Towards a quantitative kinetic theory of polar active matter

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Abstract. A recent kinetic approach for Vicsek-like models of active particles is reviewed. The theory is based on an exact Chapman-Kolmogorov equation in phase space. It can handle discrete time dynamics and "exotic" multi-particle interactions. A nonlocal mean-field theory for the one-particle distribution function is obtained by assuming molecular chaos. The Boltzmann approach of Bertin et al., Phys. Rev. E \textbf{74}, 022101 (2006) and J. Phys. A \textbf{42}, 445001 (2009), is critically assessed and compared to the current approach. In Boltzmann theory, a collision starts when two particles enter each others action spheres and is finished when their distance exceeds the interaction radius. The average duration of such a collision, $\tau_0$, is measured for the Vicsek model with continuous time-evolution. If the noise is chosen to be close to the flocking threshold, the average time between collisions is found to be roughly equal to $\tau_0$ at low densities. Thus, the continuous-time Vicsek-model near the flocking threshold cannot be accurately described by a Boltzmann equation, even at very small density because collisions take so long that typically other particles join in, rendering Boltzmann's binary collision assumption invalid. Hydrodynamic equations for the phase space approach are derived by means of a Chapman-Enskog expansion. The equations are compared to the Toner-Tu theory of polar active matter. New terms, absent in the Toner-Tu theory, are highlighted. Convergence problems of Chapman-Enskog and similar gradient expansions are discussed.

1 Introduction

The past decade has seen a surging interest in active matter. According to Ref. 3, active matter systems are defined by “their unifying characteristic that they are composed of self-driven units, active particles, each capable of converting stored or ambient free energy into systematic movement”. Describing these intrinsic nonequilibrium systems analytically poses a big challenge because there is no powerful general framework such as the free-energy formalism for equilibrium systems. Systems have to be treated on a case by case basis, and often uncontrolled approximations are employed. Even the simplest active matter models show a wealth of interesting phenomena and are not completely understood. For this reason I focus on one of the

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The simplest models of active matter – the Vicsek model (VM) – with the goal of custom-making a quantitative theory for it. The rationale behind this strategy is that by not modifying a computationally-efficient microscopic model, the theory can be directly compared to existing agent-based numerical simulations and new simulation data can be easily created. Contrary to theories without a direct link to experiment or simulation, if we find there is no good quantitative agreement, we immediately know that the approximations must be too crude or the calculations must be flawed. I believe that such a direct feedback will be very helpful in constructing accurate theories of active matter. For example, the kinetic approach presented in this article has been shown to quantitatively reproduce the shape and properties of strongly nonlinear waves in the Vicsek-model, in the limit of large mean free path.

In 1998 Toner and Tu proposed hydrodynamic equations for the density and momentum density of active particles and performed a dynamic renormalization. While they were able to explain how long-range orientational order can be achieved in a two-dimensional system of active particles, this theory, to my knowledge, has not been able to reproduce the details of the phase transition from a disordered state to a state of collective motion in the VM.

The terms in the hydrodynamic equations of Ref. were postulated based on rotational symmetry and relevance in the renormalization group sense. The coefficients of these terms are undetermined by construction. In reality, the coefficients are all related to just a few parameters of the underlying microscopic interactions, and therefore typically cannot be modified independently of each other. A direct derivation of the macroscopic equations from the microscopic model is beneficial because it strongly reduces the parameter space of allowed coefficients and can reveal relevant terms that might have been overlooked.

Using the Vicsek-model as a paradigm of active matter, a number of important fundamental questions can be studied, such as (i) is the Toner-Tu hydrodynamic theory sufficient to quantitatively describe active matter, is there relevant terms missing, does one need more than two equations or nonlocal equations instead?, (ii) Is it possible to rigorously derive the coefficients in the Toner-Tu theory from a microscopic model?, (iii) how to calculate the scaling behavior near the transition to collective motion, and (iv) how can one extend the theory for the Vicsek-model to more realistic models?

The first two questions are actually the active matter equivalent of Hilbert’s famous problem about how to establish a direct link between microscopic dynamics and macroscopic equations. To my knowledge, there has been quite some progress on the solution of this problem for regular Hamiltonian systems but, recently, serious doubts on its solution have been raised. By restricting ourselves to simple microscopic models like the VM which has particles of zero volume and employs external uncorrelated noise terms, it is interesting to explore whether Hilbert’s problem is solvable for active systems, at least in certain limits.

