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Effects of short-range attraction on Jamming transition*

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Enormous progresses to understand the jamming transition have been driven via simulating purely repulsive particles which were somehow idealized in the past two decades. While the attractive systems are both theoretical and practical compared with repulsive systems. By studying the statistics of rigid clusters, we find that the critical packing fraction ϕ_c varies linearly with attraction μ for different system sizes when the range of attraction is short. While for systems with long-range attractions, however, the slope of ϕ_c appears significantly different, which means that there are two distinct jamming scenarios. In this paper, we focus our main attention on short-range attractions scenario and define a new quantity named "short-range attraction susceptibility" χ_p, which describes the degree of response of the probability of finding jammed states p_j to short-range attraction strength μ. Our central results are that χ_p diverges in the thermodynamic limit as $\chi_p \propto |\phi - \phi_c^\infty|^{-\gamma_p}$, where ϕ_c^∞ is the packing fraction at the jamming transition for the infinite system in the absence of attraction. χ_p obeys scaling collapse with a scaling function in both two and three dimensions, illuminating that the jamming transition can be considered as a phase transition as proposed in previous work.

Keywords: short-range attraction, Jamming transition, short-range attraction susceptibility

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1. Introduction

As the packing fraction increases, complex fluids such as colloids, emulsions, foams, and granular materials often undergo a transition from a liquid-like state to a solid-like state when the jamming transition occurs.[1–3] A large number of theoretical and numerical studies on the jamming transition have been carried out by studying packings of frictionless spheres interacting via pure repulsions.[4–13] As the repulsive systems are too idealized and attractive interaction often exists between particles which can potentially change the physics of jamming transition, the jamming of sticky particles has attracted much more attention in recent years.[14–17]

The earliest study of jamming transition of attractive particles can be traced back to an early experimental study,[14] which proved that the glass transition temperature or the non-vanishing yield stress may extend to low packing fractions because of the presence of attraction. Lois *et al.*[18] showed that jamming transition in particulate systems with strongly attraction belongs to a new universality class, distinct from repulsive jamming and percolation transition without force balance constraints. Zheng *et al.*[19] showed that considering the presence of weak attraction in particle system, the static structure of shear-driven solids was sensitive to the change of packing fraction and shear stress. By simulating the soft particles with an attractive shell, Koeze *et al.*[20] presented an evidence for two distinct jamming scenarios. For weak attraction systems, a spanning cluster appears suddenly at the jamming transition point ϕ_c while for strongly attraction systems, the rigid cluster undergoes a continuous growing. And they proposed that the weakly attractive scenario is a finite size effect, means that sufficiently large systems will fall in the strongly attractive universality class no matter how weak the attraction is. But it remains unclear when the attraction tends to disappearance, what are the characteristics of the susceptibility of short-range attraction.

As we all know that the magnetic susceptibility can be defined by assuming a "ghost spin" in the limit of vanishing density in spin systems.[21] In the case of percolation or correlated percolation, susceptibility corresponds to the addition of low-probability "short routes to the infinite cluster".[22,23] The pinning susceptibility can be calculated by considering the responses of "ghost pins" in the limit of vanishing pinning.[24] Similarly, if the attraction acts as a small perturbation, another way to compute a susceptibility is to calculate the response to a perturbation. We expect the "short-range attraction susceptibility" to show critical behavior in the thermodynamic limit on jamming systems by calculated the responses of "ghost attractions" when the attraction of particles is vanishing. We define the short-range attraction susceptibility in the limit of vanishing attraction

$$\chi_p = \lim_{\mu \to 0} \frac{\partial p_j(\phi, N, \mu)}{\partial \mu}, \tag{1}$$

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which describes the degree of response of the probability of finding jammed states p_j to short-range attraction strength μ.

