Large-Scale Chaos and Fluctuations in Active Nematics

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We show that "dry" active nematics, *e.g.* collections of shaken elongated granular particles, exhibit large-scale spatiotemporal chaos made of interacting dense, ordered, band-like structures in a parameter region including the linear onset of nematic order. These results are obtained from the study of the relatively simple and well-known (deterministic) hydrodynamic equations describing these systems in a dilute limit, and of a self-propelled particle Vicsek-like model for this class of active matter. In this last case, revisiting the status of the strong fluctuations and long-range correlations now considered as landmarks of orientationally-ordered active phases, we show that the giant number fluctuations observed in the chaotic phase are a trivial consequence of density segregation. However anomalous density fluctuations are present in the homogeneous quasi-ordered nematic phase and characterized by a non-trivial scaling exponent.

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Many of the recent studies on active suspensions and active gels have reported the existence of instabilities leading to spontaneous flows [1–4]. At the nonlinear level, the term "bacterial turbulence" has been used to describe the fast, collective but chaotic motion of swimmers evolving in what remains a very low Reynolds number, inertialess, world [5–8]. In remarkable in vitro experiments on actomyosin motility assays, the fluid in which filaments and motors evolve seems to play a key role in the emergence of local order leading in turn to erratic large-scale flows [9]. Other actomyosin systems, like the active nematics suspensions studied by Dogic *et al.*, display spontaneous large-scale dynamics mediated by the nucleation and motion of topological defects [10–13].

In contrast, most of the recent studies of "dry" active matter (where the fluid in which active particles move can be safely neglected), have not reported widespread occurence of large-scale chaos or turbulence [14]. Following the seminal papers of Vicsek *et al.* [15] and Toner and Tu [16], a lot of attention has been paid to the nature of the onset of orientational order/collective motion and to the existence of generic long-range correlations and anomalous fluctuations in spatially-homogeneous ordered phases [17, 18, 21]. The existence of long-wavelength instabilities of homogeneous ordered states leading, in dilute systems, to some phase separation between high-density high-order structures (bands, waves) is now recognized as a generic feature [18–20, 22–29], but the stability and large-scale dynamics of these structures remain largely unknown.

In this Letter, we show that large-scale spatiotemporal chaos arises generically in dry active nematics. We first demonstrate that the solutions of the relatively simple and well-known (deterministic) hydrodynamic equations describing these systems are chaotic in a region of parameter space including the linear onset of nematic order. We show in particular that the nonlinear ordered band solution found before [30] is unstable, leading to a disordered phase in which elongated dense and ordered structures curve, extend, merge, and split on very large time- and length-scales. Returning to the Vicsek-style model for dry active nematics introduced in [32] to investigate further the effect of fluctuations, we provide evidence that its segregated regimes where dense, ordered structures form are also actually chaotic on large scales, rendering this phase asymptotically disordered. The giant number fluctuations reported in [32] to be in agreement with the predictions of Ramaswamy *et al.* [33] are thus a trivial consequence of phase separation. Non-trivial fluctuations are nevertheless present in the homogeneous quasi-ordered phase overlooked in [32] but found here at larger densities. Their scaling exponent, though, differs from the simple one derived in [33] using a linearized theory. Interestingly, we find that it takes a value similar to that calculated by Toner and Tu for *polar* ordered phases [16].

We start by recalling the Vicsek-style model for active nematics defined in [32], where point particles carrying a (uniaxial) nematic degree of freedom align locally and are forced to move randomly along one of the two directions defined by their axis. In two spatial dimensions

the positions $\mathbf{x}_j^t$ and directors $\mathbf{n}_j^t \equiv \left(\cos\theta_j^t, \sin\theta_j^t\right)^T$ with $\theta_j^t \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ of particles $j = 1, \ldots, N$ are updated synchronously at discrete timesteps according to:

$$\theta_j^{t+1} = \frac{1}{2}\mathrm{Arg}\left[\sum_{k\in V_j} e^{i2\theta_k^t}\right] + \psi_j^t \; ; \;\; \mathbf{x}_j^{t+1} = \mathbf{x}_j^t \pm v_0\, \hat{\mathbf{n}}_j^t \quad (1)$$

where V_j is the set of neighbors of particle j within unit distance, the sign in the second equation is chosen randomly with equal probability, and the random angle $\psi_j^t \in [-\eta\frac{\pi}{2}, \eta\frac{\pi}{2}]$ (with $\eta \in [0, 1]$) is drawn from a uniform distribution. As a matter of fact, this model has not been much studied beyond the initial paper [32] where numerical simulations performed on square domains of linear size L at global density $\rho_0 = N/L = \frac{1}{2}$ concluded to an isotropic/nematic Berezinskii-Kosterlitz-Thouless-like transition [34] as η is decreased, with the quasi-long-range ordered phase consisting of a single dense ordered band and supporting giant number fluctuations.

