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Nonlinear diffusion and hyperuniformity from Poisson representation in systems with interaction mediated dynamics

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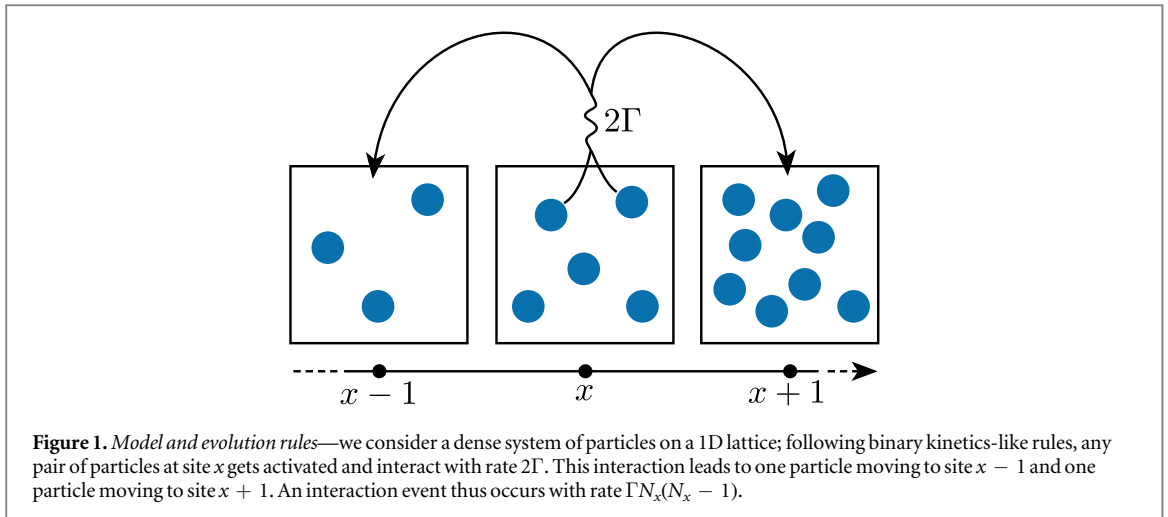
Abstract

We introduce a minimal model of interacting particles relying on conservation of the number of particles and interactions respecting conservation of the center of mass. The dynamics in our model is directly amenable to simple pairwise interactions between particles leading to particle displacements, ensues from this what we call interaction mediated dynamics. Inspired by binary reaction kinetics-like rules, we model systems of interacting agents activated upon pairwise contact. Using Poisson representations, our model is amenable to an exact nonlinear stochastic differential equation. We derive analytically its hydrodynamic limit, which turns out to be a nonlinear diffusion equation of porous medium type valid even far from steady state. We obtain exact self-similar solutions with subdiffusive scaling and compact support. The nonequilibrium steady state of our model in the dense phase displays hyperuniformity which we are able to predict from our analytical approach. We reinterpret hyperuniformity as stemming from correlations in particles displacements induced by the conservation of center of mass. Although quite simplistic, this model could in principle be realized experimentally at different scales by active particles systems.

1. Introduction

Driven many-body systems can exhibit nonequilibrium phase transitions between phases characterized by qualitatively very different dynamics. One such class of systems is represented by absorbing state models [1–3]. In these systems, the transition happens between a so-called *absorbing phase*, where the system reaches a state in which the dynamics comes to rest forever, and an *active phase* where the system converges towards nonequilibrium steady states with non zero fraction of degrees of freedom that remain active. By construction, such systems are out of equilibrium as they violate explicitly detailed balance. Examples of models leading to such absorbing phase transitions include models from the directed percolation class (which do not conserve particle number—see [1] and references therein) and the conserved directed percolation class or Manna universality class (where particle number is conserved) [4–8]. More recently, absorbing phase transition models were experimentally realized using for instance sheared suspensions of particles [9–13].

In models of the Manna class, the transition is generically controlled by the density of particles and it was found that these transitions to absorbing states display properties of continuous phase transitions with universal characteristic critical exponents, a well-defined model dependent critical density, and a correlation length diverging at the critical point. In essence, these models involve particles that can be active or passive depending on the local particle density. In dense regions (typically defined as more than 2 particles in a given neighborhood), particles are active and follow a prescribed dynamics (typically perform jumps); otherwise particles are said to be passive and remain at rest. Several microscopic models in this class have been proposed, including the Manna model, the random organization (RandOrg) model or the conserved lattice gas model and their generalizations; these are either on or off lattice, and involve different choices of kinetic rules [5, 7, 10, 14–17].