In this work, we concentrate our attention on the effects of dilute attraction on the jamming transition. We find that no matter how the system increases, we can always find such an estimated crossover attraction strength μ^* which can be defined to separate the short and long range attractions based on the behavior of the jamming transition point. In the short-range attraction regime, we define the short-range attraction susceptibility χ_p as the response of jamming probability to the increasing of attraction strength, which should be constant in the limit of small attraction.[21–23] Our central result is that the short-range attraction susceptibility diverges in the thermodynamic limit as $\chi_p \propto |\phi - \phi_c^{\infty}|^{-\gamma_p}$, with $\gamma_p = 2.0$ in two-dimensional (2D) system and $\gamma_p = 1.57$ in three-dimensional (3D) system, where ϕ_c^{∞} is the jamming threshold in the absence of attraction. Furthermore, such susceptibility obeys scaling collapse with a scaling function in both two and three dimensions, illuminating that the jamming transition can be considered as a phase transition as proposed in previous work.[24]

We simulate N attractive soft spheres in a fixed square (two dimensions, $d = 2$) or cubic (three dimensions, $d = 3$) box with periodic boundary conditions. The diameter ratio of the large to small spheres is 1.4 and their numbers in the box are equal to avoid crystallization. The inter particle potential is[7,19,25]

$$U(r_{ij}) = \begin{cases} \dfrac{\varepsilon}{2}\left(|1-\dfrac{r_{ij}}{d_{ij}}|^2 - 2\mu^2\right), & \dfrac{r_{ij}}{d_{ij}} \le 1+\mu, \\ -\dfrac{\varepsilon}{2}\left(1+2\mu-\dfrac{r_{ij}}{d_{ij}}\right)^2, & 1+\mu < \dfrac{r_{ij}}{d_{ij}} \le 1+2\mu, \\ 0, & \dfrac{r_{ij}}{d_{ij}} > 1+2\mu, \end{cases} \quad (2)$$

where r_{ij} is the separation between particles i and j, and d_{ij} is the sum of their radii, and μ is a tunable parameter used to control the range and strength of attraction. We generate static states at fixed packing fraction by applying the fast inertial relaxation engine (FIRE) method[26–28] to minimize the potential energy $U = \sum_{ij} U(r_{ij})$ of random configurations, where the sum is over all pairs of particles. The contact force law for a pair of particles with an attractive shell used in our simulations is shown in the lower inset of Fig. 1(b). We set the units to be the particle mass m, the characteristic energy scale of the potential ε, and the small particle diameter d_s.

The system is characterized by its packing fraction ϕ, number of particles N, and the attraction strength μ. We calculate the probability of finding jammed states $p_j(\phi, N, \mu)$ when the temperature changes rapidly from infinite ($T = \infty$) to zero ($T = 0$). In our simulation, each particle's initial location is generated randomly by the standard preparation protocol.[7] The probability of finding jammed states $p(\phi)$ for different values of attraction strength are calculated by minimizing the potential energy of 10000 random states. When the energy of the system is minimized, it is considered that the jammed configuration is obtained when the absolute value of pressure is greater than 10^{-12}. The pressure can be negative in a jammed solid with attractive interactions, but it has little effect on high density system.[29] Which means that the existence of negative pressure has little effect on our results.

2. Results

2.1. Critical attraction strength

As shown in Fig. 1(a), we vary the attraction strength μ from 5×10^{-5} to 5×10^{-3} to study the jamming probability $p_j(\phi, N, \mu)$ at $T = 0$, and the zero attraction case is shown as well. The black square line shows that there is a rapid increase of $p(\phi)$ at a packing fraction close to $\phi \approx 0.84$ where there is no attraction ($\mu = 0$). At fixed μ, we approximate $p_j(\phi, N, \mu)$ into a complementary error function[30]

$$p_j(\phi, N, \mu) = \frac{1}{2}\mathrm{erfc}\left[\frac{\phi_c(N,\mu) - \phi}{\sqrt{2}w(N,\mu)}\right], \quad (3)$$

where ϕ_c is the critical packing fraction at which $p_j(\phi, N, \mu) = 0.5$ and w is the width of $p_j(\phi, N, \mu)$. It is clear that with the attraction strength increasing, the change of $p(\phi)$ becomes more gradual and $\phi_c(N, \mu)$ becomes smaller, and there is a distinct