As shown in [30], the rather well known hydrodynamic equations for dry active nematics [31] can be derived in a simple and controlled way from this model, with all transport coefficients depending explicitly on ρ_0 and the noise strength, the only two parameters remaining after rescaling. In this approach, one assumes a dilute limit and a molecular chaos hypothesis, which allows to write a Boltzmann equation for the one-body distribution function $f(\mathbf{x}, \theta, t)$. By expanding f in Fourier series of θ, $f(\mathrm{x}, \theta, t) = \frac{1}{\pi}\sum_{k=-\infty}^{k=\infty} \hat{f}_k(\mathrm{x}, t)e^{-i2k\theta}$, the kinetic equation becomes a hierarchy which can be truncated and closed, assuming a diffusive scaling ansatz and the proximity of the onset of nematic order. The first non-trivial order yields a nonlinear equation governing the nematic complex field $Q \equiv \hat{f}_1$, together with the continuity equation governing the density field $\rho \equiv \hat{f}_0$ [40]:

$$\partial_t \rho \;=\; \frac{1}{2}\Delta\rho + \frac{1}{2}\mathrm{Re}\left(\nabla^{*2} Q\right) \quad (2)$$

$$\partial_t Q \;=\; \left(\mu(\rho) - \xi\,|Q|^2\right) Q + \frac{1}{4}\nabla^2\rho + \frac{1}{2}\Delta Q \quad (3)$$

where $\mu(\rho) = \mu'(\rho - \rho_\mathrm{t})$ and we have used the complex operators $\nabla \equiv \partial_x + i\partial_y$, $\nabla^* \equiv \partial_x - i\partial_y$, and $\Delta \equiv \nabla\nabla^*$. The transport coefficients μ', ρ_t, and ξ are positive constants depending on the noise strength σ [41].

The phase diagram of Eqs.(2) and (3) is given in Fig. 1a. The condition $\rho = \rho_\mathrm{t}$, defining the line σ_t, marks the linear instability of the disordered solution $Q = 0$ and the emergence of the homogeneous ordered solution $|Q| = \sqrt{\mu/\xi}$ (for $\mu > 0$). But this ordered solution is itself linearly unstable to long-wavelength perturbations transversal to nematic order in a region bordering the basic line $\rho_\mathrm{t}, \sigma_\mathrm{t}$. Deeper in the ordered phase, below the line $\rho_\mathrm{s}, \sigma_\mathrm{s}$, the homogeneous ordered solution is linearly stable.

It was shown in [30] that Eqs.(2) and (3) support an inhomogeneous solution in the form of a band of nematic order with density $\rho_\mathrm{band} > \rho_\mathrm{s}$ surrounded by a disordered gas with $\rho_\mathrm{gas} < \rho_\mathrm{t}$. Supposing the nematic order is along x, for this solution we obtain $\rho = R_0(y) \equiv Q_0(y) + \rho_\mathrm{gas}$ and

$$Q_0(y) \;=\; \frac{3(\rho_t - \rho_\mathrm{gas})}{1 + a\cosh\left(\sqrt{4\mu'(\rho_t - \rho_\mathrm{gas})}y\right)} \quad (4)$$

with $a = \sqrt{1 - 9\xi(\rho_t - \rho_\mathrm{gas})/2\mu'}$, ρ_gas being a constant fixed by density conservation [30]. Its existence domain $(\sigma_\mathrm{min}, \sigma_\mathrm{max})$ actually extends beyond the region of linear instability of the homogeneous ordered solution ($\sigma_\mathrm{min} < \sigma_\mathrm{s}$ and $\sigma_\mathrm{max} > \sigma_\mathrm{t}$). Its ordered part occupies a *fraction* of the y dimension of the system going continuously from zero (near σ_max) to one (near σ_min).