Recently, a renewed interest in this class of models was triggered by [15, 16], where it was found that the fluctuations in density in models belonging to the Manna class scale differently than usual random systems. More precisely, for a system of spatial dimension d , density fluctuations in a region of volume $V = \lambda^d$ can be written

$$\sigma_\lambda^2 = \langle \rho_\lambda^2 \rangle - \langle \rho_\lambda \rangle^2, \quad (1)$$

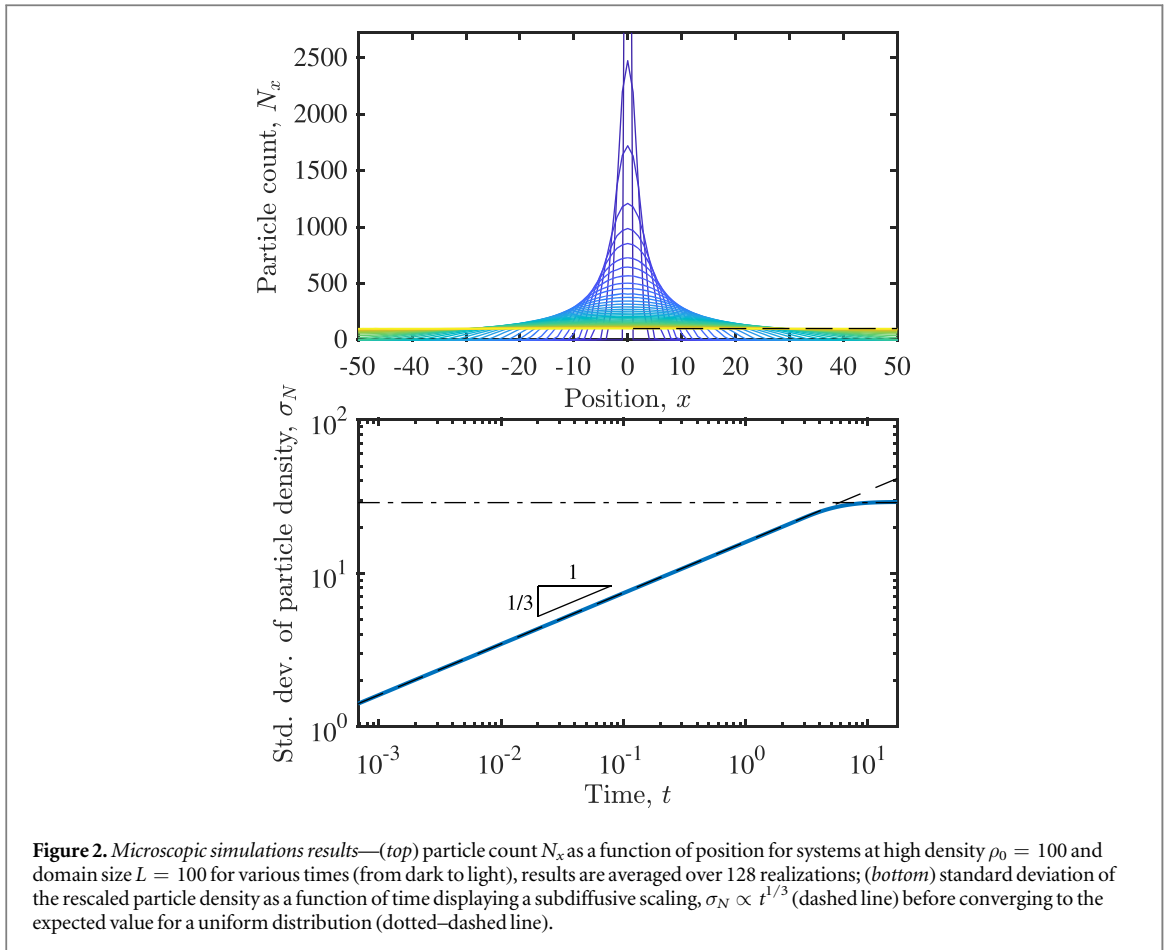
where ρ_λ is the number of particles in the region divided by its volume V and the $\langle \dots \rangle$ denotes an average over many such volumes; these density fluctuations generically follow a scaling behavior $\sigma_\lambda^2 \propto \lambda^{-\gamma}$, with $\gamma > 0$. Random systems such as those stemming from Poisson processes display the expected scaling with $\gamma = d$. In systems for which $\lambda > d$, particles are distributed more uniformly than random; these systems are called hyperuniform [18–21].

