Lattice Model to Derive the Fluctuating Hydrodynamics of Active Particles with Inertia

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We derive the hydrodynamic equations with fluctuating currents for the density, momentum, and energy fields for an active system in the dilute limit. In our model, nonoverdamped self-propelled particles (such as grains or birds) move on a lattice, interacting by means of aligning dissipative forces and excluded volume repulsion. Our macroscopic equations, in a specific case, reproduce a transition line from a disordered phase to a swarming phase and a linear dispersion law accounting for underdamped wave propagation. Numerical simulations up to a packing fraction $\sim 10\%$ are in fair agreement with the theory, including the macroscopic noise amplitudes. At a higher packing fraction, a dense-diluted coexistence emerges. We underline the analogies with the granular kinetic theories, elucidating the relation between the active swarming phase and granular shear instability.

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Introduction.—Active particles (APs) encompass several different out-of-equilibrium systems where many interacting agents continuously convert internal energy into self-propulsion [1]. Living or manmade instances of such systems can be found at the microscale, such as bacteria, spermatozoa, and Janus spheres [2,3], or at the macroscale, such as vibrated polar granular particles [4,5] and animal groups (mammal herds, bird flocks, fish schools), where inertia becomes relevant [6,7]. APs display intriguing collective phenomena in the form of disorder-order transitions: Their complexity implies the existence of many symmetries that can be broken and several types of possible ordered patterns, one of the most spectacular being "flocking" [8,9].

The difficulty to fit the behavior of APs into equilibrium statistical mechanics explains the lack of a unified theoretical approach and the unsolved debate about the nature or specificity of the observed transitions [10]. This is reflected in a plethora of AP models which—even containing similar microscopic ingredients—may display subtly different macroscopic features; see, for instance, the comparison between the "run and tumble" model [11,12], the "active Brownian" model [13–15], and the recent "Gaussian-colored noise" model [16]. The situation is even more complex if looking at the many macroscopic theories: These include phenomenological field equations based upon fundamental symmetries [2,10], local mean field approximations [17–21], and theories starting from a Boltzmann kinetic equation. The latter describe systems with short-range (collisionlike) interactions, mainly applied to Vicsek-like models [22–24] or self-propelled *elastic* hard spheres [25]. Given that systems of APs do not contain a huge number of particles, fluctuations are observable and can even be very large [26–28]: The fundamental problem of computing macroscopic noise from microscopic models has been approached through the kinetic theory basically only for active nematics [29].

A fertile ground for further insights into the collective behavior of APs with inertia is the study of macroscopic patterns in fluidized granular materials [30], a connection made stronger by experiments and models of polar granular particles [4,5,31–33]. Inertial APs (including animals) and granular materials seem to share similar theoretical mechanisms: Such an analogy stimulates the transposition, into the realm of inertial APs, of features and methods of granular kinetic theories [34,35]. Granular active particles (GAPs) have been revealed to be important also for the study of giant fluctuations [4,36]. Moreover, the general theory of fluctuating hydrodynamics received important inputs from the granular realms in recent years [37–39] also within simplified lattice gas models [35,40–43] inspired by lattice gases with conservative interactions [44]. Notwithstanding such intense activity, a theory of fluctuating hydrodynamics for GAP models is lacking.

Here we introduce a model of GAPs on the lattice where pairwise interactions combine excluded volume and dissipative alignment, quite similarly to the off-lattice model in Ref. [31] and to the one in Ref. [45], which has a slightly different evolution of the self-propulsion force. Our main result is a set of hydrodynamic equations for the density, momentum, and energy fields with fluctuating currents and source terms, in analogy with recent granular lattice models [35,42,43]. An application of these general equations is given under the assumption of local equilibrium [46], where they describe a gas-swarming phase transition through the linear instability of the homogeneous disordered state. The homogeneous swarming state arises when either the noise amplitude is small enough or the aligning force is strong enough.