If considered only as a one-dimensional function of y, the band solution Eq. (4) is linearly stable. We now show that it is always unstable with respect to long-wavelength undulations along the x-axis. To study the linear stability with respect to wavenumber k, we seek the perturbative solution in the form $(Q, \rho) = (Q_0(y), R_0(y)) + (q(y), r(y))\exp(\lambda t + ikx)$. Substituting the growth rate λ into Eqs. (2),(3), we obtain a linear system for $q(y), r(y)$. Noting that for $k = 0$ the solution to this system is the translational mode $r = q = \partial_y Q_0$, we can further simplify the problem in the long-wave limit $k \to 0$ by expanding the perturbative solution in k and employing the following anzatz: $\lambda = \lambda_1 k^2$, $q(y) = u(y) + iv(y)$ and

$$\begin{pmatrix} r(y) \\ u(y) \\ v(y) \end{pmatrix} = \begin{pmatrix} \partial_y Q_0(y) \\ \partial_y Q_0(y) \\ 0 \end{pmatrix} + \begin{pmatrix} k^2 r_1(y) \\ k^2 u_1(y) \\ ikv_1(y) \end{pmatrix} \quad (5)$$

We then obtain linear inhomogeneous self-adjoint equations for the functions r_1, u_1, and v_1. The solvability condition yields an explicit expression for the growth rate λ in terms of integrals of Q_0 and $\partial_y Q_0$. The analysis, detailed in [35], shows that $\lambda > 0$, implying that the band solution is always unstable. However, the instability can be suppressed in small systems.

At the nonlinear level, for large enough systems, the instability of the band first manifests itself as some periodic modulation in space and time localized along its borders. This then turns into localized chaotic behavior (Fig. 1b), which eventually develops into full-blown spatiotemporal chaos for large enough system sizes and integration times. There, distorted band-like structures evolve on very long timescales and large lengthscales, elongate, split, merge, without ever forming the original macroscopic band again (Fig. 1c and [35]). We have observed this spectacular dynamics all along the $(\sigma_\mathrm{min}, \sigma_\mathrm{max})$ interval [42]. As σ is varied from σ_max to σ_min, the largest structures observed have increasing sizes. We measured the global nematic order parameter $S(t) = |\langle Q\rangle_{x,y}|$ and the two-point spatial correlation function of the density field for different square systems of linear size L. For

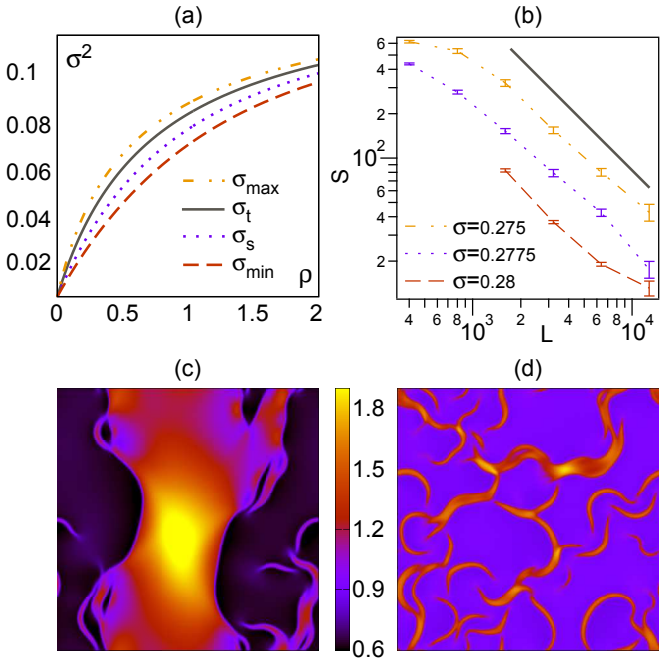

FIG. 1: (color online) Mesoscopic dynamics: (a) phase diagram of hydrodynamic equations for active nematics. (b) global order parameter vs system size at different noise values in chaotic regime (the solid line has slope -1). (c,d) snapshots of density field in chaotic regime for $L = 1600$ and $\rho_0 = 1$; (c): localized chaos ($\sigma = 0.26$); (d) fully-developed chaos ($\sigma = 0.28$)

large enough systems, the time-averaged order parameter $\langle S\rangle$ decreases like $1/L$, indicating the existence of a finite, L-independent correlation length (Fig. 1d) [43]. The segregated phase of the hydrodynamic equations for active nematics is thus asymptotically disordered.