In [15], a variety of models belonging to the Manna class were shown to display hyperuniformity ($\gamma > d$) at the critical point. This is in contrast with classical equilibrium models in which fluctuations are enhanced at the critical point ($\gamma < d$) [18]. Further, it was found in [16] that enforcing conservation of the particles center of mass during pairwise interactions in models of the Manna class, while preserving the transition to an absorbing state, leads to hyperuniformity in the active phase, even far from the critical point. Interestingly, the density fluctuations were shown to scale with exponent $\gamma = d + 1$, which can be shown to be the largest possible exponent value [22].

In this paper, we introduce a minimal model where the dynamics is directly amenable to simple pairwise interactions between particles, leading to interaction mediated dynamics. Using binary reaction kinetics-like rules, such model can therefore be interpreted as a system of agents that can get activated upon pairwise contacts, which leads to a finite range irreversible transient repulsion (see figure 1). While obviously simplistic, we suggest that this model could in principle be realized experimentally beyond the examples of sheared suspensions mentioned below, at different scales, with particles with pairwise interactions (e.g. molecular motors, cells, active colloids, bioinspired robots), which are controlled by active processes (e.g. hydrolysis of a chemical fuel). By a systematic approach based on Poisson representations, we obtain an exact nonlinear stochastic differential equation governing this dynamics. In the hydrodynamic limit of the high density active phase, we show that this model leads to a porous medium type nonlinear diffusion equation valid even far from steady state. The dynamics of this system is entirely controlled by the reaction kinetics governing the active repulsion between particles; in turn, our model exhibits subdiffusive behavior and aging. Finally, in its nonequilibrium steady state, this model displays hyperuniformity, which we also predict quantitatively using our macroscale stochastic differential equation; this allows to reinterpret hyperuniformity in this system as originating from correlations in particles displacements induced by conservation of the center of mass, in agreement with [16].

2. Model and simulations

First, we introduce a one-dimensional discrete model of driven many-body system, where the dynamics is entirely mediated by pairwise interactions between the particles. We introduce N interacting particles on a lattice of size L with reflective boundary conditions at both ends. In turn, we have *conservation of the number of particles*. In our model, a site x on the lattice may have any number of particles N_x . Each pair of particles on the same lattice site may interact with rate 2Γ with the result of one of them moving to site $x + 1$, while the other moves to site



$x - 1$. In our model, such interaction events are thus controlled via combinatorial kinetics and happen at rate proportional to $N_x(N_x - 1)/2$. This type of interaction leads to *conservation of the center of mass*.

This absorbing state model admits a density-controlled nonequilibrium phase transition between an absorbing phase and an active phase. It is easy to see that the critical density in this one-dimensional model is $\rho_c = 1$. In what follows, we will only study the resulting dynamics at high density, deep in the active phase away from the critical density where $N_x \gg 1$ in steady state. As defined here, while our model is similar to the so-called COMCon model introduced in [16], it differs in the definition of the kinetic rules, which has striking consequences for the dynamics. In particular, we show in what follows that the dynamics of our system is governed by a nonlinear diffusion equation of porous medium type leading to anomalous spreading dynamics. In addition, we make use of a different methodology, based on Poisson representation, which allows us to obtain an exact nonlinear stochastic differential equation as well as its hydrodynamic limit. This leads to a nonlinear diffusion equation that describes the system dynamics at all times, and in particular far from the steady state. Note that we expect our model to display an absorbing phase transition of the same nature as that of the COMCon model.

We perform simulations of this system in the high density regime $\rho_0 = N/L \gg 1$. We study the classical problem of diffusion from a point source and fix $\Gamma = 1$ in all simulations. Starting from a Dirac delta distribution at the center of the domain, we use Gillespie's algorithm [23, 24] to predict the time increment and location of the next interaction based on the local number of particles at each lattice site. Figure 2 quantifies the expansion of the initial distribution to a nonequilibrium steady state at uniform average density ρ_0 . We define the standard deviation of the rescaled particle density as $\sigma_N^2 = \langle \tilde{\rho}^2 \rangle - \langle \tilde{\rho} \rangle^2$, with the rescaled particle density $\tilde{\rho}(x) \equiv (N_x/L)/\rho_0$ (i.e. the fraction of particles at site x) and $\langle \dots \rangle$ representing an average over space. In turn, we show that the standard deviation of the rescaled particle density strikingly displays a subdiffusive scaling, $\sigma_N \propto t^{1/3}$ before converging to the value expected for a uniform density over the L lattice sites, $\sigma_u = L/\sqrt{12}$.