Model.—We consider a square lattice in d dimensions of volume $V = L^d$, with $1 \ll N \leq V$ self-propelled particles moving on it. A lattice site $i \in \{1, L\}^d = \Lambda$ can be

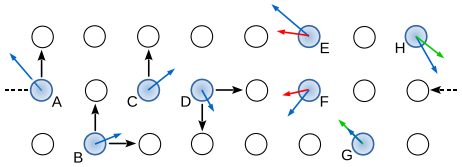

FIG. 1. Sketch of APs in a lattice. Particles A–D show hopping (black arrows) to neighbor sites according to the directions of their active velocity (blue arrows), including periodic conditions (A) and excluded volume (C,D). Next neighbors interact (E,F), with a force which aligns velocities (from blue to red arrows). Self-propulsion acts in the direction of the velocity and brings the speed toward a fixed value (G, from blue to green arrow). The velocity of a particle can be modified also by external noise (H, from blue to green).

occupied at most by one particle (excluded volume) and is described by its occupation number $n_i \in \{0,1\}$ and its "active velocity" $\mathbf{v}_i \in \mathcal{R}^d$ (the meaning of this variable is discussed later). The elementary moves of our dynamics amount to (see Fig. 1) (1) hopping, (2) self-propulsion, (3) nearest-neighbor interaction, and (4) noise. A particle hops from i to an adjacent j with a probability, per unit of time, proportional to the projection of $\mathbf{v}_i$ along the direction connecting i to j. Self-propulsion consists in a velocity-dependent force

$$\mathbf{f}^{(1)}(\mathbf{v}) = \omega_s \mathbf{v}\left(1 - \frac{v^2}{v_s^2}\right); \tag{1}$$

i.e., it acts along the direction of the particle's velocity and induces the relaxation of its speed toward a set value v_s with a characteristic rate ω_s. Pairwise interaction is a nonconservative force, exerted on $\mathbf{v}$ by its nearest neighbor $\mathbf{v}'$, of the kind

$$\mathbf{f}^{(2)}(\mathbf{v},\mathbf{v}') = -\omega_d(\mathbf{v}-\mathbf{v}'), \tag{2}$$

which—as in granular collisions—satisfies momentum conservation and dissipates relative kinetic energy at a typical rate ω_d. Finally, a white noise force acts independently upon each component of the velocity, making it follow a Wiener process with diffusion coefficient D, when self-propulsion and interactions are switched off. Here noise represents the coupling with hidden degrees of freedom, i.e., surrounding fluids, internal fluctuations in the self-propulsion mechanism, etc. In Supplemental Material [47], one can find the detailed stochastic finite-difference equations for the evolution of n_i, $n_i\mathbf{v}_i$, and $e_i = n_i v_i^2/2$ for each site i. The probability of a configuration $\{n_i,\mathbf{v}_i\}$ is defined as $\mathcal{P}(\{n_i,\mathbf{v}_i\};t)$. The two-site marginalized probability for sites i and j is also defined as $\mathcal{P}_{ij}(n_i,n_j,\mathbf{v}_i,\mathbf{v}_j;t)$.

Locally averaged fields are defined as

$$\rho_i(t) = \langle n_i\rangle, \tag{3a}$$
$$\rho_i(t)u_{i,k}(t) = \langle n_i v_{i,k}\rangle, \tag{3b}$$
$$\rho_i(t)T_i(t) = \langle n_i|\mathbf{v}_i-\mathbf{u}_i|^2\rangle/d, \tag{3c}$$

defining the average of an arbitrary function $f()$ as

$$\langle f(n_i,\mathbf{v}_i)\rangle = \prod_{i\in\Lambda}\left(\sum_{n_i=0,1}\int d\mathbf{v}_i\right)\mathcal{P}(\{n_i,\mathbf{v}_i\};t)f(n_i,\mathbf{v}_i), \tag{4}$$

and in Eq. (3c) we assumed isotropy of the local temperature.

Fluctuating hydrodynamics.—Our investigation has led to equations for local averages in the large volume limit $L\to\infty$, $N\to\infty$ at constant number density $\phi = N/V$. In this limit, the physical spacing between two adjacent sites is sent to 0 as $\Delta x = 1/L$, such that a spatial position in the system is denoted by a continuous $\mathbf{x}\in[0,1]^d$.

