Glass-like behavior of a hard-disk fluid confined to a narrow channel

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Disks moving in a narrow channel have many features in common with the glassy behavior of hard spheres in three dimensions. In this paper we study the caging behavior of the disks which sets in at characteristic packing fraction \( \phi_d \). Four-point overlap functions similar to those studied when investigating dynamical heterogeneities have been determined from event driven molecular dynamics simulations and the time dependent dynamical length scale extracted. It increases with time and on the equilibration time scale is proportional to the static length scale associated with the zigzag ordering in the system, which grows rapidly above \( \phi_d \). The structural features responsible for the onset of caging and the glassy behavior are easy to identify as they show up in the structure factor, which we have determined exactly from the transfer matrix approach.

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I. INTRODUCTION

It has been frequently observed that disks moving in a narrow channel can provide useful insights into glassy behavior [1–6]. In a recent paper two of us studied the static and dynamic properties of \( N \) disks of diameter \( \sigma \), which move in a narrow channel consisting of two impenetrable walls (lines) spaced by a distance \( H_d \) such that \( 1 < H_d/\sigma < 1 + \sqrt{3}/2 \) (see Fig. 1). With channels of this width only nearest-neighbor disks can interact with one another and neighboring disks cannot pass each other so that their ordering is preserved: \( 0 \leq x_1 < x_2 < \cdots < x_N \leq L \), where \( x_i \) is the position of the center of disk \( i \), measured along the channel, and \( L \) is the total length available to the disk centers. The coordinate \( y_i \) of the \( i \)th disk is measured from the center of the channel, and can vary between \( \pm h/2 \), where \( h = H_d - \sigma \). It is the chief purpose of this paper to illustrate the many glass-like features of this simple system, whose equilibrium properties can be determined exactly with the transfer matrix [5, 7–9]. We shall find interesting similarities and also some instructive differences with three dimensional glassy systems. The dynamical properties of our system have to be determined from simulations and to this end we have used event-driven molecular dynamics to handle the collisions of the disks with each other and the channel walls.

It was found some time ago that in this system there is a packing fraction \( \phi_d \approx 0.48 \) above which the dynamics is activated [1]. For hard spheres in three dimensions there is a dramatic increase in their relaxation times above a packing fraction of \( \approx 0.58 \) [10]. The packing fraction \( \phi \) in our system of disks is defined as

\[
\phi = \frac{N \pi \sigma^2}{4 H_d L},
\]

and \( N \) is the number of disks in the channel. We have observed that when \( \phi > \phi_d \approx 0.48 \) zigzag ordering of the disks also started to rapidly increase [5]. In other words, the onset of the slow dynamics is connected with the growth of this particular kind of order. There is a long tradition of associating glassy behavior with geometrical features associated with the arrangements of particles around a given particle, see e.g. [11–15], and our work on disks in a narrow channel is entirely consistent with these ideas. A length scale \( \xi \) associated with zigzag order can be determined from the decay with \( s \) of the correlation function

\[
(y_i, y_{i+s}) \sim (-1)^s \exp(-s/\xi).
\]

It is a measure of the distance over which the zigzag order, a form of bond-orientational order, persists and is of order of the distance between the defects in the zigzag order of the kind shown in the top and bottom panels of Fig. 2. In three dimensional systems the ordering associated with glassy behavior is complicated [15]. Furthermore, the ordering associated with glassy behavior is not apparent in changes to the structure factor as it is cooled through the glass transition. In Sec. II we calculate the structure factor of our system, defined as

\[
S(k_x, k_y) = \frac{1}{N} \sum_{i,j} \exp[ik_x(x_i - x_j) + ik_y(y_i - y_j)],
\]

at packing fractions close to \( \phi_d \) by use of the transfer matrix formalism. One can see (via cumulant averaging of Eq. (3)) that it will change rapidly near \( \phi_d \) because such averages will bring in the correlations in Eq. (2) and this
The average is over different initial states. There is caging of particles in our system, i.e. there is at large enough packing fractions a plateau in $\Delta^2(t)$ (before its long time limit is reached). We find that in our system there are two distinct time scales, which we shall call $\tau$ and $\tau_D$ following Ref. [5], and we can obtain both of them from the behavior of $\Delta^2(t)$. $\tau$ is the typical time scale for a defect to cross from one side of the system to the other as in Fig. 2. It marks the time at which the particle starts to escape from its cage or the end of the plateau in $\Delta^2(t)$; in three dimensional systems this would be called the alpha relaxation time $\tau_\alpha$. At packing fractions above $\phi_d$, escape from a cage can be regarded as a displacement of a defect in the zigzag ordering of the disks as illustrated in Fig. 2. We are able to determine from the simulation the diffusion constant for the movement of such defects. Its dependence on packing fraction is consistent with the general picture of a crossover from fragile glass behavior at low packing fractions to strong glass behavior at high packing fraction, which has been investigated previously in Ref. [2].