3. Nonlinear diffusion equation from first principles

The dynamics of this system being entirely controlled by combinatorial kinetics, it is natural to expect the diffusion coefficient of a single particle to be proportional to the local particle density. Here, we proceed to a

systematic derivation of an exact stochastic differential equation giving access to all moments of the random variables N_x , defined as the number of particles at site x . We start by writing the master equation for $P(\{N_x\}, t)$ the probability to have at each site x a number of particles N_x at time t

$$\partial_t P = \Gamma \sum_x [(N_x + 2)(N_x + 1)P(N_{x-1} - 1, N_x + 2, N_{x+1} - 1) - N_x(N_x - 1)P], \quad (2)$$

where for the sake of simplicity we only write the terms changing. To treat this many-body system in a simple way, we make use of the Poisson representation introduced by Gardiner and Chatuverdi [25–27]. This method is a formally exact analytical approach based on the following projection of the particle numbers at site x on Poisson states

$$P(\{N_x\}, t) = \int \prod_x d\alpha_x e^{-\alpha_x} \frac{\alpha_x^{N_x}}{N_x!} f(\{\alpha_x\}, t), \quad (3)$$

where $f(\{\alpha_x\}, t)$ is a quasi-probability function of the Poisson fields α_x . The Poisson representation can be reinjected in the master equation. By choosing the region of integration such that $f(\{\alpha_x\}, t)$ vanishes at the boundary, one can obtain after straightforward integrations by part the following Fokker–Planck equation

$$\partial_t f(\{\alpha_x\}, t) = \Gamma \sum_x \frac{\partial}{\partial \alpha_x} \Delta \alpha_x^2 f(\{\alpha_x\}, t) - \frac{1}{2} \left[\frac{\partial^2}{\partial \alpha_x^2} - \frac{\partial^2}{\partial \alpha_{x-1} \partial \alpha_{x+1}} \right] 2\alpha_x^2 f(\{\alpha_x\}, t) \quad (4)$$

equivalent to the following exact stochastic differential equation for the Poisson fields

$$\partial_t \alpha_x = \Gamma \Delta \alpha_x^2 + \eta_x \quad (5)$$

with Δ is the second finite difference operator and η_x is a Gaussian noise with zero mean value whose correlations are given by

$$\langle \eta_x(t) \eta_x(t') \rangle = 2\Gamma \langle \alpha_x^2 \rangle \delta_{t,t'} \quad (6)$$

$$\langle \eta_{x-1}(t) \eta_{x+1}(t') \rangle = 2\Gamma \langle \alpha_x^2 \rangle \delta_{t,t'} \quad (7)$$

with $\delta_{i,j}$ is the Kronecker delta. Note that the factorial moments of the particles numbers $\langle N_x \rangle_n$ are equal to the moments of the Poisson fields $\langle \alpha_x^n \rangle$ [26]. In particular, this means that

$$\langle N_x \rangle_n \equiv \langle N_x [N_x - 1] \cdots [N_x - (n - 1)] \rangle = \int \prod_x d\alpha_x \alpha_x^n f(\{\alpha_x\}, t) \equiv \langle \alpha_x^n \rangle \quad (8)$$

Thus, equations (5)–(7) define exactly the dynamics of the system and give access in principle to all moments of N_x . The correlations in particle displacements imposed by the conservation of the center of mass in the interactions induce a correlated noise term. In turn, the form of the noise (as expressed in equation (7)) induces correlations among lattice sites.