The used assumptions amount to (i) molecular chaos (expected to be valid in the dilute limit $\phi\to 0$) with isotropic velocity factorization:

$$\mathcal{P}_{ij}(n_i,n_j,\mathbf{v}_i,\mathbf{v}_j;t) = \mathcal{P}_i(n_i,\mathbf{v}_i;t)\mathcal{P}_j(n_j,\mathbf{v}_j;t), \tag{5}$$

$$\mathcal{P}_i(n_i,\mathbf{v}_i;t) = p_i(n_i;t)\prod_{k=1}^{d}P_{i,k}(v_{i,k};t); \tag{6}$$

(ii) smoothness in the space of averages of generic observables $F(n,v)$:

$$\langle F\rangle_{i+1,t} = \langle F\rangle(\mathbf{x},t) + \frac{1}{L}\partial_{x_l}\langle F\rangle|_{(\mathbf{x},t)} + O(1/L^2), \tag{7}$$

l being a Cartesian direction $l\in\{1,d\}$, and $i+1$ denotes the next-neighbor site in the lth direction.

With the above assumptions, through a direct local averaging procedure and in the large volume limit [47], one gets the following "hydrodynamic" equations:

$$\partial_t\rho = -\nabla\cdot\mathbf{j}, \tag{8a}$$

$$\rho\partial_t\mathbf{u} = -\nabla\cdot\mathcal{J} + \mathbf{u}(\nabla\cdot\mathbf{j}) + \rho\mathbf{f}^s, \tag{8b}$$

$$\rho\partial_t T = \left(T - \frac{u^2}{d}\right)\nabla\cdot\mathbf{j} + \frac{2}{d}\mathbf{u}\nabla:\ \mathcal{J} - \frac{2}{d}\nabla\cdot\mathbf{J} - 2\rho^2\Delta^d + 2\rho(\Delta^s + D). \tag{8c}$$

In the above equations, we have introduced the local averages for (i) the self-propulsion force $\mathbf{f}^s(\mathbf{x},t) = \int d\mathbf{v}P(\mathbf{v};\mathbf{x},t)\mathbf{f}^{(1)}(\mathbf{v})$, (ii) the power dissipated by pairwise interaction $\Delta^d(\mathbf{x},t) = \int d\mathbf{v}d\mathbf{v}'P(\mathbf{v};\mathbf{x},t)P(\mathbf{v}';\mathbf{x},t)\times(\mathbf{v}-\mathbf{v}')\cdot\mathbf{f}^{(2)}(\mathbf{v},\mathbf{v}')$, and (iii) the power injected by self-propulsion $\Delta^s(\mathbf{x},t) = \int d\mathbf{v}P(\mathbf{v};\mathbf{x},t)\times[\mathbf{v}-\mathbf{u}(\mathbf{x},t)]\cdot\mathbf{f}^{(1)}(\mathbf{v})/d$. The fluctuating currents up to orders smaller than $1/L$ read

$$j_l = \rho(1-\rho)u_l + \sigma_l, \tag{9a}$$

$$\mathcal{J}_{kl} = \rho(1-\rho)\langle v_k v_l\rangle + \varsigma_{kl}, \tag{9b}$$

$$J_l = \rho(1-\rho)\frac{1}{2}\sum_{k=1}^{d}\langle v_k^2 v_l\rangle + \Sigma_l, \tag{9c}$$

for density, momentum, and energy, respectively. Equations (9) are isotropic, even if on a squared lattice, as opposed to previous lattice gas automata [48,49], possibly because of the different modeling of microscopic velocities. The terms σ_l, ς_{kl}, and Σ_l are current noises with zero average. Our calculation indicate that such noises are Gaussian and white, with amplitudes given explicitly in Supplemental Material [47].

It is interesting to discuss the terms $\rho(1-\rho)$ appearing in the currents. These are an effect of the excluded volume and clarify the meaning of our active velocity $\mathbf{v}_i$: It is not equivalent to the actual infinitesimal displacement of the particle. The active velocity rather represents the tendency to go at a given speed in a certain direction, such as self-propulsion: a tendency which can be frustrated by excluded volume and that can be immediately resumed when the target site becomes free. In the dilute limit $\rho \to 0$, this is not a relevant difference, but it can be appreciated at relatively moderate densities.