The second time scale $\tau_D$ is essentially the longest time scale in the system. In equilibrium defects are thermally nucleated in pairs and the defects produced then diffuse and annihilate with each other. It is this process of diffusion with creation/annihilation which takes place on the time scale $\tau_D$. There is a simple relation between $\tau$ and $\tau_D$: $\tau_D \sim \tau \xi^2$ [5]. Note that $\xi$ is the typical distance between defects in equilibrium, so that $\xi^2/D$ is the time it would take for a defect to move a distance $\xi$: this gives a diffusion coefficient $D$ for the defects which varies as $1/\tau^2$ [5]. $\tau_D$ is determined from the time at which $\Delta^2(t)$ approaches its equilibrium limit.

A characteristic of glassy dynamics is the appearance of a plateau in the decay of some time-dependent correlation functions. This plateau eventually decays to zero after the time $\tau_\alpha$, the alpha relaxation time. The time to reach the plateau is the beta relaxation time $\tau_B$. Correlation functions with this feature have not previously been studied in our narrow channel system. The existence of a plateau in $\Delta^2(t)$ implies that there will be such a plateau in the decay of

$$R(t) = \frac{1}{N} \sum_i \langle y_i(0) y_i(t) \rangle ;$$

at long times $R(t)$ approaches zero. As noted above, our results support a model in which the diffusion of defects leads to equilibrium. In models of this kind, $R(t)$ is expected to decay with a stretched exponential form $\exp(-t/\tau_D)^{1/\xi^2}$, where $\tau_D$ is the equilibration time of the system [16].

We have also studied a correlation function related to the $\chi_4(t)$ which has been much studied in three dimensions [13, 17]. In three dimensions $\chi_4(t)$ rises to a peak at the alpha relaxation time and then decays away to zero as the particles escape their cages; that is, for times longer than the alpha relaxation time, $\chi_4(t)$ decays to zero. Our $\chi_4(t)$ increases to a constant, plateau value as

$\Delta^2(t) = \langle \frac{1}{N} \sum_{i=1}^{N} (y_i(t) - y_i(0))^2 \rangle$.
t increases and stays at this value as $t \to \infty$. In this regard the narrow channel system behaves more like a spin glass than a structural glass [18]. We have also extracted a dynamical correlation length $\xi(t)$ from a four-point correlation function. In our system as $t \to \tau_D$, $\xi$ grows towards the static correlation length $\xi$, which measures the extent of zigzag, i.e., structural order.

In Sec. II we show how the structure factor can be determined exactly from the transfer matrix procedure, and demonstrate that it is rapidly changing at densities close to $\phi_d$. Our dynamical studies are in Sec. III. We conclude with a discussion in Sec. IV.

II. STRUCTURE FACTOR

The structure factor is familiar from the part it plays in the scattering of electromagnetic radiation by liquids [19]. It is the Fourier transform of the density–density correlation function and so provides information on the relative positions of scatterers within the system. Like a liquid, our system of disks in a channel has no long-range order (along the channel) for finite values of the longitudinal force $f$; but, unlike in the bulk of a liquid, the short-range order is strongly affected by the presence of confining walls, leading to the zigzag correlations discussed in Sec. I. In this section we show that the structure factor can be calculated essentially exactly for disks in a narrow channel. Our numerical results for the case $h = \sqrt{3}\sigma/2$ show a rapid change in the short-range order for $\beta f\sigma$ in the range 0.5 to 8, which corresponds to packing fractions $\phi$ in the range 0.45 to 0.50. This range of packing fractions correlates closely with the onset of activated dynamics, as we discuss later in Sec. III.