4. Hydrodynamic limit

We turn to the continuous space limit (where the lattice spacing $\ell \rightarrow 0$) and consider x to be a continuous variable. To take the continuous space limit accurately, we also need to rescale the rates and Poisson fields accordingly [28, 29]. Taking this into account, we have by definition of the Poisson fields,

$$\langle \alpha(x, t) \rangle = u(x, t) \quad (9)$$

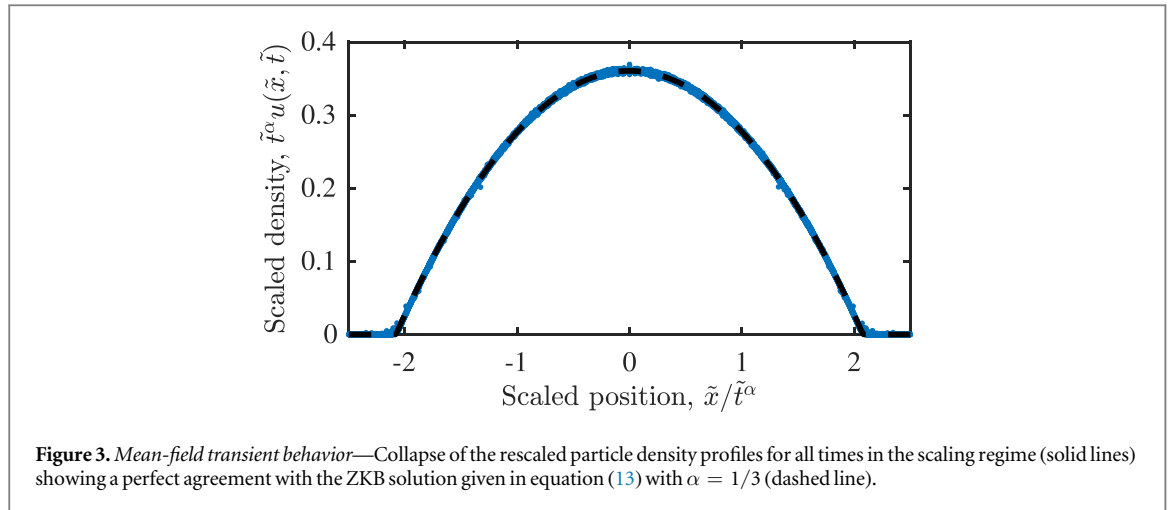
with $\langle \cdots \rangle$ an average over the noise. We can thus write that

$$\alpha(x, t) = u(x, t) + \delta\alpha(x, t) \quad (10)$$

where u is the space- and time-dependent particle density averaged over the noise while $\delta\alpha(x, t)$ denotes local deviations from the mean values; by definition, we have $\langle \delta\alpha(x, t) \rangle = 0$. In the large density limit ($N \rightarrow \infty$), the fluctuations in the particle density can be neglected in comparison to the mean particle density, i.e. $|\delta\alpha(x, t)| \ll u(x, t)$. Thus, the hydrodynamic limit is well-defined and we obtain the following nonlinear diffusion equation

$$\partial_t u(x, t) = \Gamma \partial_{xx} u^2(x, t) \quad (11)$$

which is exact in this limit. This equation is a special case of a wider class of equations known as porous medium equations, $\partial_t u = \partial_{xx} u^m$ [30]. Self-similar solutions of the form $u(x, t) = t^{-\alpha} f(xt^{-\beta})$ were obtained in the case of the point-source problem studied here [30–32]. It can easily be shown that the similarity exponents are given by



$$\alpha = \frac{d}{d(m-1)+2} \text{ and } \beta = \frac{1}{d(m-1)+2}. \quad (12)$$

Which leads to $\alpha = \beta = 1/3$ in the case $d = 1$ and $m = 2$ which is consistent with the scaling observed in figure 2. Furthermore, the so-called ZKB solutions are given by

$$u_{\text{ZKB}}(x, t) = \max\left(0, t^{-\alpha} \left[C - \kappa \frac{x^2}{t^{2\alpha/d}} \right]^{\frac{1}{m-1}}\right), \quad (13)$$

where $\kappa = (m-1)\alpha/2md$ and C is determined by conservation of mass and the initial condition. For all times such that the boundary of the domain have not been reached the ZKB solution (equation (13)) should represent well our microscopic model. Figure 3 shows a perfect agreement between the ZKB solution and the rescaled particle density in nondimensional quantities for all times in the scaling regime.

5. Self-similar dynamics and aging

Note that equation (11) can be written $\partial_t u = D(u) \partial_{xx} u$ (with $D(u) = 2\Gamma u(x, t)$) which is consistent with our intuition and a direct mean-field argument. So far, we have only quantified the dynamics at the macroscopic scale; at the single particle scale, we measure the time-dependent mean-squared displacement (or increment function)

$$\mathcal{G}(\tau, t) = \langle |x(t+\tau) - x(t)|^2 \rangle, \quad (14)$$

where $\langle \dots \rangle$ denotes an average over particles and realizations but not origin of time t .

