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Correlations of plasticity in sheared glasses

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In a recent paper [Mandal *et al.*, Phys. Rev. E **88**, 022129 (2013)], the nature of spatial correlations of plasticity in hard-sphere glasses was addressed both via computer simulations and in experiments. It was found that the experimentally obtained correlations obey a power law, whereas the correlations from simulations are better fitted by an exponential decay. We here provide direct evidence—via simulations of a hard-sphere glass in two dimensions (2D)—that this discrepancy is a consequence of the finite system size in the 3D simulations. By extending the study to a 2D soft disk model at zero temperature [Durian, Phys. Rev. Lett. **75**, 4780 (1995)], the robustness of the power-law decay in sheared amorphous solids is underlined. Deviations from a power law occur when either reducing the packing fraction towards the supercooled regime in the case of hard spheres or changing the dissipation mechanism from contact dissipation to a mean-field-type drag in the case of soft disks.

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I. INTRODUCTION

It is well established that dynamic correlations grow in glass forming liquids as the glass transition is approached [1–7]. This growth is, however, generally found to be limited to a few particle diameters [2,4,5,7]. A dramatic change may occur if the glass is driven by an applied shear that forces structural rearrangements [8]; such external driving can lead to an avalanchelike plastic response, mediated by a long range elastic field [9].

Some of us recently addressed this issue for a hard-sphere glass both via computer simulations and experiments with a focus on the direction dependence of correlations and the crossover from the thermal regime of supercooled liquids to the athermal limit of strongly driven glasses [10,11]. Qualitative agreement was found between simulations and experiments regarding both the behavior of single particle fluctuations (found to be isotropic) and the anisotropy of their spatial correlations. The specific functional form of these correlations was, however, found to be different. While experimental data were best described by a power-law decay—recalling a self-similar behavior—simulations suggested an exponential decay with a characteristic length of the order of a few particle diameters.

Here we provide strong evidence that a reason for this discrepancy is the finite system size of simulations. When performing event-driven finite-temperature simulations in two dimensions (2D) (which allows for much larger linear sizes, L), we find that the exponential decay found for smaller sizes changes to an algebraic decay at larger L.

We also perform simulations of a Durian-type 2D soft disk model at zero temperature [12] with two different types of hydrodynamic drag: (i) contact dissipation (CD), where the dissipative force is proportional to the relative velocity of interacting particle pairs, and (ii) mean-field or reservoir dissipation (RD), where a drag force relative to an externally imposed background linear velocity field is used (see Sec. II for details). These simulation studies are accompanied by experiments on granular particles. Results obtained for the CD case are in line with experiments, thus showing that power-law correlations are the generic response of driven amorphous solids.

In the case of reservoir dissipation, on the other hand, there are strong deviations from a power-law decay even for the largest L simulated. We attribute this behavior to the simplified dissipation mechanism which couples the particle dynamics to an externally imposed flow, without any influence of the particle motion on the flow velocity [13–15].

II. SIMULATION MODEL AND EXPERIMENTAL SYSTEM

Our first simulation model is a polydisperse hard-sphere system of mass $m = 1$ and average diameter $\sigma = 0.8$. Lengths are measured in units of σ and time in units of $\sigma\sqrt{m/k_BT}$, where T is temperature and k_B, the Boltzmann constant, are both set to unity for convenience. Event-driven molecular dynamics simulations are performed using the DYNAMO code [16]. Periodic boundary conditions are used along all directions. When combined with the Lees-Edwards boundary condition [17], this leads to a shear deformation of $\gamma = t\dot{\gamma}$. The simulated shear rates reported here are $\dot{\gamma} = 5 \times 10^{-5}$ and 10^{-4}. The packing fractions studied are around the glass transition point, which, for the present polydisperse system, is located at a packing fraction of $\phi_g \approx 0.58$ (3D) [18] and $\phi_g \approx 0.80$ (2D) [19,20]. The quiescent properties of the 3D system have been studied extensively in Ref. [21]. The temperature is fixed at $T = 1$ via velocity rescaling. We present all the measurements after 100% shearing to ensure that the system has reached a steady state.

We also perform simulations with soft bidisperse particles with size ratio 1.4 in two dimensions and at zero temperature.

