Gardner Transition in Physical Dimensions

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(Received 18 August 2017; revised manuscript received 19 January 2018; published 29 May 2018)

The Gardner transition is the transition that at mean-field level separates a stable glass phase from a marginally stable phase. This transition has similarities with the de Almeida–Thouless transition of spin glasses. We have studied a well-understood problem, that of disks moving in a narrow channel, which shows many features usually associated with the Gardner transition. We show that some of these features are artifacts that arise when a disk escapes its local cage during the quench to higher densities. There is evidence that the Gardner transition becomes an avoided transition, in that the correlation length becomes quite large, of order 15 particle diameters, even in our quasi-one-dimensional system.

DOI: 10.1103/PhysRevLett.120.225501

In a remarkable series of papers (see Ref. [1] for a review and references) the large-dimension limit of the hard sphere fluid has been solved. This program of calculation provides the mean-field description relevant for the dynamical glass phase transition, the Kauzmann ideal glass transition, the Gardner transition, and the geometrical description of the properties of jammed states. The next step is of course to understand what happens in finite dimensions. In this Letter we argue that at least the Gardner transition is not a real transition in physical dimensions, $d \leq 3$. The Gardner transition is the transition associated with the emergence of a complex free-energy landscape composed of many marginally stable sub-basins contained within a larger glass metabasin [2]. It is thus similar to a state of a spin glass in a phase with broken replica symmetry [3]. In fact the field theory of the Gardner transition is closely related to that of the Ising spin glass problem in a random magnetic field—the de Almeida–Thouless transition [4].

It has been argued for some time that the de Almeida–Thouless transition only occurs in systems with dimensions $d > 6$ [5–7], but this is still controversial [8–11]. Furthermore, in two dimensions there is not even a spin glass transition in zero field, and none has been detected either in a finite field. Nevertheless, both simulations [12] and experiments on hard disks in two dimensions [13,14] seem to provide evidence for a Gardner transition during compression; i.e., that glass systems that start with the same particle positions but with different particle velocities, can, by the end of the compression, be in mutually inaccessible states. To understand what might be going on, we have applied the methods of Ref. [12] to a system of hard disks moving in a narrow channel, which is a model that has previously been studied in some detail [15–25]. Our system, being one dimensional, cannot have a true phase transition. We find that we can produce the same kinds of behavior that other investigators studying two- and three-dimensional hard sphere systems have explained in terms of the state-following Gardner transition. However, because of the simplicity of our system we can give a full explanation of our observations. We find that some of the behavior that has been ascribed to the Gardner transition (such as a nontrivial change in the distribution of an order parameter) arises when the timescales associated with the quench used in the state-following investigations are long enough for there to be a significant chance of a disk escaping its cage by crossing the channel. Our results thus do not imply that there are glasses that are stable and glasses that are marginal, with the Gardner transition separating the two [12]. Effects that have been attributed to the Gardner transition in two- and three-dimensional hard-sphere systems may also have a simple explanation, connected with just a few disks or spheres escaping their cages on the time scale of the quench. In a recent preprint, Scalliet *et al.* [26] have invoked a similar mechanism to help explain the absence of a Gardner transition in a system of particles that interact via a soft potential. However, for our system of hard disks we can provide evidence that there is an avoided Gardner transition at which the correlation length grows to a large value, ≈15 particle diameters, but does not diverge. For hard spheres in three dimensions, which is closer to the mean-field limit of infinite dimension, we suspect that the equivalent length scale will be larger still and exceed the linear dimensions of the systems that were simulated [12], making it impossible to distinguish a true phase transition from an avoided one.

Details of the system that we are studying are given in Fig. 1. The packing fraction ϕ is defined as $\phi = N\pi\sigma^2/(4H_dL)$, where N is the number of disks in a channel of length L. The channel width H_d was taken to be 1.95σ, where σ is the diameter of a disk; we have previously made extensive transfer-matrix [27] calculations of thermodynamic properties and correlation functions for this case [16].

The dynamics in this system start to slow as “zigzag” order sets in above a packing fraction $\phi = \phi_d \approx 0.48$

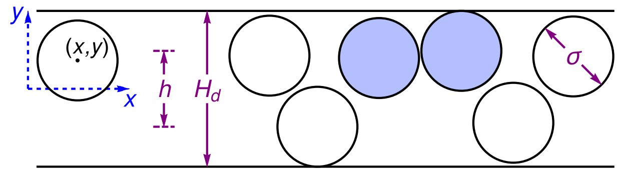

FIG. 1. The system of hard disks in a channel. The distance H_d is the width of the channel, σ is the diameter of each disk, and $h = H_d - \sigma$ is the width of the channel accessible to the centers of the disks. For the coordinates (x, y) of the disk, y is measured from the center line of the channel. The blue shaded disks can be regarded as a *defect* in the zigzag arrangement of the disks that is favored at high density.