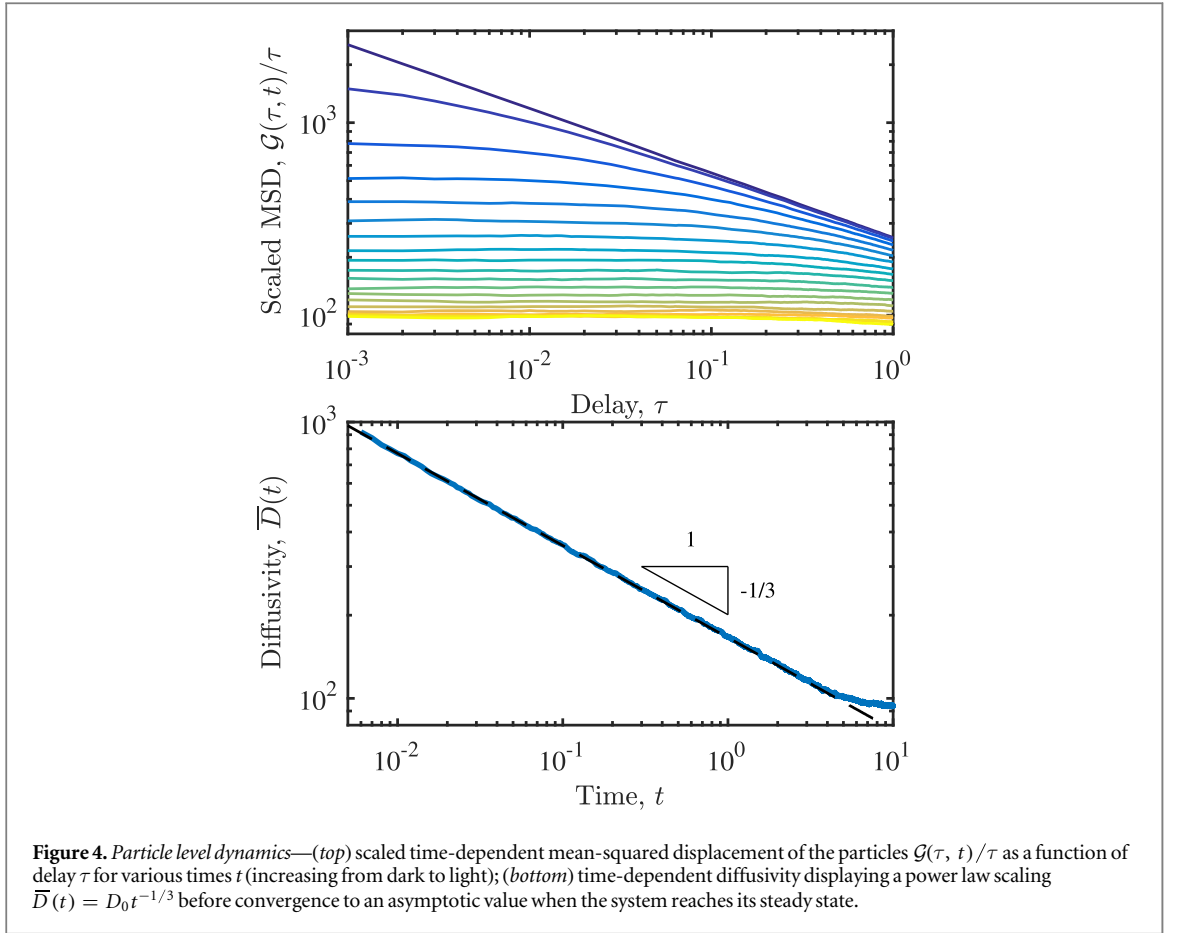
We find that for all times t , $\mathcal{G}(\tau, t)$ is linear in the delay τ at short times and thus displays a diffusive scaling $\mathcal{G}(\tau, t) \underset{\tau \rightarrow 0}{\sim} 2\bar{D}(t)\tau$ (see figure 4). Writing out the definition of the average diffusion coefficient, one has in the $\tau \rightarrow 0$ limit:

$$\mathcal{G}(\tau, t) \sim \frac{2\tau}{N} \int D(u) u(x, t) dx, \quad (15)$$

Together with $D(u) = 2\Gamma u(x, t)$ and the density of particles which admits the following scaling form $u(x, t) = t^{-1/3} f(xt^{-1/3})$, we can easily predict the scaling of the average diffusivity with time to obtain $\bar{D}(t) \sim D_0 t^{-1/3}$. This is confirmed by our numerical results for which we find that the diffusivity at short delay time τ is time-dependent, a signature of aging, and scales as $\bar{D}(t) \propto t^{-1/3}$ before converging to a constant when the particle density profile reaches its uniform steady state (see figure 4). Thus, it is interesting to note that this interaction mediated dynamics leads to short time aging, single particle diffusion and subdiffusive scaling at the population scale.

6. Density fluctuations and hyperuniformity

In the long time limit, we find that the density of particles converges to a profile with anomalously small density fluctuations. We find that the model under study here displays a power law decay of the density fluctuations with exponent $\gamma > d$. Thus, the nonequilibrium steady state of our model is hyperuniform deep in the active phase (at large densities). Moreover, we measure an exponent $\gamma = 2 = d + 1$ corresponding to the fastest decay



possible [18, 20, 22] (see figure 5). This is in agreement with recent studies [16] as the conservation laws (conservation of particles and conservation of center of mass) introduced in our model have been shown to lead in other models to hyperuniform behavior at long times.

Another way to measure hyperuniformity is to check that the structure factor $S(k)$ vanishes as the wavenumber $k \rightarrow 0$. Defined as

$$S(k) = \frac{1}{N} \left| \sum_{i=1}^N \exp(ikr_i) \right|^2 \quad (16)$$

the structure factor is asymptotically typically characterized by a power law with exponent ξ , $S(k) \sim k^\xi$. When $\xi < 1$, the density fluctuations decay as $\sigma_\lambda^2 \propto \lambda^{-\xi-d}$; while when $\xi > 1$, the density fluctuations decay as $\sigma_\lambda^2 \propto \lambda^{-(d+1)}$ and are then maximally hyperuniform [19]. We show in figure 5 that in our model the structure factor does indeed vanish as $k \rightarrow 0$ with exponent $\xi = 2$ implying a maximally hyperuniform system.

To confirm this result analytically, we linearize equation (5) around the uniform state. Writing $\alpha(x, t) = n_0 + \delta\alpha(x, t)$, we obtain in Fourier space

$$\partial_t \delta\tilde{\alpha} = -2\Gamma n_0 k^2 \delta\tilde{\alpha} + \tilde{\eta} \quad (17)$$