In the limit $N \to \infty$, the definition of the structure factor, Eq. (3), may be rewritten in the form

$$S(k_x, k_y) = \sum_{n=-\infty}^{\infty} S_n = 1 + 2 \text{Re} \sum_{n=1}^{\infty} S_n, \quad (6)$$

where

$$S_n = \langle e^{i(k_x x_n - x_0) + k_y (y_n - y_0)} \rangle. \quad (7)$$

At $k_x = 0$, $S(k_x, k_y)$ has a delta-function singularity and the sum on the right-hand side of (6) diverges. As we now show, for $k_x \neq 0$ the sum can be evaluated relatively simply by solving a pair of integral equations. One of these equations is known from the transfer-matrix formalism introduced by Barker [7] and applied by Kofke and Post [8] to the problem of hard disks in a channel. We follow the latter authors in using an ensemble in which the longitudinal force $f$ is constant and we refer the reader to their paper [8] for details.

Let $\psi_n(y)$ be the eigenfunctions of Kofke and Post’s integral equation

$$\lambda_n \psi_n(y_1) = \int_{-h/2}^{h/2} e^{-\beta f\sigma_1 c} \psi_n(y_0) dy_0, \quad (8)$$

where $y_0$ and $y_1$ are the $y$-coordinates of a neighboring pair of disks and $\sigma_{1,0} = [\sigma^2 - (y_1 - y_0)^2]^{1/2}$ is the distance of closest approach of their centers, measured along the $x$-axis. Approximations to the $\psi_n$ and the eigenvalues $\lambda_n$ can be found by discretizing Eq. (8), which converts it to a real-symmetric matrix eigenvalue problem. The
eigenfunctions (taken to be real) can be normalized so that
\[
\int [\psi_n(y_1)]^2 dy_1 = 1. \tag{9}
\]
In this and subsequent equations, the limits of the \( y \) integration are \(-h/2 \) and \( h/2 \), the same as in Eq. (8).

Equilibrium expectation values, such as those needed for the quantities \( S_n \) defined in (7), can be expressed as integrals involving the eigenfunction \( \psi_1 \) which corresponds to the largest eigenvalue \( \Lambda_1 \). We illustrate this for the calculation of \( S_1 \) below.

Accordingly, \( S_1 \) is given by
\[
S_1 = \langle e^{ik_x(s+\sigma_1,a)+ik_y(y_1-y_0)} \rangle = \frac{\int \psi_1(y_1) \int \int_0^\infty e^{(ik_x-\beta f(s+\sigma_1,a)+ik_y(y_1-y_0))} \psi_1(y_0) \, ds \, dy_0 \, dy_1}{\int \psi_1(y_1) \int \int_0^\infty e^{-\beta f(s+\sigma_1,a)} \psi_1(y_0) \, ds \, dy_0 \, dy_1}. \tag{11}
\]

After completing the integrals with respect to \( s \) and using the eigenvalue equation (8) and the normalization condition (9) to simplify the denominator, we obtain
\[
S_1 = \int \psi_1(y_1) \left\{ \frac{\beta f}{\lambda_1(\beta f - ik_x)} \int e^{(ik_x-\beta f)\sigma_1,a+ik_y(y_1-y_0)} \psi_1(y_0) \, dy_0 \right\} dy_1 \tag{12}
\]
in which the bracketed expression in the first line defines the action of the integral operator \( \hat{S} \) on \( \psi_1 \). More generally, for \( n \geq 1 \) one can write
\[
S_n = \int \psi_1 \hat{S}^n \psi_1 \, dy_1, \tag{13}
\]
so that the sum in Eq. (6) becomes
\[
\sum_{n=1}^\infty S_n = \sum_{n=1}^\infty \int \psi_1 \hat{S}^n \psi_1 \, dy_1 = \int \psi_1 \hat{S} \phi \, dy_1, \tag{14}
\]
where \( \phi \) is the solution of
\[
\phi = \psi_1 + \hat{S} \phi, \tag{15}
\]
which is a Fredholm equation of the second kind. Given the function \( \psi_1 \) found by solving the discretized Eq. (8), the calculation of \( \phi \) requires only the solution of the set of linear equations obtained by discretizing Eq. (15).

Finally, in terms of \( \psi_1(y_1) \) and \( \phi(y_1) \), the structure factor is given by
\[
S(k_x, k_y) = 1 + 2 \Re \int \psi_1 \hat{S} \phi \, dy_1, \tag{16}
\]
which depends on \( k_x \) and \( k_y \) via \( \phi \) and the operator \( \hat{S} \).