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The diameter of the smaller particles is $\sigma = 1$. With σ_i for the diameter of particle i, the mass is $m_i = \pi\sigma_i^2/2$. We make use of Lees-Edwards boundary conditions with shear rates $\dot{\gamma} = 10^{-6}$ through 10^{-4}. At the densities considered here, there is no strong dependence on shear rate, and the data in this Rapid Communication are only for a single shear rate, $\dot{\gamma} = 10^{-5}$. The number of particles in the simulations is mostly $N = 262\,144$, though smaller systems are also simulated to examine finite size effects. In the model, there is both a conservative elastic force and a dissipative force. The elastic force depends on the position coordinates only. With $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ for the distance between particles i and j, $\sigma_{ij} = (\sigma_i + \sigma_j)/2$, and the overlap $\delta_{ij} = (\sigma_{ij} - r_{ij})/\sigma_{ij}$, the elastic force is $f^{\rm el} = k_e\delta_{ij}\hat{\mathbf{r}}_{ij}$ with $\hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}|$. We note that at shear rate $\dot{\gamma} = 10^{-5}$, the particles deform only marginally, $\delta_{ij} \approx 1.1 \times 10^{-4}$ at $\phi = 0.82$. This means that we expect this soft disk model to behave essentially as a hard disk model; the softness of the particles should not play any significant role. We report on results obtained both with contact dissipation (CD) for which the dissipative force is given by the velocity difference to all particles in contact, $f_{\rm CD}^{\rm diss} = -k_d \sum_j (\mathbf{v}_i - \mathbf{v}_j)$, as well as with reservoir dissipation (RD), $f_{\rm RD}^{\rm diss} = -k_d[\mathbf{v}_i - \mathbf{v}_R(\mathbf{r}_i)]$, where $\mathbf{v}_R(\mathbf{r}_i) = \dot{\gamma}\, y_i\hat{\mathbf{x}}$ (with $\hat{\mathbf{x}}$ the unit vector along the x direction). The latter model has sometimes been called the mean-field model, as the particles dissipate against the average velocity $\dot{\gamma}\, y_i\hat{x}$. In the simulations, we take $k_d = 1$ and $k_e = 1$.

For the experimental measurements, we use suspensions of both Brownian and granular particles. The Brownian system consists of sterically stabilized polymethylmethacrylate (PMMA) particles with diameter of $\sigma = 1.3\ \mu$m, suspended in a mixture of cycloheptyl bromide and *cis*-decalin. This solvent mixture matches both the density and refractive index of the particles. The particles have a polydispersity of 7% to prevent crystallization. The particle volume fraction is fixed at $\phi \sim 0.6$, well inside the glassy state [22]. We apply shear at a constant rate in the range of 1.5×10^{-5} to 2.2×10^{-4} s^{-1}, corresponding to modified Peclet numbers $\dot{\gamma}\tau$ between 0.3 and 2.2, respectively [8]. Here, the structural relaxation time is $\tau = 2 \times 10^4$ s, as determined from the mean-square displacement of the particles. The granular system consists of PMMA particles with a diameter of 3.9 mm, and a polydispersity of ∼5% suspended in a mixture of dimethyl-sulfoxide, water, and salt (NaI), carefully tuned to match both the refractive index and the density of the particles [23]. Individual particles are imaged in three dimensions using a laser sheet, while the suspension is sheared at a rate of $\sim 5 \times 10^{-5}$ s^{-1} with a constant confining pressure of ∼7 kPa [23].

III. SPATIAL CORRELATIONS OF PLASTICITY

We define a quantitative measure of plastic activity as follows [24]. For a reference particle (noted here with index 0), we follow the evolution of the distance vectors $\mathbf{d}_i = \mathbf{r}_i - \mathbf{r}_0$ for a short time interval δt, where i runs over the nearest neighbors of the reference particle. We then define a measure for plastic activity as $D^2 = (1/n)\sum_{i=1}^{n}[\mathbf{d}_i(t+\delta t) - \mathbf{d}_i(t) - \boldsymbol{\epsilon}\cdot\mathbf{d}_i(t)]^2$, where $\boldsymbol{\epsilon}$ is the linear (affine) transformation tensor which best describes the time evolution of $\mathbf{d}_i$. D^2 is the mean-square deviation from a local affine deformation, and is known as an excellent measure of local plasticity [24].