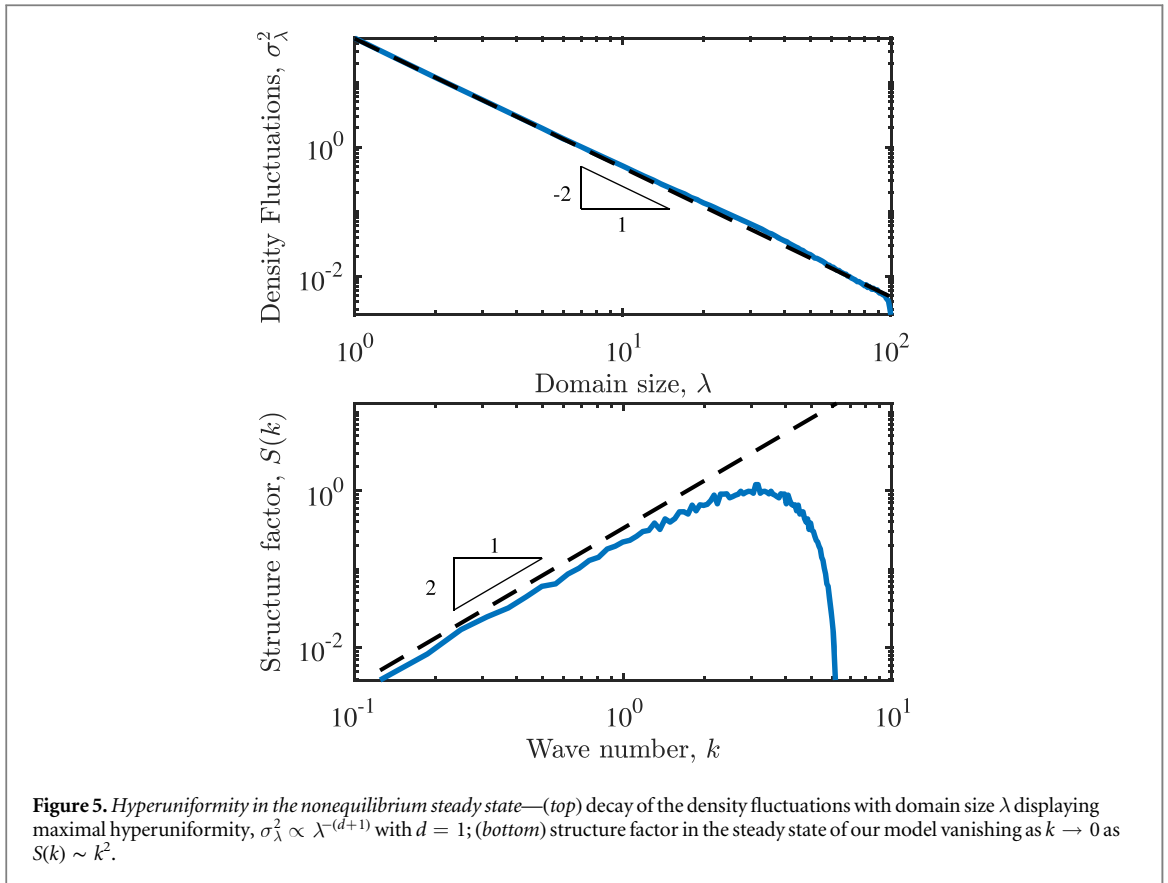
whose solution is given by

$$\delta\tilde{\alpha} = \int_{-\infty}^t dt' e^{-2\Gamma n_0 k^2 (t-t')} \tilde{\eta}. \quad (18)$$

The structure factor can be expressed via the Fourier transform of the particle density, $S(k) = \langle \delta n(k) \delta n(-k) \rangle / N$ with $\delta n(k, t) = \int \delta n(x, t) e^{-ikx} dx$. By the nature of the Poisson fields, we have

$$\langle \delta n(x) \delta n(y) \rangle = \langle \delta\alpha(x) \delta\alpha(y) \rangle + n_0 \delta(x - y). \quad (19)$$

From the solution of the linearized Langevin equation, we can compute the scaling of the structure factor at small wavenumber to obtain



$$NS(k) = \frac{n_0}{2k^2}[\cos 2k - 1] + n_0 \xrightarrow{k \rightarrow 0} \frac{n_0 k^2}{3}, \quad (20)$$

where we recover the scaling observed in figure 5. It was argued that hyperuniformity stems from a competition between a noise term which generates fluctuations and a deterministic term which reduces them. Further, it was suggested that particle conservation *and* center of mass conservation diminish drastically large wavelength fluctuations leading to the far-reaching consequence of hyperuniformity in the active phase. In particular [16], established that the noise term in the Langevin equation for the particle density appears as a second spatial derivative as a consequence of the center of mass conservation. Our approach based on Poisson representation gives us another interpretation, where hyperuniformity stems from correlations in particles displacements, which induce a correlated noise term in our exact stochastic differential equation. Here, we observe this at the level of the Poisson fields. Indeed, correlations in the noise term (equation (7)) are crucial in determining the scaling of $S(k)$ in equation (20). Our model differs from the COMCon model established in [16] in the definition of their kinetic rules (and thus, the transition rates) but not in the definition of their transition rules. While we have shown that this has striking consequences for the dynamics of the system which in our case displays a nonlinear diffusion equation with anomalous spreading, hyperuniformity is insensitive to this change of kinetic rules. Thus, our work provides a complementary approach to that of [16] in understanding the mechanism behind the observed hyperuniformity.

7. Conclusion

To summarize, we have introduced a simple model of interaction mediated dynamics with center of mass conservation. Our model is based on binary reaction kinetic rules, and can be recast in an exact nonlinear stochastic differential equation by using Poisson representations. This allows us to derive its hydrodynamic limit, which turns out to be a nonlinear diffusion equation of porous medium type for which exist exact self similar solutions with subdiffusive scaling and compact support. In addition, our Poisson representation approach provides a direct way to demonstrate hyperuniformity in the model. We reinterpret hyperuniformity as stemming from the non trivial correlations between particles displacements.

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