Numerical results are shown in Figs. 3–7. In Fig. 3, the structure factor is plotted as a function of \( \beta f \sigma \) and \( k_x \) for the case \( k_y = 0 \). For \( k_y = 0 \), the structure factor is sensitive only to correlations in the \( y \)-averaged density. Zigzag order grows rapidly for \( \beta f \sigma \) in the range 6.5 to 8, and this appears in the structure factor as a rapid movement of the first maximum with respect to \( k_x \), which follows the change in spatial periodicity. At very large values of \( \beta f \sigma \), the \( y \)-averaged density has periodicity \( \sigma/2 \), so that the position of the first maximum in \( S(k_x, k_y = 0) \) approaches \( k_x = 4\pi/\sigma \).

Figure 4 illustrates the evolution of the structure factor for \( k_y = \pi/h \). This value of \( k_y \) selects information about the difference in density between the upper and lower walls. The growing zigzag order is accompanied by the growth of a peak in the structure factor near \( k_x = 4 \) for \( \beta f \sigma > 4 \). For very large values of \( \beta f \sigma \), the difference in density between the upper and lower walls has periodicity \( \sigma \) in \( x \), so the position of the first maximum tends towards \( k_x = 2\pi/\sigma \).

Figures 5–7 show the structure factor for three values of the force for which \( S(k_x, k_y) \) is changing most rapidly: \( \beta f \sigma = 5, 7.5 \), and 10. The maxima in \( S \) grow and become narrower (in the \( k_x \) direction) as \( f \) increases and the zigzag correlations strengthen. For very large \( f \), the widths of the peaks decrease as \( (\beta f \sigma)^{-2} \). We note that this \( f \)-dependence of the peak-width is the same as is found for a one-dimensional gas of hard rods, whose structure factor was derived analytically by Zernike and Prins [20].
III. TIME-DEPENDENT BEHAVIOR

In order to study time dependent effects we have used event driven molecular dynamics based upon the code in Ref. [21]; the speed of the program was improved by using the fact that in our narrow-channel system only nearest-neighbor disks can collide. The initial state from which the dynamics evolves was created by means of the Lubachevsky–Stillinger algorithm [22], starting from a random configuration of small disks. Their diameters were slowly increased to the desired value during the course of a simulation which preceded the long runs used to study dynamics in the equilibrated system.

The force $f$ along the channel was computed by using

$$fL = \frac{N}{\beta} + \frac{1}{\tau_{\text{sim}}} \sum_c \Delta x(c) \Delta p_x(c),$$

where the sum includes all disk–disk collisions $c$ that occur during the simulation time $\tau_{\text{sim}}$.

All of our simulations were performed with $N = 10000$, $m = \beta = \sigma = 1$, and $h = \sqrt{3}/2$. To check their accuracy we calculated the equation of state and compared it with the results of the exact transfer matrix calculation [5], as shown in Fig. 8. The agreement is excellent up to $\phi = 0.65$. There is a discrepancy at $\phi = 0.70$ (but too small to be visible in the figure) as at this packing fraction the time scale for equilibration, $\tau_D$, is becoming comparable to our simulation time.

A. Time scales

To see the emergence of caging behavior it is convenient to study

$$\tilde{\Delta}^2(t) = \frac{1}{N} \sum_{i=1}^N \langle |y_i(t) - y_i(0)|^{-2} \rangle,$$

where the angled brackets indicate an average over runs with different initial states. Though it appears unnatural at first sight, this quantity was introduced in Ref. [23].
to minimize the contribution of rattlers. The ability of rattlers to move a distance of $O(\sigma)$ tends to dominate the mean-squared displacements at small times $t$. We have a similar problem here in that a few disks which border gaps are able to cross from one side of the channel without hindrance. In Fig. 9 one can see the emergence of a plateau as $\phi$ increases from 0.45 to 0.50, which suggests that caging of the disks is setting in as the zigzag order develops around $\phi_d$. It was in Ref. [1] that $\phi_d \approx 0.48$ was first identified as the onset point for activated dynamics.

It is easier to understand the behavior of the unmodified mean-square displacement $\Delta^2(t)$ as defined in Eq. (4). However, Fig. 10 shows that for this quantity the plateau is only clearly visible at values of $\phi$ above 0.60, which is well into the density regime where the timescales have a similar problem here in that a few disks which sides of the channel.

1. Final long-time limit: In the limit $t \rightarrow \infty$, $\Delta^2(t)$ reaches a finite value. (In three dimensions in the same limit, the mean-square displacement of a particle increases without limit linearly with $t$.) From its definition, $\Delta^2 = \langle y_i^2(t) + y_i^2(0) - 2y_i(t)y_i(0) \rangle$; the last term in the brackets gives $2R(t)$, which tends to zero in the long time limit, so $\Delta^2$ tends to $2\langle y_i^2 \rangle$, a quantity which is close to $2(h/2)^2$ in the limit of large $f$ when the disks are mostly pushed to the sides of the channel.