As a step in this direction, in this paper I will discuss a kinetic theory approach for self-driven particles. The theory does not start at the coarse-grained Boltzmann-level for the one particle distribution function, \( f(x, v, t) \). Instead it is based on an exact equation, the Chapman-Kolmogorov equation, in the full phase space of the model. A mean-field kinetic equation is then derived by using Boltzmann’s principle of molecular chaos. The kinetic equation has been evaluated analytically and numerically and extended to topological interactions. Hydrodynamic equations are derived from it by means of the Chapman-Enskog expansion and will be discussed in this paper. Surprisingly, these equations contain terms which are not included in the Toner-Tu theory, even if one makes the coefficients of this theory density-dependent.

The kinetic theory presented in this paper, which I will call phase space approach (PSA), has been thoroughly tested for a model with passive particles. The
regular Navier-Stokes equations have been derived \cite{27} and all transport coefficients were found to agree within a few percent with direct simulations and with alternative theoretical predictions \cite{28,29}. In addition to the PSA approach, there has been other attempts to derive the Toner-Tu equations from a microscopic model. One of the first attempts is due to Bertin et al. \cite{30,31}, one of the most recent approaches was presented by Großmann et al. \cite{32}. The common characteristic of these approaches is that they do not treat the original VM with discrete time step and genuine multiparticle collisions but other, often simpler, models related to it. The method presented in this paper deals with the Vicsek model as is. It keeps the original time-discrete dynamics and the multi-particle collisions. Moreover, it distinguishes between the so-called forward- and backward updating schemes and could be used to calculate the differences in the phase diagrams and density waves due to different updating methods, \cite{33,36}.

Kinetic theory approaches work best if there is a strong mixing of particles, e.g. when collision partners change rapidly. When cluster formation occurs, particles have a stronger tendency to recollide and to stay together for longer. Theoretical approaches for strong clustering of self-propelled particles which is in some sense the opposite limit to what is treated by kinetic theories, have been presented recently by Peruani et al. \cite{37,38}. The ultimate theory for active particles should contain both scenarios – clustering and strong mixing – as limit cases. Exploring the mixing side of this problem, the PSA approach presented in this paper can hopefully contribute to the construction of such a general framework.

2 Vicsek model

2.1 Definition

Consider the two-dimensional Vicsek-model (VM) \cite{4,5} with \( N \) point particles at number density \( \rho \), which move at constant speed \( v_0 \). The particles with positions \( x_i(t) \) and velocities \( v_i(t) \) undergo discrete-time dynamics with time step \( \tau \). The evolution consists of two steps: streaming and (microscopic) collision. In the streaming step all positions are updated according to

\[
x_i(t + \tau) = x_i(t) + \tau v_i(t) .
\]

(1)

Because the particle speeds stay the same at all times, the velocities are parametrized by the “flying” angles, \( \theta_i, v_i = v_0(\cos \theta_i, \sin \theta_i) \). In the collision step, the directions \( \theta_i \) are modified. Particles align with their neighbours within a fixed distance \( R \) plus some external noise: a circle of radius \( R \) is drawn around the focal particle \( i \), and the average direction \( \Phi_i \) of motion of the particles (including particle \( i \)) within the circle is determined according to

\[
\Phi_i = \arctan\left[\frac{\sum_{(j)} \sin(\theta_j)}{\sum_{(j)} \cos(\theta_j)}\right],
\]

(2)

Eq. (2) means that the vector sum of all particle velocities in every circle is computed and the direction of this summed vector is taken as average angle \( \Phi_i \). Once all average directions \( \Phi_i \) are known, the new directions follow as

\[
\theta_i(t + \tau) = \Phi_i + \xi_i
\]

(3)

where \( \xi_i \) is a random number with zero mean and probability distribution \( w_n(\xi) \). The distributions are assumed to be even, \( w_n(\xi) = w_n(-\xi) \) and normalized on the
interval $[-\pi, \pi]$ by $\int_{-\pi}^{\pi} \omega_n \, d\xi = 1$. In the original VM, $\omega_n(\xi)$ is a simple rectangular distribution, where $\xi$ is uniformly distributed in the interval $[-\eta/2, \eta/2]$. Here, I use a more general definition and assume that the shape of $\omega$ can depend on the number of particles encountered in a collision circle. For example, self-interaction or simple diffusion where particle $i$ finds itself alone in a circle can be described by a different probability distribution $\omega_1$ than binary collisions with distribution $\omega_2$.

The so-called standard Vicsek-model uses a forward-updating rule, as discussed in Ref. [33]. The already updated positions $x_i(t + \tau)$ are used to determine the average directions $\Phi_i$. In the so-called original VM, an Euler-like backward-updating rule is implemented. Here, the old locations $x_i(t)$ are used to calculate the average directions $\Phi_i$.