[15–17]. This kind of order is characterized by successive values of y_i taking opposite signs (see Fig. 1). The zigzag order can be interrupted by defects where successive y_i are of the same sign; the correlation length ξ for zigzag order is approximately half the average distance between defects [17]. These defects play an important role in our analysis of the dynamics of the system. (Defects of one kind or another seem to play an important role across the whole of glass physics [28–31].) Their spacing increases rapidly with increasing ϕ, such that ξ passes 2000 at $\phi = 0.7206$ and reaches $\xi = 2.3 \times 10^6$ at $\phi = 0.76$.

We use event-driven molecular dynamics for our simulations. The number of disks N is taken to be 4000 and periodic boundary conditions are applied in the x direction. We start the system in an initial "equilibrium" state of packing fraction $\phi_i \geq 0.70$ and use the Lubachevsky-Stillinger algorithm [32] to compress it to values of $\phi > \phi_i$ on a time scale much less than the α relaxation time at the packing fraction ϕ_i. We put the word equilibrium in quotes as for the packing fractions studied there should be no or very few defects present in the system, but we have found there are typically ~10 present, owing to imperfect equilibration. During the compression, the diameter of the disks is increased at a rate $\dot{\sigma}$ and the width of the channel is also increased so that the relation $H_d = 1.95\sigma$ is maintained throughout the compression [19]. Such a compression is "state following" if on the time scale of the quench most of the disks remain caged and do not move far from their initial positions. The kinetic energy of the disks increases during the compression, so, after the quench, the disks are assigned new velocities drawn from a Maxwellian distribution for particles of mass $m = 1$ at a reciprocal temperature $\beta = 1$. The unit of length is chosen so that $\sigma = 1$.

We judge the extent of caging by studying the mean-squared y displacements (MSD) of the disks from their initial positions $y_i(t_W)$,

$$\Delta(t, t_W) = \frac{1}{N}\sum_{i=1}^{N}\langle[y_i(t + t_W) - y_i(t_W)]^2\rangle, \qquad (1)$$

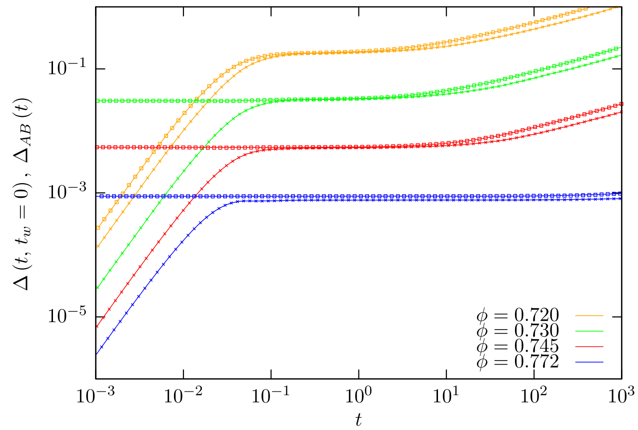

FIG. 2. Mean-squared displacements $\Delta(t, t_W = 0)$ [crosses] and $\Delta_{AB}(t)$ [squares] as a function of time t, where the quench was started from the initial equilibrium state of packing fraction $\phi_i = 0.720$, which contains defects, and compressed to packing fractions $\phi = 0.730$, 0.745, and 0.772. Data have been multiplied by 5^k, with $k = 0, \ldots, 3$ for $\phi = 0.772, \ldots, 0.72$, respectively, so the data points do not obscure each other. Note that for $\phi = \phi_i = 0.720$ there was no quench; no disks crossed the channel in this case, so Δ_{AB} follows Δ closely.