The above applies directly to both the experiments and the event-driven (finite-temperature) simulations. The analyses in the zero-temperature simulations (the RD and CD models) work the same except that $\mathbf{d}_i(t+\delta t) - \mathbf{d}_i(t)$ is replaced by $\mathbf{v}_i(t)\delta t$, where $\mathbf{v}_i(t)$ is the instantaneous velocity of the particle i relative to the reference particle. Note that, here, δt affects the magnitude of the optimum affine transformation tensor (and thus D^2) by a constant factor only and has no effect on the spatial correlations of D^2 addressed in this Rapid Communication.

We then use the above introduced scalar quantity D^2 to define the correlation function [8],

$$C_{D^2}(\Delta\mathbf{r}) = \frac{\langle D^2(\mathbf{r}+\Delta\mathbf{r})D^2(\mathbf{r})\rangle - \langle D^2(\mathbf{r})\rangle^2}{\langle D^2(\mathbf{r})^2\rangle - \langle D^2(\mathbf{r})\rangle^2}. \qquad (1)$$

The function $C_{D^2}(\Delta\mathbf{r})$ provides a measure of correlations between plastic activity at two points in space separated by a vector $\Delta\mathbf{r}$.

IV. RESULTS ON SPATIAL CORRELATIONS

A. Motivation—experiments and event-driven simulations in 3D

We compare correlations of plastic activity in experiments and the 3D simulations in Fig. 1. Figures 1(a) and 1(b), which are the experimental correlations, show robust power-law correlations with exponent $\alpha \sim 1.3$ for a range of Peclet numbers. These power-law correlations extend out to the distance $r \sim 50\sigma$, which equals the vertical system size. (In the horizontal directions, the experimental system is macroscopically large.) In contrast, Figs. 1(c) and 1(d), which are the correlations from the event-driven 3D simulations, give strong evidence of an exponential decay. This discrepancy was noted by some of us in an earlier publication [11].

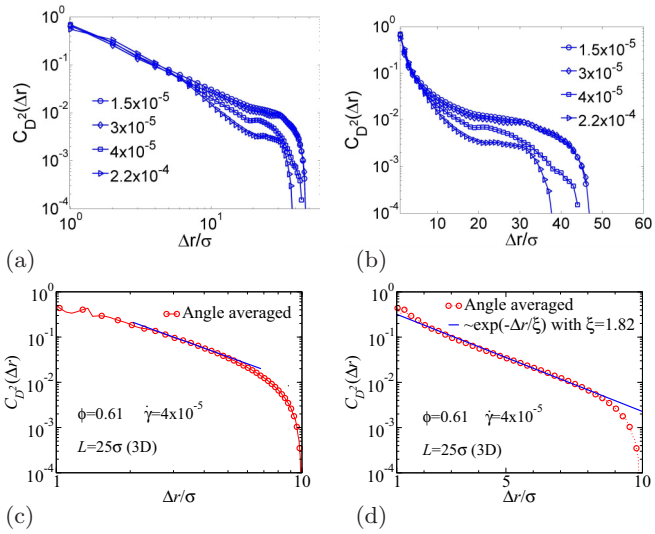

FIG. 1. (Color online) Correlation of plastic activity in (a),(b) experiments and (c),(d) simulations of hard-sphere glasses. The same data are shown both in double logarithmic (left panel) and semilogarithmic (right panel) scales. The experimental data show robust power-law decay, while the simulations rather show exponential decay.

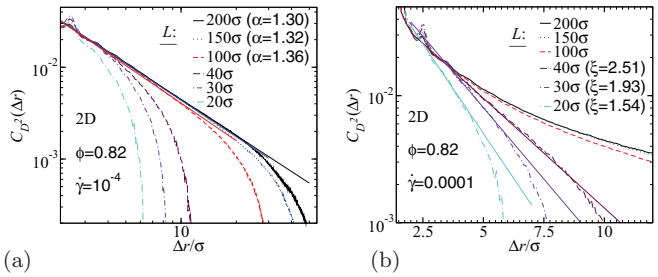

FIG. 2. (Color online) Angle averaged correlation of plastic activity in 2D simulations of hard disks for various system sizes in (a) double logarithmic and (b) semilogarithmic scale. The packing fraction is $\phi = 0.82 > \phi_g \approx 0.80$ (glassy phase). The straight lines are fits to (a) $A(\Delta r)^{-\alpha}$ and (b) $B\exp(-\Delta r/\xi)$ with values of α and ξ as indicated.