### 2.2 Continuous versus discrete time evolution

In gases with Hamiltonian dynamics, two important length scales immediately come to mind, the effective range of interaction, $R$, and the average distance between molecules, $l_D = \frac{1}{\sqrt{\rho}}$ (all expressions in this paper are given for two dimensions). Both lengths enter the well-known expression for the average distance particles travel between subsequent binary collisions,

$$l_{\text{coll}} = \frac{1}{2\sqrt{2}\rho} = \frac{l_D^2}{2R^2},$$

(4)

with the 2D cross section $\sigma = 2R$. To solve the equations of motions numerically, a small time-step $\tau$ is introduced. This creates a new length scale, $\lambda = v\tau$ which is irrelevant if it is much smaller than all other physical length scales, $\lambda \ll \min(R, l_D, l_{\text{coll}})$. If this condition is met in the Vicsek-model, I will call this the continuous-time VM. However, if the new scale $\lambda$ becomes larger or of the order of one of the previous lengths, $\lambda$ becomes relevant and I label the model discrete-time VM. It is easy to check that the original numerical work by Vicsek [4] was done in the continuous-time regime [13]. Why do we care about about the other regime? One reason is that kinetic and hydrodynamic theories are traditionally based on the smallness of some parameter. For example, Boltzmann and later Bogolyubov [34] exploited the smallness of the ratio $(R/l_D)^3$ at small density; Landau and Vlasov [35] used the smallness of the interaction energy compared to the kinetic energy of molecules for their theories. In our case, the new length scale $\lambda$ allows the definition of a different expansion parameter, $\varepsilon = R/\lambda$. The mean-field kinetic theory presented in the next chapter exploits the smallness of $\varepsilon$, and, in fact, is actually the zeroth order contribution in a formal expansion in powers of $\varepsilon$. The advantage of introducing $\varepsilon$ is that it allows to control the Molecular Chaos approximation.

For the VM defined by Eqs. (1,3) the length $\lambda$ takes on the role of the mean free path (mfp) which is defined by the distance a particle travels between collision steps. This is because at every time increment $\tau$, particle directions will change, even if a particle has no collision partner and just undergoes self-interaction.

### 3 Kinetic theory

In the VM, a given particle $i$ is specified by three numbers, its location $x_i$, $y_i$, and the flying angle $\theta_i$. Hence, the microstate of a system of $N$ such particles is completely specified by $3N$ numbers and corresponds to a point in $3N$-dimensional phase space. The time-evolution of the Vicsek model in this phase space is completely Markovian
because information about microstates from earlier times is irrelevant for further evolution. This allows us to write down the Chapman-Kolmogorov equation for a Markov chain,

\[ P(B, t + \tau) = \int P(A, t) W_{AB} dA. \tag{5} \]

where \( P \) is the \( N \)-particle probability density \[11\]. Eq. (5) describes the transition from a microscopic state \( A \) to the state \( B \) during one time step with transition probability \( W_{AB} \). The microscopic state of the system at time \( t + \tau \) is given by the 3N-dimensional vector, \( B \equiv (\theta^{(N)}, X^{(N)}) \), where \( \theta^{(N)} \equiv (\theta_1, \theta_2, \ldots, \theta_N) \) contains the flying directions of all \( N \) particles, and \( X^{(N)} \equiv (x_1, x_2, \ldots, x_N) \) describes all particle positions. The initial microscopic state at time \( t \) is denoted as \( A \equiv (\tilde{\theta}^{(N)}, \tilde{X}^{(N)}) \). The integral over the initial state translates to \( \int dA \equiv \prod_{i=1}^{N} \int_{-\pi}^{\pi} d\theta_i \int d\tilde{x}_i \) and ensures that all possibilities to create the state \( B \) are included. Pre-collisional angles and positions are given by \( \theta_i \) and \( \tilde{x}_i \), respectively. The transition probability \( W_{AB} \) encodes the microscopic collision rules,

\[ W_{AB} = \prod_{i=1}^{N} \delta(\tilde{x}_i - x_i + \tau v_i) \int_{-\pi}^{\pi} w_n(\xi_i) \, \delta(\theta_i - \xi_i - \Phi_i) \, d\xi_i, \tag{6} \]

and consists of two parts: the first \( \delta \)-function describes the streaming step which changes particle positions. The second part contains the periodically continued delta function, \( \delta(x) = \sum_{m=-\infty}^{\infty} \delta(x + 2\pi m) \), which accounts for the modification of angles in the collision step. The particle velocities \( V^{(N)} \equiv (v_1, v_2, \ldots, v_N) \), are given in terms of angle variables \( \theta_i \),