averaged over both thermal fluctuations and initial states. The time t starts after a waiting time t_W, when the compression has reached a chosen target packing fraction ϕ. The MSD $\Delta(t, t_W)$ grows initially as t^2 from zero at $t = 0$ (see Fig. 2). For our choice of channel width the disks cannot pass each other so the ordering $0 \leq x_1 < x_2 < \cdots < x_N < L$ is preserved at all times, and the disks are always caged in the x direction. Caging in the y direction is indicated by the presence of a plateau in $\Delta(t, t_W = 0)$; the plateau is present for packing fractions $\phi > 0.7$ (see Fig. 2), rather than for $\phi \gtrsim \phi_d$, as seen in two- and three-dimensional systems. Caging is a prerequisite for seeing the state-following Gardner transition [12]. In contrast to the studies of two- and three-dimensional systems, $\Delta(t, t_W)$ cannot increase indefinitely as $t \to \infty$ since in our system $|y_i| \leq h/2$. The α relaxation time τ_α is defined as the time at which Δ leaves the plateau, which in our system is the result of disks crossing from one side of the channel to the other; quantitative estimates for τ_α are given in the Supplemental Material [33]. Channel crossing is catalyzed by the presence of the defects; if defects are absent, they must first be nucleated in pairs [15,16], and this is a process that takes much longer than the α relaxation time [15]. We have prepared initial states free of defects and have found for such states that we cannot observe the end of the plateau on the times for which we could run the simulation; this is shown in Fig. 3. In such systems there is no channel crossing on accessible time scales.

To see Gardner-like behavior, one must study independent copies A and B of the system [12]. Initially, the disks in A and B have identical coordinates (x_i, y_i), taken from the

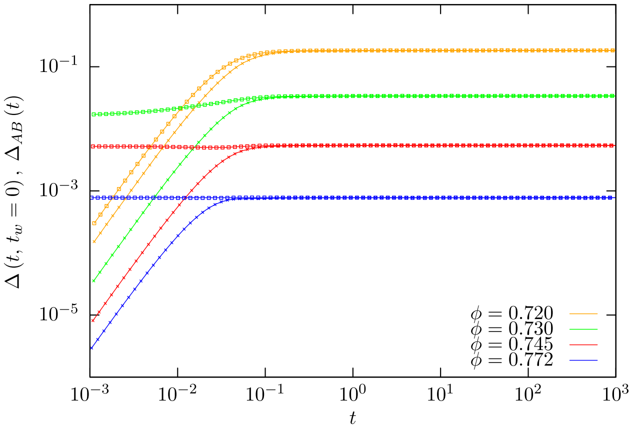

FIG. 3. Mean-squared displacements $\Delta(t, t_W = 0)$ [crosses] and $\Delta_{AB}(t)$ [squares] as a function of time t, where the quench was started from an initial state of packing fraction $\phi_i = 0.720$, which contained *no defects*, and compressed to packing fractions 0.730, 0.745, and 0.772. Data have been multiplied by 5^k, with $k = 0, \ldots, 3$ for $\phi = 0.772, \ldots, 0.72$, respectively, so the data points do not obscure each other. Notice that there is no splitting on the plateau between Δ and Δ_{AB}.

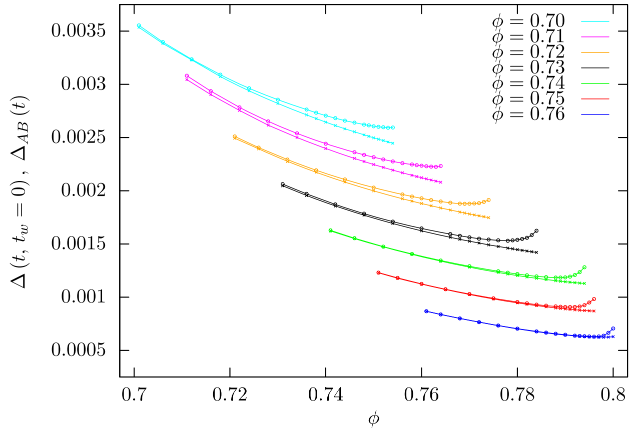

FIG. 4. Comparison of the plateau values of Δ and Δ_{AB} for the system with defects showing that the two separate, with $\Delta_{AB} > \Delta$, as ϕ increases. For clarity, the data have been shifted up by $0.00025k$, where $k = 0, 1, \ldots, 6$ for $\phi = 0.76, 0.75, \ldots, 0.70$, respectively. Error bars are insignificant in comparison to the size of the data points.

equilibrium state at ϕ_i, but they are assigned different velocities drawn from a Maxwellian distribution. The quantity studied is the MSD of their separation,

$$\Delta_{AB}(t) = \frac{1}{N}\sum_{i=1}^{N}\langle[y_{A,i}(t) - y_{B,i}(t)]^2\rangle. \qquad (2)$$

In Fig. 2 we show our results for Δ and Δ_{AB} as a function of time for various initial packing fractions. At the larger packing fractions, they show a feature that has been previously been regarded as a signature of the Gardner transition, a difference between the plateau values of $\Delta(t, t_W)$ and $\Delta_{AB}(t)$ [12]. These have been plotted against ϕ in Fig. 4. To extract the plateau values, we used the method of Ref. [12], in which the MSD starting from a given equilibrium state are rescaled to a universal curve of Δ/Δ_m against t/t_m, where Δ_m and t_m are ϕ-dependent scaling factors.