We now investigate the robustness of the above results with respect to fluctuations by coming back to the Vicsek-like model defined by Eq. (1). This also provides an opportunity to gauge the faithfulness —at a qualitative level— of the hydrodynamic equations (2)-(3) to the model they were derived from. We performed extensive simulations of Eq. (1) at various global densities ρ_0, varying the noise strength η and the system size L.

At large enough ρ_0, we do observe, for low enough η, a spatially-homogeneous, non-segregated, quasi-ordered phase (not shown). Because it possesses unusually strong density fluctuations (see below) which may be hard to distinguish from the fluctuating structures of the segregated phase, the location of $\eta_{\rm low}$, the noise value marking the lower extent of the inhomogeneous phase, is difficult to characterize beyond visual inspection provided by movies and snapshots such as in Fig. 2 and [35]. We used scaling and fluctuation properties of the global nematic order parameter S, whose full probability distribution $P(S)$ can be measured with good statistics only for moderate system sizes (up to $L=256$). In the homogeneous phase, its mean $\langle S\rangle$ decreases algebraically with L with an exponent $\zeta(\eta)<\frac{1}{8}$ (quasi-long-range order), and $P(S)$ quickly converges, as L is increased, to the Bramwell-Holdsworth-Pinton (BHP) distribution, well-known to describe almost perfectly the quasi-ordered, vortex-free phase of the equilibrium XY model [36] (Fig. 2a). The inhomogeneous segregated phase, by contrast, is characterized by a departure of $P(S)$ from the BHP distribution which becomes more important as the system size is increased (Fig. 2c). During the corresponding events, the main dense ordered band typically observed at such moderate system sizes reorganizes itself. We used the finite-size behavior of $P(S)$ to define —admittedly rather roughly— the threshold value $\eta_{\rm low}$: for $\eta < \eta_{\rm low}$, $P(S)$ falls on the BHP distribution, whereas for $\eta > \eta_{\rm low}$ $P(S)$ deviates from BHP, and these deviations eventually become so important that the initial algebraic decay of $\langle S\rangle$ with L accelerates at large L values (inset of Fig. 2c).

Using the above approach, we find that $\eta_{\rm low}$, decreases with ρ_0 (Fig. 2b). For $\rho_0 = \frac{1}{2}$, the density used in [32], we estimate $\eta_{\rm low} \simeq 0.02$, relegating the homogeneous regime to numerically difficult, very small noise strengths regimes not probed in [32]. For even smaller ρ_0 values the homogeneous phase is practically unobservable.

For the $\eta_{\rm high}$ line of the phase diagram separating the segregated from the homogeneous *disordered* phases, we used the location of the peak of the susceptibility of the nematic order parameter. Even though both phases are disordered, the segregated one still shows sizeable S values at the finite sizes we can probe numerically.

Our numerical results obtained for $\eta_{\rm low} < \eta < \eta_{\rm high}$ show that the decay of $\langle S\rangle$ accelerates at large system sizes as $P(S)$ gradually departs from the BHP distribution. We thus conjecture that our system is then, asymptotically, in a *disordered*, not a quasi-ordered phase. This occurs even when the initial decay of $\langle S\rangle$ displays an exponent $\zeta < \frac{1}{8}$, its value at the Berezinskii-Kosterlitz-Thouless transition used in [32] to define the isotropic/nematic transition (inset of Fig. 2c). In particular, at the onset of density segregation ($\eta \simeq \eta_{\rm low}$), the decay exponent ζ is typically rather small (e.g. $\zeta \simeq 0.03$ for $\rho_0 = 0.5$).

Observing full-blown disordered inhomogeneous regimes for η values such that the early decay of $\langle S\rangle$ occurs with an exponent $\zeta < \frac{1}{8}$ is however numerically very difficult, requiring huge system sizes and simulation times. The snapshots shown in Fig. 2e-f are actually taken in such a case: several dense, curved bands of various orientations are present. They evolve on very long timescales, elongating, merging, splitting, in a manner reminiscent of the band chaos reported in Fig. 1 (see [35]). Only the largest system sizes (Fig. 2f) reveal the existence of a finite characteristic length, in agreement with the nonlinear analysis of the equations (2)-(3).