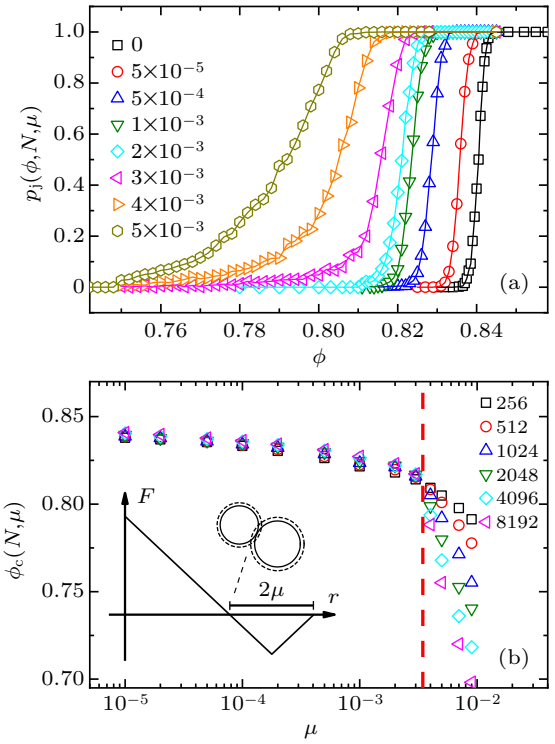


Fig. 1. (a) Probability of finding jammed states $p_j(\phi, N, \mu)$ versus packing fraction ϕ for varying attraction strength μ from 5×10^{-5} to 5×10^{-3} in 2D system with size $N = 1024$. The solid curves are the fits using Eq. (3). (b) The critical packing fraction ϕ_c as a function of attraction strength μ for 2D systems with different system sizes $N = 256$, 512, 1024, 2048, 4096, and 8192. Lower inset shows the contact force law for a pair of particles with an attractive shell used in our simulations.

difference between the two fitting results of $\mu = 2 \times 10^{-3}$ and 3×10^{-3}. The error function is no longer applicable on the bottom-left when the attraction strength is greater than a certain value. To determine the transition attraction strength μ^* quantitatively, we study the relationship between the critical packing fraction ϕ_c and attraction strength μ. As shown in Fig. 1(b), for different system sizes, their ϕ_c curves are almost identical at the lower attraction strength. However, they diverge suddenly from each other when $\mu > 2.5 \times 10^{-3}$. This result is in excellent agreement with previous work.[20,31] Therefore we find an estimated crossover attraction strength $\mu^* = 2.5 \times 10^{-3}$ to distinguish the short and long range attractions. In the rest of this paper, we will focus on the short-range attraction regime ($\mu < \mu^*$) to investigate the susceptibility χ_p.

2.2. Short-range attraction susceptibility

The probability curves of $p_j(\phi, N, \mu)$ versus packing fraction ϕ for varying short-range attraction strength μ and different system sizes are redisplayed in Fig. 2(a). It is clear that with the increasing of μ, p_j at any given value of ϕ increases. Meanwhile, as the system size N increases, the change of p_j as a function of ϕ becomes steeper. The relationship between the critical packing fraction ϕ_c and the attraction strength μ is shown in the inset of Fig. 2(a). We find that ϕ_c varies linearly with μ for a given system size. It supports the idea that when the attraction strength is lower than the estimated crossover value μ^*, this short-range attraction can be regarded as perturbation which is different to the repulsive system, validating the calculation of the attraction susceptibility.

In Fig. 2(b), the probability p_j of different system sizes can be collapsed by plotting versus $(\phi - \phi_c)N^\nu$. We find that data collapse for positive values of the exponent ν, when p_j approaches a step function in the system size infinite. However, the values of ν providing the best collapse for the plotted range of N is different for 2D and 3D systems. We obtained $\nu = 0.5$ in 2D and $\nu = 0.42$ in 3D systems, this is exactly the same as what is observed for systems without attraction.[7,32]

As the attraction strength μ is an independent control parameter for small values. By the finite-difference method, we can approximate the short-range attraction susceptibility as

$$\chi_p \approx \frac{p_j(N, \mu') - p_j(N, \mu)}{\mu' - \mu}, \tag{4}$$

where both μ and μ' are in the short-range attraction regime.

Using $\mu' = 5 \times 10^{-6}$, $\mu = 0$ in the finite difference, we obtain smooth curves for 2D (Fig. 3(a)) and 3D (Fig. 3(b)) systems. Choosing other values of μ in the short-range attraction regime to compute χ_p does not change our results.