Plateau values of $\Delta(t, t_W)$ and $\Delta_{AB}(t)$ can also be calculated on the assumption that no disk crosses the channel, so that in Eq. (1), $y_i(t + t_W)$ and $y_i(t_W)$ take the same sign; similarly, $y_{A,i}(t)$ and $y_{B,i}(t)$ take the same sign in Eq. (2). Then, on the plateau, $\Delta(t, t_W)$ and $\Delta_{AB}(t)$ can be approximated by

$$\Delta(t, t_W) = \Delta_{AB}(t) \approx 2(\langle y^2\rangle - \langle|y|\rangle^2). \qquad (3)$$

We calculate $\langle y^2\rangle$ and $\langle|y|\rangle^2$ using the transfer-matrix method of Ref. [16]; the results from Eq. (3) are indistinguishable from the plateau values of Δ and Δ_{AB} seen in Fig. 3.

In recent work, Scalliet *et al.* [26] have shown that a splitting of the plateau values of Δ and Δ_{AB} is not of itself sufficient to show that there is a state-following Gardner transition that requires the stable glass to split into marginally stable sub-basins where the two copies A and B sometimes end up. The split can instead be due to a small subset of the particles being frozen into slightly different locations in the two copies. As we shall see, an explanation of this kind also applies to our system of disks in a channel.

For very large times, $t \gg \tau_\alpha$, disks may cross the channel, so that $\langle y_i(t + t_W) y_i(t_W)\rangle \to 0$; thus, $\Delta(t, t_W)$ and $\Delta_{AB}(t)$ will both reach a *second* plateau at the equilibrium value, $2\langle y_i^2\rangle \approx h^2/2$. However, this long-time limit is not relevant to the state-following Garder transition, where one is interested in times such that $\Delta(t, t_W)$ and $\Delta_{AB}(t)$ are still on their first plateau. At the α relaxation time disks begin to escape their cages by crossing from one side of the channel to the other. Channel crossing is strongly suppressed in the absence of defects; thus, for a system with no defects there can be no splitting in the first plateau values of Δ and Δ_{AB} at large packing fractions; this is confirmed by the results shown in Fig. 3. When defects are present, Δ_{AB} and Δ separate, as shown in Fig. 4.

To understand the cause of the splitting we turn to the histograms of the plateau values of Δ and Δ_{AB} in Fig. 5. In all cases, one can see that the distribution of Δ_{AB} has acquired additional peaks compared to the distribution for Δ. These arise because, during the quench from ϕ_i to ϕ, in some of the copies of the system one or more disks belonging to defects have managed to escape their cages and have crossed to the other side of the channel. The splitting of the peaks due to channel crossing would be approximately h^2/N, which is consistent with the data in Fig. 5. It should be understood that this process is possible

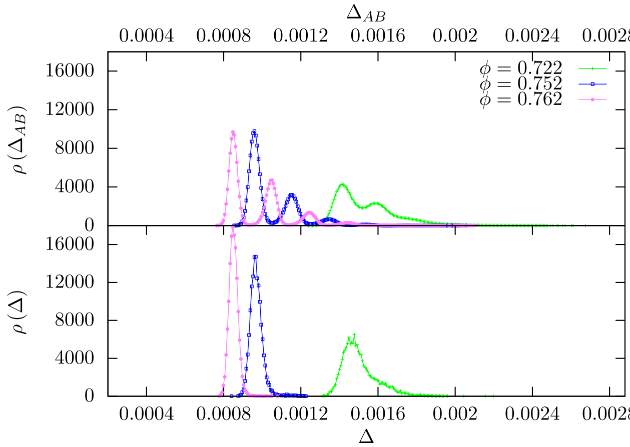

FIG. 5. Distribution of plateau values of Δ, $\rho(\Delta)$ and of Δ_{AB}, $\rho(\Delta_{AB})$ following a quench from $\phi_i = 0.71$ to the packing fractions $\phi = 0.722$, 0.752, and 0.762. The smaller peaks in $\rho(\Delta_{AB})$ are due to one or more disks crossing the channel during the quench.