Stability analysis.—In order to understand the relevance of our hydrodynamic equations, we discuss the stability of homogeneous steady states—i.e., states where fields do not depend upon spatial coordinates. We adopt adimensional variables, using $1/\omega_s$ and v_s/ω_s as units of time and length, respectively. The only free parameters left are density ϕ, relative rate of dissipation $\gamma = \omega_d/\omega_s$, and relative strength of noise $\Gamma = D/(\omega_s v_s^2)$. Moreover, to close our equations, we assume a Gaussian local velocity distribution: $P(\mathbf{v};t) = [2\pi T(t)]^{-d/2} \exp[-|\mathbf{v}-\mathbf{u}(t)|^2/2T(t)]$. Such an assumption rests upon the fact that in the limit of large noise or small self-propulsion one recovers the driven granular gas model, yielding a nearly Gaussian velocity distribution [50]. It is also corroborated by observing (see below) that the disordered-swarming instability is reproduced already within such an approximation. The equations for the homogeneous speed u and temperature T then read

$$\dot{u} = u\{1-[(d+2)T+u^2]\},$$
$$\dot{T} = -4d\phi\gamma T + 2T\left[1-(d+2)\left(T+\frac{1}{d}u^2\right)\right] + 2\Gamma, \quad (10)$$

which have three possible fixed points: the fully disordered point ($u=0, T=T_0$), with $T_0 = \{[1-2d\phi\gamma + \sqrt{(1-2d\phi\gamma)^2+4(d+2)\Gamma}]/[2(d+2)]\}$ which always exists; and two "swarming" points with $u=u_-, T=T_-$ and $u=u_+, T=T_+$, which exist only in a certain (γ,Γ) range [47]. Small—spatially dependent—fluctuations around the fully disordered fixed point are denoted as $\delta\rho(\mathbf{x},t)=\rho(\mathbf{x},t)-\phi$, $\delta\mathbf{u}=\mathbf{u}(\mathbf{x},t)$, and $\delta T = T(\mathbf{x},t)-T_0$. After converting to Fourier space, decomposing $\hat{\mathbf{u}}_\mathbf{k}$ in a parallel (to $\mathbf{k}$) and $d-1$ transverse components ($\hat{u}^\parallel_\mathbf{k}$, $\hat{\mathbf{u}}^\perp_\mathbf{k}$), and defining $\delta\mathbf{f} = (\hat{\rho}_\mathbf{k}, \hat{u}^\parallel_\mathbf{k}, \hat{\mathbf{u}}^\perp_\mathbf{k}, \hat{T}_\mathbf{k})$, the time evolution of the modes, linearized near that fixed point, reads

$$\partial_t \delta\mathbf{f} = M(\mathbf{k})\delta\mathbf{f}, \quad (11)$$

with $M(\mathbf{k})$ equal to

$$\begin{pmatrix} 0 & -\phi(1-\phi)2\pi ik & 0 & 0 \\ -\frac{1-2\phi}{\phi}T_0 2\pi ik & B(\gamma,\Gamma) & 0 & -(1-\phi)2\pi ik \\ 0 & 0 & B(\gamma,\Gamma) & 0 \\ -4d\gamma T_0 & -\frac{2}{d}(1-\phi)T_0 2\pi ik & 0 & -2A(\gamma,\Gamma) \end{pmatrix}, \quad (12)$$

where

$$A(\gamma,\Gamma) = \sqrt{(1-2d\phi\gamma)^2+4(d+2)\Gamma},$$
$$B(\gamma,\Gamma) = \frac{1}{2}[1+2d\phi\gamma - A(\gamma,\Gamma)]. \quad (13)$$

The first outcome is that the shear mode—reminiscent of swarming phases—separates from other modes, and it is stable only when $B(\gamma,\Gamma)<0$, i.e., for large enough noise

$$\Gamma > \frac{2d}{d+2}\phi\gamma. \quad (14)$$

At zero dissipation, the shear mode is stable for any nonzero noise amplitude. Conversely, at zero noise amplitude, the shear mode is *always* unstable. Noticeably, in the absence of a k-dependent competing mechanism for stability (such as shear viscosity), the stability of the shear mode is lost synchronously at any k. Among the other three eigenvalues of $M(\mathbf{k})$, one is always real and two are complex conjugate (apart from a small region at low k where they are real). At a given γ, at least in the range $0<\gamma<1/(2\phi)$, the eigenvalue associated with shear is the first to change sign when Γ is reduced; i.e., shear instability is the leading one. Most importantly, in the region where the disordered state is stable, at large k and in the dilute limit, we recover a linear dispersion law (see [47]): This demonstrates the existence of underdamped wave propagation, which is an interesting consequence of our inertial microscopic dynamics, possibly related to observations in natural active systems [7].