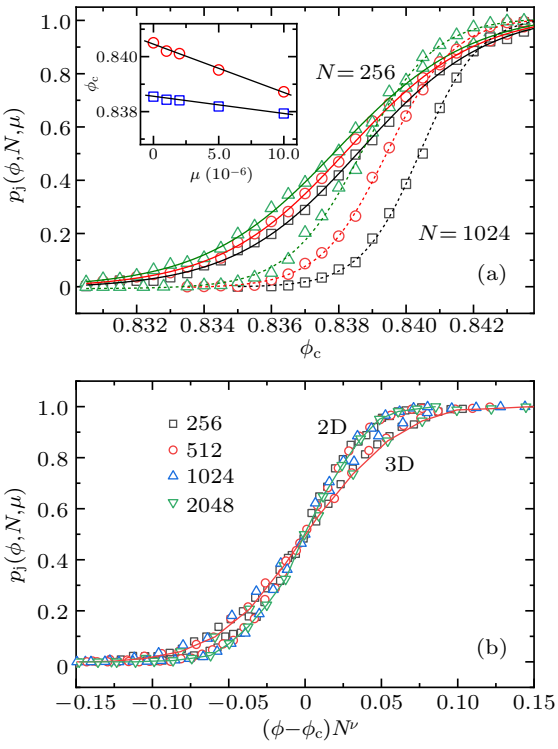


Fig. 2. (a) Probability of finding jammed states $p_j(\phi, N, \mu)$ versus packing fraction ϕ for varying attraction strength in 2D system. Square, circle, and diamond symbols correspond to different attraction $\mu = 0$, 5×10^{-6}, and 1×10^{-5}. The solid and dashed lines represent the different system sizes $N = 256$ and $N = 1024$. The fitting curves based on error function (3). Inset: $\phi_c(N, \mu)$ vs. μ for $N = 256$ (square) and $N = 1024$ (circle). (b) Data collapse of the fraction of jammed states for varying system sizes $N = 256$, 512, 1024, 2048 with $\mu = 1 \times 10^{-5}$ in 2D and 3D, respectively. The solid lines are the data collapse for varying system sizes without attraction $\mu = 0$.

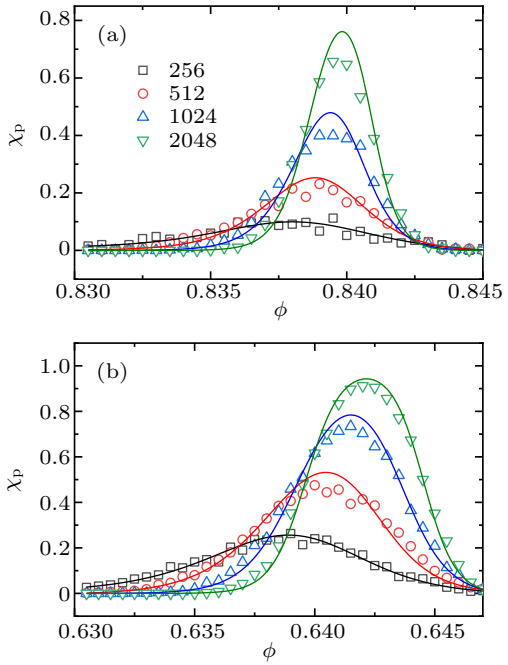


Fig. 3. (a) The attraction susceptibility curves in 2D system with different system sizes $N = 256$, 512, 1024, and 2048 calculated by finite difference method. (b) The short-range attraction susceptibility curves in 3D system with different system sizes $N = 256$, 512, 1024, and 2048. The solid lines are the derivative of the fitting lines in Fig. 2(a) with respect to μ.

We find that the short-range attraction susceptibility exponent χ_p is clearly different between 2D and 3D systems.

2.3. Finite size scaling

Since we have two control parameters, the packing fraction and the attraction strength, a two-variable finite-size scaling function can be constructed for the jamming probability. There is significant evidence that the upper critical dimension of the jamming transition is $d = 2$.[33,34] For $d \geq 2$, we could expect that finite scaling depends not on linear system size, but on particle number N. So we propose that

$$p_{\rm j} = F(\Delta\phi N^{\nu}, \mu N^{\gamma_{\rm p}\nu}), \tag{5}$$

where $\Delta\phi$ is the distance from the jamming transition for the infinite system without attraction $\Delta\phi = \phi - \phi_{\rm c}^{\infty}$.