Next, we investigated anomalous, "giant" number fluctuations, which we characterize by the scaling of Δn^2,

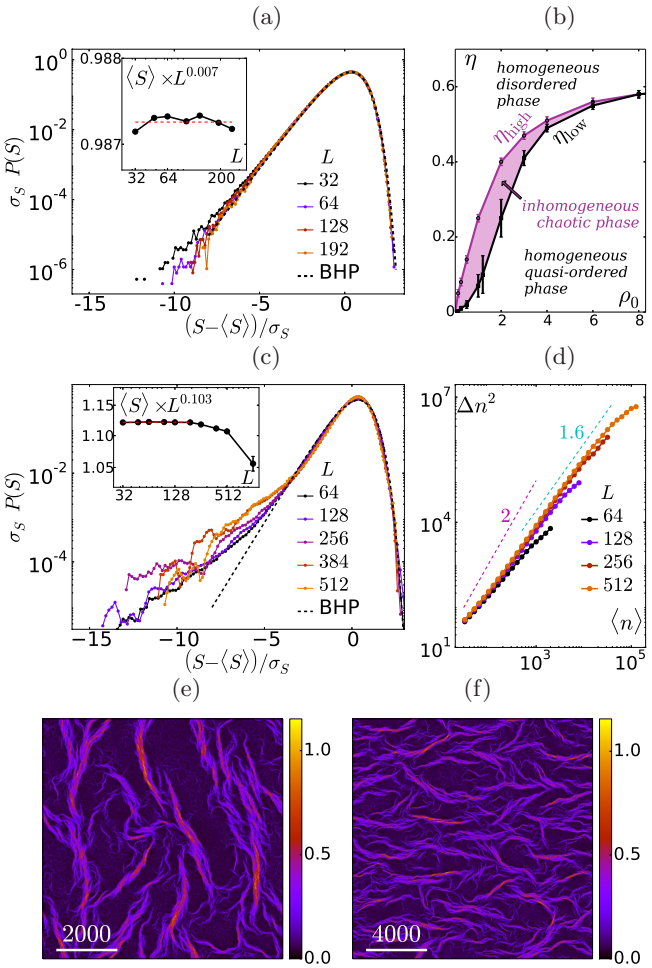

FIG. 2: (color online) Microscopic dynamics: (a,c) Rescaled distribution of S at various system sizes in the homogeneous ordered (a) and inhomogeneous (c) phases. Insets of (a,c): log log plots of $\langle S\rangle \times L^{-\zeta}$ vs L, where ζ is estimated from a fit of the initial decay of $\langle S\rangle$. (b) Phase diagram in the (η, ρ_0) plane. (d) Variance Δn^2 as a function of mean number of particle $\langle n\rangle$, in the homogeneous ordered phase. Dashed lines: power laws with exponents 2 (magenta) and 1.6 (cyan). (e-f) Snapshots of coarse-grained density in the chaotic phase of panel (c) for system sizes $L=8192$ (e) and $L=16384$ (f). Parameters: in all cases $v_0 = 0.3$, for (a,d): $\rho_0 = 2$, $\eta = 0.1$, $\zeta = 0.007$ and for (c,e,f): $\rho_0 = \frac{1}{8}$, $\eta = 0.038$, $\zeta = 0.103$.

the variance of the number n of particles contained in a square sub-system. Even though this anomalous scaling is a landmark of fluctuating active ordered phases, it can be probed in the fluctuation-free context of the fully chaotic regime of the hydrodynamic equations (2) and (3). We find $\Delta n^2 \sim n^2$ for boxes of sizes up to the characteristic lengthscale of chaos, followed by a crossover to normal fluctuations ($\Delta n^2 \sim n$) for larger boxes (not shown). For the inhomogeneous disordered phase of the Vicsek-like model (1), as already reported in [32], we also find $\Delta n^2 \sim n^2$ but are numerically unable to see the expected crossover to normal fluctuations. These observations are the trivial result of the segregation of density in dense bands [37] and not due to the sophisticated mechanism put forward by Toner, Ramaswamy, *et al.* as a typical feature of ordered, non-segregated, active phases. However, the homogeneous regimes found for $\eta < \eta_{\rm low}$ in the microscopic model do constitute such a phase. Measuring number fluctuations in this case, we find anomalous fluctuations, $\Delta n^2 \sim n^\alpha$, but with a characteristic scaling exponent α close to 1.6, not 2 (Fig. 2d). In other words, we do *not* find the value $\alpha = 2$ derived by Ramaswamy *et al.* from a linearized theory, but, surprisingly, a value close to that calculated by Toner and Tu for active *polar* ordered phases.

