GCP} \approx (\varphi_{GCP} - \varphi)^{-1/4} \).

**Summary and discussion.** — In this letter, we considered a one-dimensional chain of \( d \)-dimensional boxes each of which contains \( N \) hard spheres as a model system of liquids under confinement. By focusing on the large-dimensional limit, we analytically computed the phase diagram of the model. From the chain length dependence of the transition densities, we derived the critical behavior of two relevant length scales of the glass transition. We also showed that there are two relevant length scales of the jamming transition, whose critical behaviors are similar to those of the glass transition as long as the 1RSB ansatz is assumed. One of the advantages of the model is that, although the system is under confinement, it can be regarded as a homogeneous liquid, and thus the model can be analyzed using the usual replica liquid theory.

We summarize the results in fig. 4. The upper panel is the phase diagram of the glass transition of the confined liquid, where \( \varphi \) is the normalized density \( \varphi = 2^d \varphi_d / d \), and \( L \) is the distance between the boundaries. There are two relevant length scales \( \xi_d \) and \( \xi_K \), which diverge as \( \xi_d \approx (\varphi_d - \varphi)^{-1/4} \) and \( \xi_K \approx (\varphi_K - \varphi)^{-1} \), respectively. When \( L > \xi_d \), the system holds the ergodicity and is in the liquid phase. For \( \xi_K < L < \xi_d \), the phase space splits into many sub-spaces and the ergodicity of the system is broken at least in the large-dimensional limit. In the \( L < \xi_K \) region, the number of the sub-spaces becomes sub-exponential and no longer contributes to the entropy. Thus, the equilibrium phase transition from the liquid phase to the ideal glass phase occurs. These results are consistent with the results for the \( p \)-spin mean-field spin glass model [19,20], where the critical behaviors \( \xi_d \approx (T - T_d)^{-1/4} \) and \( \xi_K \approx (T - T_K)^{-1} \) are observed. This confirms that the proposed model is considered to be a hard-sphere extension of the \( p \)-spin mean-field spin glass model under confinement. The result for \( \xi_d \) is also consistent with the prediction of the inhomogeneous mode-coupling theory for the dynamic correlation length diverging at the mode-coupling transition point [18]. In

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finite dimensions, the correlation length does not diverge at \( \varphi_d \) since the singularity at \( \varphi_d \) is avoided due to the thermal activation process. In this case, one can expect that there is a crossover at around \( \varphi_d \) from the region in which the correlation length is controlled by \( \xi_d \) to the region in which \( \xi_k \) plays a dominant role [13,15,26]. However, a general understanding of this crossover is still lacking, though interestingly a non-monotonic behavior of the correlation length at around \( \varphi_d \) was detected in a specific model glass former [13].

The lower panel of fig. 4 is the phase diagram of the jamming transition. There are two relevant length scales \( \xi_{th} \) and \( \xi_{GCP} \) which diverge as \( \xi_{th} \approx (\hat{\varphi}_{th} - \hat{\varphi})^{-1/4} \) and \( \xi_{GCP} \approx (\hat{\varphi}_{GCP} - \hat{\varphi})^{-1} \), respectively. When \( L > \xi_{th} \), there are no jammed states. For \( \xi_{GCP} < L < \xi_{th} \), there exist exponentially many jammed states. The number of the jammed states decreases with \( L \), and becomes sub-exponential when \( L < \xi_{GCP} \).

We should emphasize that the computation of \( \xi_{th} \) and \( \xi_{GCP} \) in this work is not exact, since the 1RSB ansatz has been recently found to give unstable solution near the \( m \rightarrow 0 \) limit [7]. If we use a better ansatz, the critical exponents may change [8]. Regarding this point, we wish to indicate the following two points: 1) Even though the solution is unstable, the physics of the 1RSB solution can still survive in certain situations [27] and thus the analysis given here is still useful. 2) In case of \( \xi_{GCP} \), the results would not be affected by this instability at least in the large-dimensional limit, because the expression of the configurational entropy is \( m \) independent.

Finally we discuss the physical meaning of \( \xi_{th} \) and \( \xi_{GCP} \). Several different types of lengths are known to diverge at the jamming transition and the relations between the lengths are still not clear enough [28–38]. Since \( \xi_{th} \) and \( \xi_{GCP} \) represent the distance between boundaries at which the jammed configurations first appear/disappear, we expect that these lengths correspond to the length detected in the finite-size scaling analysis \( \xi_{FS} \sim (\varphi - \varphi_j)^{-1.09} \) [34]. However, this is a tentative expectation, because we applied a specific boundary condition (amorphous boundary) which is suitable to compute the PS length at the glass transition. It is not clear which length should be detected by this condition for the jamming transition. To resolve this question, it should be useful to study the present model under various different types of confinements such as the flat walls [39] or random boundary [20].

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