Numerical results.—We have simulated the microscopic dynamics on the lattice at several values of ϕ (up to $\phi \approx 15\%$), γ, and Γ. In the explored region of parameters, we have observed many transient states and substantially

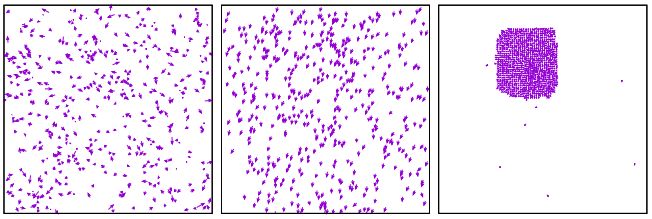

FIG. 2. Typical configurations in the three main stable states observed in the simulations. Left: A uniform disordered state. Middle: A uniform swarming state. Right: A nonuniform clustered state with a converging radial velocity field.

only three kinds of stable states (or superpositions of them): a uniform disordered state, a swarming state, and a clustered state, as shown in Fig. 2. All observed stable clustered configurations display a similar almost-radial (asterlike) velocity field, reminiscent of topological defects for polar particles or in active nematics [2]. Such a state is compatible with our hydrodynamic equations (see [47]). We focus upon two main global observables: (i) a swarming order parameter identified to be

$$r(t) = \left| \frac{1}{N} \sum_{j=1}^{N} e^{i\theta_j(t)} \right|, \tag{15}$$

where θ_j is the direction of velocity of the jth particle, so that $r(t) \approx 0$ in the fully disordered state and ≈ 1 in the case of all particles' velocities aligned along the same direction; and (ii) the number $N_l(t)$ of pairs of first neighbors at time t, a number that goes from $N_l \approx 2\phi N$ in the nonclustered case up to $N_l \approx 2N$ in the fully clustered case, so that $C(t) = N_l(t)/(2N) \in [\phi, 1]$ is a good estimate of the clustering degree in the system. Simulations start in the fully disordered case: Particle initial positions are chosen with a uniform probability in space and normal distribution for their initial velocity. Monitoring $r(t)$ and $C(t)$ up to times $t_{\max}$ larger than the inverse of the minimum of the eigenvalues of $M(\mathbf{k})$ gives a reasonable idea of the fate of this initial condition and allows us to compare the system's phase diagram with the predictions of linear stability analysis. In Fig. 3, we show the swarming order parameter r averaged on long times after the system has settled in the stationary regime, for three values of density ϕ, together with the line predicted in Eq. (14). The comparison is fair at all values of ϕ. A study of the dependence of the order parameters with the system's size tells us that the transition gets sharper for increasing L [47]. The study of the C order parameter [47] shows that at large $\phi \sim 10\%$ clusters (coexisting with a dilute background) appear in the region where the disordered regime is linearly stable. This may signal the presence of a different globally stable fixed point [22,23,29,51] or the necessity of refining our assumptions.

Numerical simulations also confirm our predictions about current noises, defined in Eq. (9). In the case of a Gaussian local velocity distribution, the noise correlation for the hopping current reads

$$\langle \sigma_l(\mathbf{x}, t)\sigma_{l'}(\mathbf{x}', t')\rangle = \delta(\mathbf{x} - \mathbf{x}')\delta(t - t')\delta_{l,l'}\phi(1 - \phi) \times \sqrt{\frac{2}{\pi}T(t)}(\Delta x)^{d+1}. \tag{16}$$

In the simulation, we measure the microscopic current $j_{i,p,l} = 0, \pm 1$, representing the number of particles hopping —in the pth time step—from site i to its neighbors in the lth direction. In the homogeneous fully disordered state, Eq. (16) is equivalent, assuming ergodicity, to

$$\sum_{i,i'}^{1,V} \sum_{p,p'}^{1,t_{\max}/\Delta t} j_{i,p,l} j_{i',p',l'} \simeq L^3 \phi(1 - \phi)\sqrt{\frac{2}{\pi}T_0 t_{\max}}. \tag{17}$$

The verification of this relation is shown in Fig. 4: We see that for $\phi < 10\%$ the simulation tends to the theoretical value as $L \to \infty$. This trend is broken when $\phi > 10\%$, which is reasonable as, in that regime, the homogeneous disordered state is replaced by a nonhomogeneous one, as put in evidence by the simulations.