B. Event-driven simulations in 2D

One possible reason for the discrepancy noted above could be the limited system size, $L/\sigma = 25$, in the event-driven 3D simulations, which is due to limitations in computational resources. To achieve larger linear system sizes with similar computational effort, we turn to two dimensions. In this way, we are able to reach sizes of up to $L/\sigma = 200$. We thus performed a systematic study of the finite size effects of C_{D^2} at a density of $\phi = 0.82$ above $\phi_g \approx 0.80$ (Fig. 2). For $L/\sigma < 50$, we find that correlations decay exponentially, in perfect agreement with the 3D simulations in Figs. 1(c) and 1(d). For larger sizes, the figure shows clear evidence of a power-law decay. This observation suggests that it is the rather limited system size in the 3D simulations that is the main cause for the observed exponential decay, and that a power-law decay is the true behavior for sufficiently large system sizes. These results therefore point to a good agreement between experiments and simulations.

In contrast to the glassy phase, C_{D^2} decays in the supercooled state exponentially, regardless of the system size (Fig. 3). This observation is interesting and suggests that the glassy state is distinct from the supercooled state: spatial correlations of plastic activity are mediated by the elastic field [9,25,26]. In the supercooled state, the elasticity is not well established (though observable for sufficiently fast processes [27]), and correlations are short ranged; in the glassy phase, on the other hand, the glass has developed a system-spanning elastic field. A local plastic rearrangement

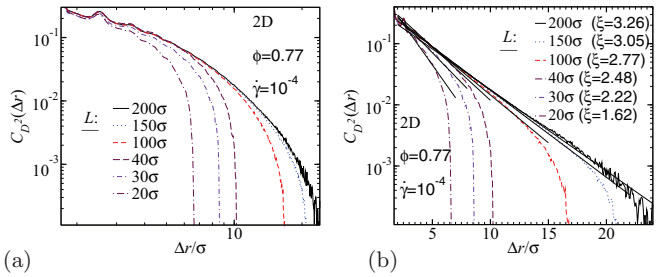

FIG. 3. (Color online) Same quantity as in Fig. 2, but for a lower packing fraction of $\phi = 0.77 < \phi_g \approx 0.80$ (supercooled state).

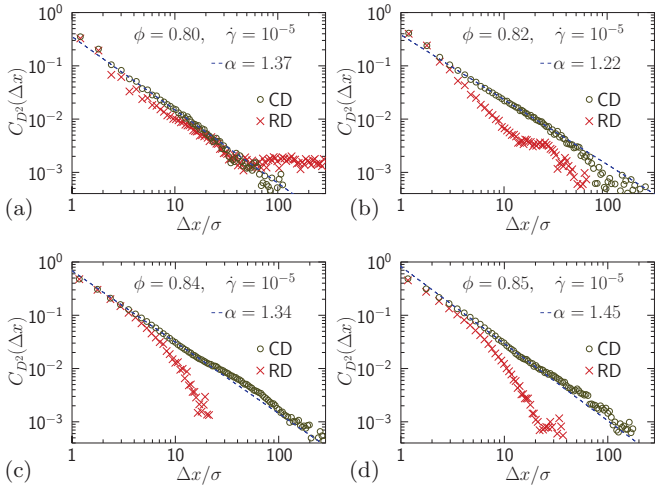

FIG. 4. (Color online) Correlation of plastic activity along the flow direction from simulations of a Durian-type model with contact dissipation (CD) and reservoir dissipation (RD) for different densities across the jamming transition ($\phi_J \approx 0.843$). The dashed lines and quoted exponents are obtained by fitting C_{D^2} for the CD model to an algebraic decay for $2 \leqslant \Delta x/\sigma \leqslant 20$.

may then influence a region far away by distorting this elastic field. This has been discussed in mean-field models [25,28].