We finally mention results obtained on the Vicsek-like model defined by Eq. (1), but where neighbors are chosen to be those forming the first shell of Voronoi polygons around a given particle. In this "metric-free" model, the basic instability of the homogeneous ordered state leading to the segregated phase is suppressed [28]. Accordingly, our simulations reveal only two phases, the homogeneous disordered one, and the homogeneous quasi-ordered one, separated by a Berezinskii-Kosterlitz-Thouless-like transition. The quasi-ordered phase also exhibits anomalous number fluctuations, also with a non-trivial scaling exponent $\alpha \simeq 1.6$ (not shown).

To summarize, we showed that dry active nematics exhibit large-scale spatiotemporal chaos consisting of moving, elongating, splitting, merging high-density high-order band-like structures. At the level of the (deterministic) hydrodynamic equations (2) and (3), this chaos is the outcome of the linear instability, in two dimensions, of the band solution (4), and is observed in the whole region of existence of the solution, *i.e.* between the $\sigma_{\rm min}$ and $\sigma_{\rm max}$ lines in Fig. 1a, a region which encompasses the linear onset of nematic order. At the level of the Vicsek-like microscopic model defined by (1), the corresponding lines are the $\eta_{\rm low}$ and $\eta_{\rm high}$ lines of Fig. 2b. The phase diagram of dry active nematics thus comprises three different phases, a homogeneous disordered phase at strong noise, an inhomogeneous disordered chaotic phase at intermediate noise values, and a homogeneous ordered phase. In the microscopic model, this last phase is only quasi-ordered and displays anomalous number fluctuations. The order-disorder transition is thus located between the ordered phase and the chaotic inhomogeneous phase. Its nature, even at the "mean-field" level of the hydrodynamic equations, remains unclear: if the correlation scales of chaos were found to diverge when $\sigma \to \sigma_{\rm min}$, then the transition would probably be continuous. Unfortunately, the numerical determination of these scales in this limit is a very difficult task beyond the scope of this Letter [44].

Our results should eventually be completed by a study of the mesoscopic theory derived in [30], either by numerical integration of these Langevin equations or by some renormalization group analysis. (This could in particular provide some explanation to the anomalous scaling expo-

nent for number fluctuations found here similar to that of polar ordered phases.) This difficult task is left for future studies. At the experimental level, we believe that microtubule motility assays of the type studied in [38] should be able to demonstrate the phenomena described here [39].

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[40] Eqs.(2) and (3) can be written in terms of the more familiar symmetric traceless tensor field $\mathbf{Q}$ since $\rho[\mathbf{Q}]_{xx} = -\rho[\mathbf{Q}]_{yy} = \frac{1}{2}\mathrm{Re}\hat{f}_1$ and $\rho[\mathbf{Q}]_{xy} = \rho[\mathbf{Q}]_{yx} = \frac{1}{2}\mathrm{Im}\hat{f}_1$ but the complex notations are very convenient and we keep them in the following.
[41] They read $\mu(\rho) = \frac{8}{3\pi}\left[\left(2\sqrt{2}-1\right)\hat{P}_1 - \frac{7}{5}\right]\rho - \left(1-\hat{P}_1\right)$ and $\xi = \frac{32\nu}{35\pi^2}\left[\frac{1}{15}+\hat{P}_2\right]\left[\left(1+6\sqrt{2}\right)\hat{P}_1 - \frac{13}{9}\right]$ with $\nu = \left[\frac{8}{3\pi}\left(\frac{31}{21}+\frac{\hat{P}_2}{5}\right)\rho_0 + \left(1-\hat{P}_2\right)\right]^{-1}$, where the $\hat{P}_k$ are the coefficients of the Fourier series of the noise distribution. In the following, we used a Gaussian distribution of variance σ^2 so that $\hat{P}_k = e^{-2k^2\sigma^2}$.
[42] This was done at a global density $\rho_0 = 1$, but we do not have any reason to believe that a qualitative change of behavior occurs as ρ_0 is varied.
[43] This is corroborated by the two-point correlation function of the density field: it is axisymmetric for long enough averaging times and its radial average decreases exponentially, with a system-size independent cutoff for large enough L (not shown).
[44] Note that this would be an even harder task with the microscopic model.