2. For small $t$, $\Delta^2(t)$ increases as $t^2$; i.e., the motion is ballistic. This regime is larger at smaller values of $\phi$, for which the gaps between disks are larger.

3. A “shoulder” begins to form around $\phi \sim 0.60$, and develops into a clearly visible plateau for $\phi \gtrsim 0.65$.

4. Beyond the “glassy” plateau for $\phi \gtrsim 0.60$, and above the ballistic regime for $\phi \lesssim 0.60$, there is a time scale $\tau$ beyond which a power-law dependence on $t$ sets in, $\Delta^2(t) \propto t^{1/2}$. This dependence

This is a clear analogue of the caging effect seen in three dimensions. It sets in at higher packing fractions $\phi$, the packing fraction at which the growing zigzag order results in the dynamics becoming activated.
on $t$ is due to the slow diffusion of defects in the zigzag arrangement of disks.

We can explain some of these features in greater detail. While activated dynamics may set in around a packing fraction $\phi \approx 0.48$, some disks still find at this density that they can easily cross the channel, and it is not until a packing fraction of 0.60 that the numbers of these "rattling" disks become negligible. The plateau represents a clear caging effect, and it lasts for a time $\tau$, the time it typically takes for a disk to cross from one side of the channel to the other by the transition state mechanism depicted in Fig. 2. Once the zigzag order sets in, the motion of the defects as in Fig. 2 dominates the behavior of most of the disks. However, there are at packing fractions around 0.48 some disks which sit at edges of large gaps between the disks and which can travel from one side of the channel to the other without hindrance. Their contribution to $\Delta^2(t)$, defined in Eq. (18) is small, which enables one to see the emergence of the caging behavior in it at lower packing fractions than for $\Delta^2(t)$.

The time scale $\tau$ for a defect to move or a disk to cross from one side of the channel was studied numerically in Ref. [1] and explained using transition state theory in Refs. [5, 24]. At high packing fractions

$$\tau \sim \tau_0 \exp(\beta f \Delta_b),$$

where $\tau_0$ is of the order of a disk collision time. The argument of the exponential in Eq. (19) can be understood from Fig. 2: $\beta f \Delta_b$ is the work done against the piston in creating the extra length $\Delta_b$ in the system which allows the defect to move. In Ref. [5] it was shown that this extra length was $\Delta_b = \sqrt{4\sigma^2 - h^2} - \sigma = \sqrt{\sigma}/\sigma - h^2$, which can also be seen directly from Fig. 2. The plateau visible at larger packing fractions in Fig. 10 will end on the time scale $\tau$.

We now turn to the details of the diffusive behavior – the dashed lines – in Fig. 10. $\Delta^2(t)$ increases as $\langle y_i(t) y_i(0) \rangle$ goes to zero. The crossing of disks from one side to the other of the channel is what drives this correlation function to zero. Fig. 2 shows that this happens where there are defects in the zigzag arrangement of the disks. Let $\theta$ be the concentration of defects, so that the number of defects is $N\theta$. This number is readily determined in numerical work using the procedure given in Ref. [3]. Figure 11 shows $\theta$ as a function of packing fraction $\phi$ obtained from the simulations and compared with the analytical approach of Ref. [5], which becomes exact at large packing fractions. As time increases the number of disks flipped by the diffusion of the defects will be of order $N\theta \sqrt{Dt}$, where $D$ is the diffusion coefficient of a defect. It was argued in Ref. [5] that at large $f$, $D\tau_D \sim 1/\theta^2$. Then

$$\tau_D \sim \tau_0 \exp(\beta f \Delta_c),$$

where $\Delta_c = \sqrt{4\sigma^2 - h^2} + \sigma - 3\sqrt{\sigma^2 - h^2}$. The physical significance of the time scale $\tau_D$ is that it is the time scale on which diffusing defects meet and annihilate [5]. It appears to be the longest time scale in the system – the time scale for full equilibration. Note that in the diffusive region

$$\Delta^2(t) \sim h^2 \sqrt{t/\tau_D}. \quad (21)$$

By extending the dashed lines in Fig. 10 to the points where they meet the analytic final values of $\Delta^2(t)$ we can estimate values for $\tau_D$. Values of $\tau_D/\tau_0$ are plotted in Fig. 12. The collision timescale $\tau_0$ was estimated from the mean collision rate per disk determined from our simulations, i.e.

$$\frac{1}{\tau_0} = \frac{n_c}{N\tau_{sim}}, \quad (22)$$

where $n_c$ is the total number of collisions that occurred during the simulation time $\tau_{sim}$. The agreement with the prediction (20) is satisfactory for the results shown in Fig. 12.