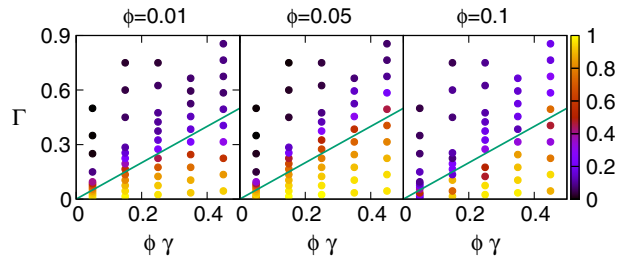

FIG. 3. Swarming phase parameter r (which goes from 0 in the disordered phase to 1 in the swarming phase; see the legend on the right) as a function of relative noise amplitude Γ and rescaled dissipation rate $\phi\gamma$ at three different average densities ϕ. The solid lines indicate the theoretical transition, Eq. (14).

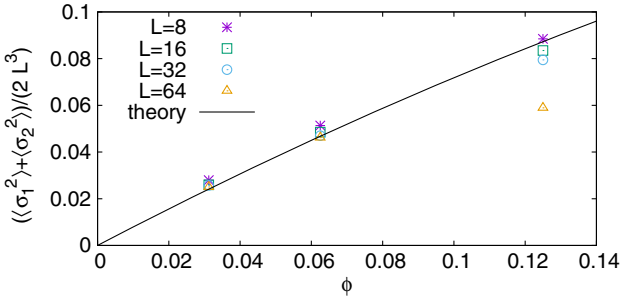

FIG. 4. Amplitude of fluctuations of the hopping current (symbols) and its theoretical prediction Eqs. (16) and (17) (solid line), as a function of ϕ for various sizes L. Here $\phi\gamma = 0.25$, $\Gamma = 4$, and the system is prepared at temperature $T_0 = 1$.

Conclusions.—In summary, we have discussed a model of inertial self-propelled particles with dissipative (aligning) interactions, inspired by GAP experiments [4] and simulations [31]. We have derived the locally averaged equations in the macroscopic ("hydrodynamic") limit, retaining also fluctuations of currents, Eq. (8). Those macroscopic equations are predictive both for the study of a phase diagram of stable and unstable phases and for the amplitude of current fluctuations which are non-negligible at finite sizes. The nonoverdamped dynamics adopted here is relevant also for other kinds of active particles, e.g., birds or insects, where inertia has proven to be crucial and a derivation of macroscopic equations from microscopic rules is lacking [7].

A key point in our results is the reduction of the necessary ingredients—in the macroscopic equations—for the existence of a disordered-swarming transition: Indeed, we have shown that viscous and heat transports are not required. A second key point is the relation between this transition and the shear instability of the homogeneous cooling state in granular gases [52]. Our results at zero noise ($\Gamma = 0$) suggest that they have the same nature, with two differences: (i) In our approximation, shear viscosity is zero; therefore, instability appears at any k, and (ii) in the dilute limit, self-propulsion makes the (unstable) homogeneous state steady, as in the so-called Gaussian thermostat or "steady state representation" [53].

Perspectives of future investigation include a study of the stability of other phases and the introduction of diffusive terms of transport (shear viscosity and heat conductivity). A numerical integration of our hydrodynamic equations can better elucidate the limits of validity of our equations, clarifying if the observed stability of inhomogeneous (e.g., clustered) states at a high density is compatible or not with our basic assumptions (e.g., molecular chaos or Gaussian local velocity distribution). Finally, contact with the large deviation theory [54–56] may foster future results on macroscopic fluctuations in systems of active particles [36].

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