Combined with Eq. (1), we obtain the scaling form of the short-range attraction susceptibility as

$$\chi_{\rm p}(\Delta\phi, N) = |\Delta\phi|^{-\gamma_{\rm p}} g_{\rm d}(\Delta\phi N^{\nu}), \tag{6}$$

Figure 4 shows the finite-size scaling of $\chi_{\rm p}$. The points and curves are perfectly matched and the peaks of $\chi_{\rm p}N^{-\gamma_{\rm p}\nu}$ are at $(\phi - \phi_{\rm c}^{\infty})N^{\nu} = -0.05$ for both 2D and 3D systems. We find an excellent scaling collapse in agreement with the prediction of Eq. (6), where $g_{\rm d}$ is the derivative of the complementary error function. By comparing the goodness of the scaling collapse as the parameters are varied, we calculate the value of critical exponents ν and $\gamma_{\rm p}$. The theoretical value of ν should be 0.5 for the jammed solid of soft vibrational modes.[35,36] We obtain the value of $\nu = 0.5$ for 2D system and $\nu = 0.42$ for 3D system, which are the same values used in Fig. 2(b). It has been shown that the value of ν is independent of the dimension of the system, but the precise numerical value varies widely throughout the previous research.[37–39] So, establishing the precise value of ν and determining whether all these values of exponent ν are the same is still a crucial issue. Our results are in good agreement with the results of theoretical analysis when $d = 2$, while the value of ν is obviously smaller in the case of $d = 3$, but this result remains in excellent agreement with previous works.[32,40]

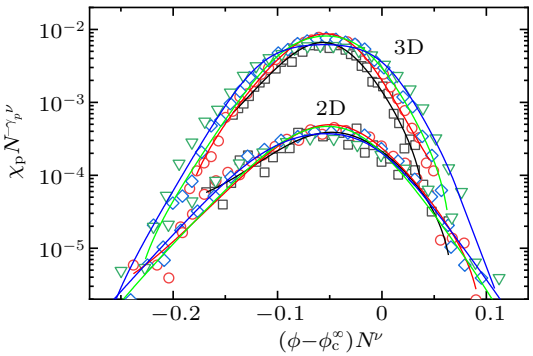


Fig. 4. Plot of scaled attractive susceptibility $\chi_{\rm p}N^{-\gamma_{\rm p}\nu}$ vs. scaled critical volume fraction $(\phi - \phi_{\rm c}^{\infty})N^{\nu}$ for the data of Fig. 3. We find a good scaling collapse using values $\phi_{\rm c} = 0.8412, \gamma_{\rm p} = 2.0, \nu = 0.5$ in 2D and $\phi_{\rm c} = 0.6442, \gamma_{\rm p} = 1.57, \nu = 0.42$ in 3D. Data point symbols correspond to those used in Fig. 3.

Further more, our results show that $\gamma_{\rm p} = 2.0$ for 2D system and $\gamma_{\rm p} = 1.57$ for 3D system. The value of $\phi_{\rm c}^{\infty}$ in 2D system is about 0.8412 (Fig. 1(a)) and in 3D system the value of $\phi_{\rm c}^{\infty}$ is 0.6442.

3. Discussion and conclusion

In conclusion, we find that the attraction strength can be divided into long and short range attractions in particle systems which exhibit distinct characteristics. Our study reveals that at the jamming point, the system is infinitely susceptible to the short-range attraction which makes the jamming transition occur at a lower value of packing fraction ϕ. By finite size scaling analysis we find that the short-range attraction susceptibility exhibits power law divergence. More work needs to be done to understand the interplay of the jamming transition and long range attraction. Foremost, we hope to validate our conclusions through experimental methods in the future. There has been a lot of research on how to systematically tune the attractive interaction in experiments.[41,42] Based on the colloidal particle system, the particle system with different attraction strength can be obtained by adjusting the temperature. Experimental verification of our predictions can be done in granular materials and non-Brownian colloids. For colloidal systems with short-range attraction, how the attractive interaction extends the jamming phase diagram to qualitatively different phenomena will be interesting to explore next.