We have also used the results shown in Fig. 10 to obtain the diffusion coefficient for defects. At high density, the diffusion coefficient should be related to $\tau$ by $D\tau_D \sim \tau_0/\tau$, and so might be expected to provide confirmation of Eq. (19). To find $D$, we make use of (21) in the form

$$\Delta^2(t) \sim h^2 \theta \sqrt{D t}. \quad (23)$$

Extrapolation of the dashed lines in Fig. 10 back to $t = 1$ gives, via (23), an estimate of $\theta \sqrt{D}$. This in turn provides $D$ when we make use of the values of $\theta$ found from
our simulations. Results for $D\tau_0$ obtained in this way are plotted in Fig. 13. The results show a significant departure from Eq. (19), but there are several reasons why we might expect our procedure to give poor results for the densities of interest here. First we note that for the smaller values of the packing fraction the lines of slope 0.5 in Fig. 10 are not very convincing fits to the data: the linear portions of the curves are very short. Secondly, the mean spacing of defects given by 1/θ is not large (see Fig. 11) for φ in the range 0.4 to 0.6: interactions between defects may well modify the diffusion coefficient significantly, leading to a θ-dependent factor in the relation $D \sim 1/τ$. Finally, as shown in Ref. [5], θ itself is not a simple exponential function of $βfσ$ at these moderate values of φ, but instead can be calculated quite accurately (see Fig. 11) from a law of mass action. Thus, even if τ has the activated form (19), it is not certain that this can be ascertained from our calculation of D at the moderate densities accessible via our simulation.

Fortunately, it is not necessary to rely on an estimate of the diffusion coefficient to verify the activated behavior of τ. Bowles and Saika-Voivod [1] have made a direct determination of the channel-crossing time from their molecular dynamics simulation. As shown in Ref. [5], their results are in satisfactory agreement with Eq. (19).

Finally we comment very briefly on the time-dependent correlation function $R(t) = \langle y_i(t) y_j(0) \rangle$, mentioned in Sec. I. $R(t)$ decays to zero because of the diffusion of the defects in the regular zigzag arrangement of disks in the channel. Such a diffusive mechanism has been much studied [16] and leads to a stretched exponential decay

Finally we comment very briefly on the time-dependent correlation function $R(t) = \langle y_i(t) y_j(0) \rangle$, mentioned in Sec. I. $R(t)$ decays to zero because of the diffusion of the defects in the regular zigzag arrangement of disks in the channel. Such a diffusive mechanism has been much studied [16] and leads to a stretched exponential decay

![FIG. 12: (Color online) Rapid increase in the $τ_D$-relaxation times with longitudinal force $f$, obtained by assigning a linear fit to the diffusive region of the mean square displacements (see Fig. 10) and extrapolating to find the time where it meets the analytic final values of $Δ^2(t)$. The dashed line fits the exponential trend and becomes an increasingly better fit as $f$ becomes large, i.e. in the limit $φ \rightarrow φ_{max}$. The circled data point, corresponding to $φ = 0.7$, deviates from this trend: as noted in the caption to Fig. 11, the system failed to reach equilibrium for this value of $φ$.

![FIG. 13: (Color online) Variation of diffusion constant $D \propto 1/τ$ with longitudinal force $f$ using the $y$-intercept of linear fits to the diffusive regions shown in Fig. 10. $R(t) \sim \exp(-1/τ_D)$. We have not attempted a direct verification of this behavior of $R(t)$, as it is expected only for very large times, $t \gg τ_D$.

### B. Dynamical heterogeneity

We turn now to a study of overlap correlations, which correlate the configuration of the system at time $t$ with a configuration drawn from the equilibrium ensemble at time $t = 0$. Studies of such correlations reveal the existence of dynamical heterogeneities. In particular we shall make use of the overlap function