C. 2D simulations of soft particles at zero temperature

In order to examine the role of drag forces for algebraically decaying correlations, we have performed 2D simulations of a Durian-type model of athermal soft disks for both CD and RD, as described in Sec. II. The two models are compared in Fig. 4, where C_{D^2} along the flow direction is shown at different densities across the jamming transition. The algebraic behavior for the CD model is very robust and changes only weakly with density. The exponent α varies slightly with ϕ and remains close to -1.3. This value coincides with both the one obtained in the 2D hard-sphere simulations and the experiments. Interestingly, the RD model exhibits a different behavior: while the decay is essentially algebraic at the lowest density, $\phi = 0.80$, it is rather exponential at higher densities, $\phi \gtrsim 0.84$. These results indicate that the dissipation mechanism plays a significant role in the correlations, as also indicated by recent works [13–15]. The results thus indicate certain pitfalls in simulation models that one has to be aware of: as the RD model is a simplified model to describe dissipation, we conclude that the CD model better describes the real experimental situation, and that power-law correlations are the generic response of athermal driven suspensions. This is indeed confirmed in experiments by direct imaging of correlations in a sheared granular suspension: As shown in Fig. 5, power-law correlations are observed in the shear direction, in agreement with the CD model, provided the system size is sufficiently large. In the experiment, correlations can only be imaged for distances $r \lesssim 10d$ due to the small size of the experimental system that can be imaged in 3D. Nevertheless, despite the limited system size, the power law becomes apparent, and the agreement between the experiments and the CD model becomes clear.

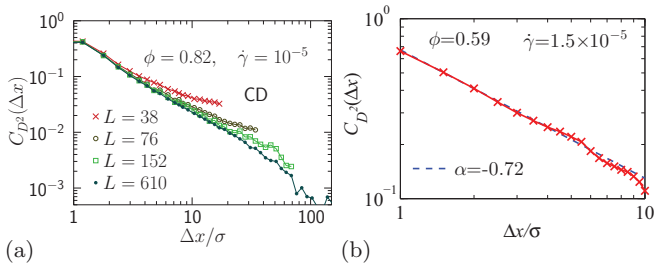

FIG. 5. (Color online) (a) Correlation of plastic activity along the flow direction from simulations of a Durian-type model with contact dissipation for different system sizes. (b) Experimental result for a granular suspension.

We note that the elastic response in amorphous solids has been studied by a number of authors [29–31]. In particular, DiDonna and Lubensky [31] proposed an analytic model for correlations in systems with random distribution of elastic modulii. For system sizes that are large compared to the correlation length of the elastic modulus, nonaffinity correlations were predicted to scale as $|\mathbf{x}|^{-1}$ in 3D, with a logarithmic decay in 2D. Interestingly, in 3D, we observe a power-law decay of correlations with an exponent of -1.3. Nevertheless, as can be inferred from the presented data, our 2D simulations suggest a power-law decay with approximately the same exponent as in 3D, rather than a logarithmic behavior. We note, however, that the correlation of plastic activity considered in this Rapid Communication is a different quantity than the correlations of nonaffine velocities—$\langle \mathbf{v}(\mathbf{r}) \cdot \mathbf{v}(\mathbf{r} + \Delta\mathbf{r}) \rangle$, studied in Ref. [31]; the latter is closely related—albeit not identical—to the correlations of plastic activity. For the simulations presented in Figs. 4 and 5, we indeed find that correlations of nonaffine velocities decay logarithmically in 2D (data not shown). The reason for this different scaling of seemingly closely related quantities is currently not clear to us.

V. CONCLUSION

In this work, we address the nature of spatial correlations of plasticity in sheared amorphous solids in experiments and simulations using different simulation models. This study is motivated by a recent publication by some of the present authors [11] reporting a power-law decay in experiments on a colloidal hard-sphere glass but an exponential decay in event-driven molecular dynamics simulations of a model hard-sphere glass (Fig. 1). By going to 2D, we find strong evidence that the exponential behavior reported in Ref. [11] is a finite size effect (Fig. 2). This conclusion is underlined by an algebraic decay of correlations in Durian-type soft disks [12] at zero temperature (Fig. 5). Furthermore, by comparing two simulation models, i.e., reservoir dissipation and contact dissipation, we find that mean-field-type drag forces that couple the dynamics of particles to an externally imposed flow field without any feedback mechanism may strongly bias the nature of correlations (Fig. 4). Thus, while this work demonstrates the robust and genuine algebraic nature of correlations in flowing amorphous solids, it also sheds some light onto the origin of possible deviations from power-law decays.