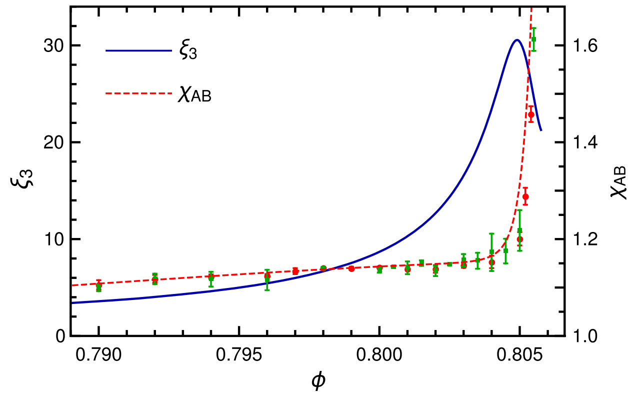

FIG. 6. The correlation length ξ_3 as a function of the packing fraction ϕ, and the susceptibility χ_{AB}, calculated using the transfer matrix procedure. Data points show values of χ_{AB} obtained in quenches from a state with no defects, starting from $\phi_i = 0.76$ (red circles) and $\phi_i = 0.78$ (green squares).

even though the compression time is much shorter than τ_α: Fig. 5 shows that disks have crossed in only a few of the copies of the system, despite the presence of $\sim$10 defects in each copy. Our explanation of why there is a splitting of Δ and Δ_{AB} does not invoke a Gardner transition and is similar to that given in Ref. [26] for soft spheres, except that in our system we can explicitly identify the localized defects associated with the disks that move.

Nevertheless, evidence for an avoided Gardner transition in our hard-disk system can be found by studying the appropriate correlation length. Following Ref. [12], we define this from the large-distance behavior of the correlation function associated with $\Delta^i_{AB} = (y_{A,i} - y_{B,i})^2$, i.e., $G^0_P(k) = \langle u_i u_{i+k} \rangle$, where $u_i = \Delta^i_{AB}/\Delta_{AB} - 1$ and Δ_{AB} is the value on the plateau which is given by Eq. (3). For our system of disks moving in a narrow channel, $G^0_P(k)$ can be obtained from a transfer-matrix calculation in the high-density regime where channel crossing can be ignored [33].

The correlation function shows a complicated behavior for small separations k, but for large k it decreases exponentially as $G^0_P(k) \sim (-1)^k \exp[-k/\xi_3]$. In Fig. 6 we show how the correlation length ξ_3 depends on the packing fraction ϕ. The length scale ξ_3 (which can also be calculated from the eigenvalues of the transfer matrix [16,33]) rises to its maximum value at $\phi = 0.8049$ before falling again. Such behavior is typical of an avoided transition. Expressed as a distance, $\xi_3 L/N \approx 0.50\xi_3\sigma$, the maximum value of the correlation length is approximately 15σ.

The susceptibility χ_{AB} is defined, following Ref. [26], as $\chi_{AB} = N\mathrm{var}(\Delta_{AB})/\mathrm{var}(\Delta^i_{AB})$, which is equivalent to

$$\chi_{AB} = \frac{\Delta^2_{AB}}{\mathrm{var}(\Delta^i_{AB})} \sum_{k=-\infty}^{\infty} G^0_P(k). \tag{4}$$

Figure 6 shows that χ_{AB} grows rapidly as the density increases, with no sign of leveling off as might have been expected for an avoided transition. This is because the sum in Eq. (4) is dominated by the small k region (see the Supplemental Material [33]).

To summarize, the splitting between the plateau values of Δ and Δ_{AB} does not provide strong evidence for a Gardner transition, as it is an artifact that arises when there is a significant chance that a disk will escape its cage during the quench. A similar explanation may apply to the observations reported in Refs. [12,13]. Our study of the correlation length ξ_3 shows that the Gardner transition is an avoided transition for our one-dimensional system of hard disks. The large magnitude of the correlation length at the avoided transition suggests that for hard spheres in three dimensions the equivalent length scale could be very large; thus we anticipate that it will be challenging for simulations to distinguish an avoided Gardner transition from a true phase transition. Nevertheless, we expect the Gardner transition to be an avoided transition for any potential, hard or soft, in dimensions $d \leq 6$.

We should like to thank Ludovic Berthier and Francesco Zamponi for sharing their insights.

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[33] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.120.225501 for explanations of how the transfer-matrix method was used to obtain approximate results for τ_α, $G_P^0(k)$, and χ_{AB}.