$$Q(t) = \frac{1}{N} \sum_{i,j} w[y_i(t), y_j(0)],$$

where $w[y_i, y_j] = \frac{1}{2}(\text{sign}(y_i) \text{sign}(y_j) + 1)$. The function $w$ is unity if $y_i$ and $y_j$ are on the same side of the channel and is zero otherwise. A very similar quantity has been studied in three dimensions: in that case, $w[r_i, r_j]$ is taken to be 1 if $|r_i - r_j| \leq 0.3σ$ and is zero otherwise [12, 13, 17]. A significant difference between this latter definition and our own $w[y_i, y_j]$ is that our quantity does not depend on the $x$-coordinates of disks $i$ and $j$. This modification eliminates the effect (specific to our one-dimensional problem) of large fluctuations in the $x$-coordinates of disks, which can lead to a small overlap between two configurations that would otherwise be identical when described in terms of defects in the zigzag arrangement of disks. A quantity much studied for three-dimensional systems is $χ_4(t)$, which is defined in terms of the variance of $Q(t)$ via

$$χ_4(t)/N = \langle Q(t)^2 \rangle - \langle Q(t) \rangle^2.$$
the timescale $\tau_\alpha$ and then decays back to zero; but for
our system there is no decay back to zero. The difference
arises because the quantity we study is similar to that
studied in spin glasses. This difference has been discussed
at length in Ref. [18].

We have also determined the dynamical length scale
from the four point correlation function $\tilde{S}_4(k_x, t)$ defined
as

$$\tilde{S}_4(k_x, t) = \frac{1}{N} \langle Q(k_x, t) Q^*(k_x, t) \rangle,$$

(26)

where

$$Q(k_x, t) = \sum_j e^{-ikxjL/N} y_j(t) y_j(0)$$

(27)

and $k_x = 2\pi m/L$, where $m = 1, 2, \ldots, N - 1$. The
$k_x$-dependence of $\tilde{S}_4(k_x, t)$ follows a roughly Lorentzian
form as in Refs. [13, 17]; i.e., it fits to the form

$$\tilde{S}_4(k_x, t) \approx \frac{A(t)}{1 + k_x^2 \xi^2(t)}$$

for $k_x \neq 0$.

We present results for the dynamical correlation length
$\xi_4(t)$ at two values of $t$. At $t = \tau_D$ the system has reached
equilibrium, so that

$$\tilde{S}_4(k_x, \tau_D) \approx \frac{1}{N} \sum_{p,q} e^{-ikx(p-q)L/N} (y_p y_q)^2.$$

(28)

Then, by using Eq. (2), one finds the correlation length
$\xi_4(\tau_D)$ to be $\xi/2$. However, $\xi$ is the number of disks for
which zigzag order persists. This dimensionless quantity
is calculated from the two largest eigenvalues, $\lambda_1$ and $\lambda_2$, of the integral equation (8), using

$$\xi = 1/\ln(\lambda_1/|\lambda_2|).$$

(29)

To convert $\xi$ to a length one has to use Eq. (1). Then
$\xi_4(\tau_D) \approx \pi \sigma^2 \xi/(8H_D\phi) \approx 0.21 \xi/\phi$. The results pre-
sented in Fig. 15 are in good agreement with this ex-
pectation.

If we choose a value for $t$ less than the equilibration
time $\tau_D$, then $\xi_4(t)$ is less than $\xi/2$. On the time scale
$\tau$, the time for which particles are caged, $\xi_4(\tau)$ is not
proportional to $\xi$ and the results in Fig. 16 show it instead
to be of the order of $\sigma$ for a wide range of $\phi$ values. This
value for $\xi_4(\tau)$ is understandable, as on the time scale $\tau$
the active regions are centered on the defects, whose size
is of order $\sigma$.

![FIG. 14: (Color online) $\chi_4(t)$ as a function of time $t$. It reaches
its largest values at a time corresponding to $\tau_D$.](image1)

![FIG. 15: (Color online) Plot of the dynamical length scale $\xi_4(\tau_D)$ versus the static length scale $\xi$ of zigzag order.](image2)

![FIG. 16: (Color online) Plot of the dynamical length scale $\xi_4(\tau)$ versus the packing fraction $\phi$.](image3)
cleated. In other words, our system displays many of the features associated with dynamical heterogeneity [27].

IV. CONCLUSIONS

There is no doubt that there are striking similarities between the behavior of our system and that found for hard spheres in three dimensions. But there are some important differences too. We believe that our work strongly supports the common idea [11–15] that glass behavior is a consequence of geometry and the local arrangements around the molecules in the supercooled liquid. Our system is sufficiently simple that we can quantitatively relate its dynamical features to structural features. The three-dimensional problem is much richer and success along these lines is probably only just starting [15].