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[1] C. Bennemann, C. Donati, J. Baschnagel, and S. C. Glotzer, Nature (London) **399**, 246 (1999).
[2] P. Scheidler, W. Kob, and K. Binder, Europhys. Lett. **59**, 701 (2002).
[3] J. Baschnagel and F. Varnik, J. Phys.: Condens. Matter **17**, R851 (2005).
[4] P. Ballesta, A. Duri, and L. Cipelletti, Nat. Phys. **4**, 550 (2008).
[5] F. Varnik and K. Binder, Int. J. Mater. Res. **100**, 1494 (2009).
[6] L. Berthier, Physics **4**, 42 (2011).
[7] W. Kob, S. Roldan-Vargas, and L. Berthier, Nat. Phys. **8**, 164 (2011).
[8] V. Chikkadi, G. Wegdam, D. Bonn, B. Nienhuis, and P. Schall, Phys. Rev. Lett. **107**, 198303 (2011).
[9] A. Lemaitre and C. Caroli, Phys. Rev. Lett. **103**, 065501 (2009).
[10] V. Chikkadi, S. Mandal, B. Nienhuis, D. Raabe, F. Varnik, and P. Schall, Europhys. Lett. **100**, 56001 (2012).
[11] S. Mandal, V. Chikkadi, B. Nienhuis, D. Raabe, P. Schall, and F. Varnik, Phys. Rev. E **88**, 022129 (2013).
[12] D. J. Durian, Phys. Rev. Lett. **75**, 4780 (1995).
[13] B. P. Tighe, E. Woldhuis, J. J. C. Remmers, W. van Saarloos, and M. van Hecke, Phys. Rev. Lett. **105**, 088303 (2010).
[14] E. Woldhuis, Ph.D. thesis, Leiden University, 2013.
[15] D. Vågberg, P. Olsson, and S. Teitel, arXiv:1312.5158.
[16] M. Bannerman, R. Sargant, and L. Lue, J. Comput. Chem. **32**, 3329 (2011).
[17] D. J. Evans and G. P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic Press, London, 1990).
[18] P. N. Pussey, E. Zaccarelli, C. Valeriani, E. Sanz, W. C. K. Poon, and M. E. Cates, Phil. Trans. R. Soc. A **367**, 4993 (2009).
[19] L. Santen and W. Krauth, Nature (London) **405**, 550 (2000).
[20] M. Bayer, J. M. Brader, F. Ebert, M. Fuchs, E. Lange, G. Maret, R. Schilling, M. Sperl, and J. P. Wittmer, Phys. Rev. E **76**, 011508 (2007).
[21] S. R. Williams, I. K. Snook, and W. van Megen, Phys. Rev. E **64**, 021506 (2001).
[22] W. van Megen, T. C. Mortensen, S. R. Williams, and J. Müller, Phys. Rev. E **58**, 6073 (1998).
[23] K. A. Lorincz and P. Schall, Soft Matter **6**, 3044 (2010).

[24] M. L. Falk and J. S. Langer, Phys. Rev. E **57**, 7192 (1998).
[25] G. Picard, A. Ajdari, F. Lequeux, and L. Bocquet, Phys. Rev. E **71**, 010501 (2005).
[26] P. Schall, D. A. Weitz, and F. Spaepen, Science **318**, 1895 (2007).
[27] J. Chattoraj and A. Lemaitre, Phys. Rev. Lett. **111**, 066001 (2013).
[28] K. A. Dahmen, Y. Ben-Zion, and J. T. Uhl, Nat. Phys. **7**, 554 (2011).
[29] C. E. Maloney, Phys. Rev. Lett. **97**, 035503 (2006).
[30] C. E. Maloney and M. O. Robbins, Phys. Rev. Lett. **102**, 225502 (2009).
[31] B. A. DiDonna and T. C. Lubensky, Phys. Rev. E **72**, 066619 (2005).