References

[1] Hecke V and Martin 2009 *J. Phys.: Condens. Matter.* **22** 033101
[2] Liu A J and Nagel S R 2010 *Annu. Rev. Condens. Matter. Phys.* **1** 347
[3] Zheng W, Zhang S Y and Xu N 2018 *Chin. Phys. B* **27** 66102
[4] Durian D 1995 *Phys. Rev. Lett.* **75** 4780
[5] Liu A J and Nagel S R 1998 *Nature* **396** 21
[6] Wyart M, Silbert L E, Nagel S R and Witten T A 2005 *Phys. Rev. E* **72** 051306
[7] O'Hern C S, Silbert L E, Liu A J and Nagel S R 2003 *Phys. Rev. E* **68** 011306
[8] Kamien R D and Liu A J 2007 *Phys. Rev. Lett.* **99** 155501
[9] Torquato S, Truskett T M and Debenedetti P G 2012 *Phys. Rev. Lett.* **84** 2064
[10] Zheng W, Shi Y and Xu N 2015 *Sci. China Chem.* **58** 1013
[11] Markus M and Wyart M 2015 *Annu. Rev. Condens. Matter. Phys.* **6** 177
[12] Baumgarten K and Tighe B P 2017 *Soft Matter* **13**
[13] Lin J and Zheng W 2017 *Phys. Rev. E* **96** 033002
[14] Trappe V, Prasad V, Cipelletti L, Segre P N and Weitz D A 2001 *Nature* **411** 772
[15] Lu P J, Zaccarelli E, Ciulla F, Schofield A B, Sciortino F and Weitz D A 2008 *Nature* **453** 499
[16] Lu P J, Peter J. and Weitz D A 2013 *Annu. Rev. Condens. Matter. Phys.* **4** 217
[17] Irani E, Chaudhuri P and Heussinger C 2013 *Phys. Rev. Lett.* **112** 188303
[18] Lois G, Blawzdziewicz J and O'Hern C S 2008 *Phys. Rev. Lett.* **110** 028001
[19] Zheng W, Liu H and Xu N 2016 *Phys. Rev. E* **94** 062608
[20] Koeze D J and Tighe B P 2018 *Phys. Rev. Lett.* **121** 188002
[21] Griffiths and Robert B 1967 *J. Math. Phys.* **8** 484
[22] Reynolds P J, Stanley H E and Klein W 1977 *J. Phys. A: Gen. Phys.* **10** L203
[23] Schwarz J M, Liu A J and Chayes L Q 2006 *Europhys. Lett.* **73** 560

[24] Graves A L, Nashed S, Padgett E, Goodrich C P, Liu A J and Sethna J P 2016 *Phys. Rev. Lett.* **116** 235501
[25] Irani E, Chaudhuri P and Heussinger C 2013 *Phys. Rev. Lett.* **112** 188303
[26] Bitzek E, Koskinen P, GaHler F, Moseler M, Gumbsch P 2006 *Phys. Rev. Lett.* **97** 170201
[27] Xiao X H, Bao K, Wang Y C, Xie H and Duan D F 2019 *Chin. Phys. B* **28** 056401
[28] Wang Y Y, Xie H Q, Wu Z H and Xing J J 2016 *Chin. Phys. B* **9** 437
[29] Head D A 2007 *Eur. Phys. J. E* **22** 151
[30] Liu H, Xie X and Xu N 2014 *Phys. Rev. Lett.* **112** 145502
[31] Wang Y C, Fang S Xu N and Deng Y J 2020 *Phys. Rev. Lett.* **124**
[32] VaGberg D, Valdez-Balderas D, Moore M A, Olsson and Teitel S 2011 *Phys. Rev. E* **83** 030303
[33] Goodrich C P, Liu A J and Nagel S R 2012 *Phys. Rev. Lett.* **109** 095704
[34] Charbonneau P, Corwin E I, Parisi G and Zamponi F 2015 *Phys. Rev. Lett.* **114** 125504
[35] Wyart M, Nagel S R and Witten T A 2005 *Europhys. Lett.* **72** 486
[36] Wyart M, Silbert L E, Nagel S R and Witten T A 2005 *Phys. Rev. E* **72** 051306
[37] Silbert L E, Liu A J and Nagel S R 2005 *Phys. Rev. Lett.* **95** 098301
[38] Henkes S and Chakraborty B 2005 *Phys. Rev. Lett.* **95** 198002
[39] Heussinger C and Barrat J L 2009 *Phys. Rev. Lett.* **102** 218303
[40] O'Hern C S, Langer S A, Liu A J and Nagel S R 2002 *Phys. Rev. Lett.* **88** 075507
[41] Zhang Z, Yunker P, Habdas P and Yodh A G 2011 *Phys. Rev. Lett.* **107** 208303
[42] Li B, Wang F, Zhou D, Peng Y, Ni R and Han Y L 2016 *Nature* **531** 485