The caging effects in our system mimic those seen in three dimensions. These are normally modeled by mode-coupling theory. Mode-coupling theory is a form of mean-field theory and becomes exact in the limit of infinite dimensions [28, 29]. In that limit it is associated with a genuine dynamical transition, but it is thought that in finite dimensions this transition is avoided. Our system is effectively one dimensional and as far as is possible from the limit of infinite dimensions. We are skeptical that the features which we see in the dynamics could be explained in any way by mode-coupling arguments. They seem instead to be more naturally explained by dynamical processes associated with the developing structural order in the system. We suspect that the same might be true of three-dimensional systems.

One feature of our system is the existence of two time scales, $\tau$ and $\tau_D$. In three dimensions only the analogue of $\tau$, which would be $\tau_\alpha$, is normally discussed. The existence of a second, perhaps much longer time scale, might possibly have been overlooked. Or the existence of this second time scale could just be a special feature of the narrow channel system. One would expect two time scales to exist in three dimensions if escaping the cage can be associated with just moving a defect; the longer time scale would then be associated with the time that the defects need to reach equilibrium.

[1] R. K. Bowles and I. Saika-Voivod, Phys. Rev. E 73, 011503 (2006).
[2] M. Z. Yamchi, S. S. Ashwin and R. K. Bowles, Phys. Rev. Lett. 109, 225701 (2012).
[3] S. S. Ashwin, M. Zaeifi Yamchi, and R. K. Bowles, Phys. Rev. Lett. 110, 145701 (2013).
[4] S. S. Ashwin and R. K. Bowles, Phys. Rev. Lett. 102, 235701 (2009).
[5] M. J. Godfrey and M. A. Moore, Phys. Rev. E 89, 032111 (2014).
[6] M. J. Godfrey, M. A. Moore, arXiv:1411.4893.
[7] J. A. Barker, Aust. J. Phys. 15, 127 (1962).
[8] D. A. Kofke and A. J. Post, J. Chem. Phys. 98, 4853 (1993).
[9] P. Gurin and S. Varga, J. Chem. Phys. 139, 244708 (2013).
[10] G. Parisi and F. Zamponi, Rev. Mod. Phys. 82, 789 (2010).
[11] A. Malins, J. Eggers, H. Tanaka, and C. F. Royall, Faraday Discuss. 167, 405 (2013).
[12] C. P. Royall and S. R. Williams, Phys. Rep. (in press); arXiv:1405.5691.
[13] C. P. Royall, A. Malins, A. J. Dunleavy, and R. Pinney, 7th IDMRC: Relaxation in Complex Systems, J. Non-Crystal Solids 407, 34 (2015).
[14] G. Tarjus, S. A. Kivelson, Z. Nussinov, and P. Viot, J. Phys.: Condens. Matter 17, R1143 (2005).
[15] E. D. Cubuk, S. S. Schoenholz, J. M. Rieser, B. D. Malone, J. Rottler, D. J. Durian, E. Kaxiras, and A. J. Liu, arXiv:1409.6820.
[16] S. Redner and K. Kang, J. Phys. A: Math. Gen. 17, L451 (1984).
[17] N. Lačević, F. W. Starr, T. B. Schröder, and S. C. Glotzer, J. Chem. Phys. 119, 7372 (2003).
[18] J-P. Bouchaud and G. Biroli, Phys. Rev. B 72, 064204 (2005).
[19] J. Frenkel, Kinetic Theory of Liquids, Oxford University Press (1946).
[20] F. Zernike and J. A. Prins, Z. Phys. 41, 184 (1927).
[21] M. Skoge, A. Donev, F. H. Stillinger, and S. Torquato, Phys. Rev. E 74, 041127 (2006).
[22] B. D. Lubachevsky and F. H. Stillinger, J. Stat. Phys. 60, 561 (1990).
[23] A. Ikeda, L. Berthier, and G. Biroli, J. Chem. Phys. 138, 12A507 (2013).
[24] M. Barnett-Jones, P. A. Dickinson, M. J. Godfrey, T. Grundy, and M. A. Moore, Phys. Rev. E 88, 052132 (2013).
[25] L. Berthier and T. A. Witten, Phys. Rev. E 80, 021502 (2009).
[26] W. Koh, S. Roldán-Vargas, and L. Berthier, Phys. Procedia 34, 70 (2012).
[27] L. Berthier and G. Biroli, Rev. Mod. Phys. 83, 589 (2011).
[28] G. Szamel, Europhys. Lett. 91, 56004 (2010).
[29] T. Rizzo, Phys. Rev. E 87, 022135 (2013).