\[ v_i = v_0 \, e_i(\theta) = v_0 (\cos \theta_i, \sin \theta_i). \tag{7} \]

with unit velocity vectors \( e_i \). For the standard VM, a flat noise distribution with noise strength \( \eta \) is used that does not depend on the actual particle number \( n \) in the interaction circle,

\[ w_n(\xi) = \begin{cases} \frac{1}{\eta} & \text{for } -\frac{\eta}{2} \leq \xi \leq \frac{\eta}{2} \\ 0 & \text{elsewhere}. \end{cases} \tag{8} \]

Note that Eq. (6) corresponds to the forward-update rule (standard VM) \[33\] as used in the agent-based simulations of Ref. \[41\]. Results for backward-updating will be given elsewhere.

Equation (5) can be interpreted as the discrete time analogue of the Liouville equation of statistical mechanics. It is exact but intractable without simplification. The easiest way to proceed is to make Boltzmann’s molecular chaos approximation by assuming that the particles are uncorrelated just prior to a every microscopic interaction, which amounts to a factorization of the \( N \)-particle probability into a product of one-particle probabilities, \( P(\theta^{(N)}, X^{(N)}) = \prod_{i=1}^{N} P_i(\theta_i, x_i) \) on the right hand side of Eq. (5). This approximation is useful at sufficiently large noise strength and when the mean free path (mfp) is large compared to the radius of interaction \( R \). As discussed in Chapter \[2,3\] the mfp is given by the distance a particle travels between collision steps, \( \lambda = \tau v_0 \). This expression differs from the usual density-dependent formula in regular gases, Eq. (4), because of the special discrete time dynamics of the VM and the fact that particles in the VM do not interact during streaming. A large mfp and sufficiently large noise ensure that particles are well mixed and that the probability of subsequent re-collisions of the same particles is small, which suppresses memory and correlation effects. These correlations only vanish completely in extreme limits, for example, when the noise \( \eta \), defined in Eq. (5), is exactly equal to \( 2\pi \) and
particles just diffuse but do not interact at all, or when the mean free path and the system size are infinite while \( \eta \) is nonzero. However, even under more realistic conditions, the molecular chaos assumption can lead to very accurate results, see for example, Refs. 29, 25, 30. Because molecular chaos neglects pre-collisional correlations and leads to an effective one-particle picture, the final outcome will be a mean-field theory. So far, to my knowledge, all treatments of active particles by kinetic theory, for example \([49,31,51,57,58,59]\), or Fokker-Planck equations \([50,32]\) make such a mean-field assumption, either explicitly or implicitly.

To derive this mean-field theory, we multiply eq. (5) by the phase space density \( \sum_{i} \delta(x - x_i) \delta(x - x_i) \). A subsequent integration over all particle positions \( x_i \) and angles \( \theta_i \) leads, in the large \( N \)-limit, to a kinetic equation for the one-particle distribution function, \( f(\theta, x, t) = NP_1(\theta, x, t) \)

\[
f(\theta, x + \tau v, t + \tau) = \int_{0}^{2\pi} f(\phi, x, t) G(x, \theta, \phi, t) \, d\phi
\]

with the nonlocal (in velocity space) mean-field potential \( G \) that acts like an external potential. Particles are assumed to move in an uncorrelated fashion and the effect of their mutual interactions being such that any one particle experiences the average potential field \( G \) that depends nonlinearly and nonlocally on \( f \) itself. This picture is thus similar to the Vlasov kinetic equation, the Hartree and the Debye-Hückel theory. The potential \( G \) is given by

\[
G(x, \theta, \tilde{\theta}_1, t) = \left\langle \left\langle \sum_{n=1}^{N} \int_{-\pi}^{\pi} w_n(\xi) \, d\xi \, \frac{e^{-M_R}}{(n-1)!} \right. \right.
\]
\[
\times \delta[\theta - \xi - \Phi_1(\tilde{\theta}_1, \ldots, \tilde{\theta}_n)] \prod_{i=2}^{n} f(\tilde{\theta}_i, x_i, t) \right\rangle \right\rangle_x
\]

where \( M_R(x, t) = \int_{R} \rho(y, t) \, dy \) is the average number of particles in a circle of radius \( R \) centered around \( x \) and can be position dependent. The subscript “R” at the integral denotes integration over this circle. The local particle density \( \rho \) is given as a moment of the distribution function, \( \rho(x, t) = \int_{0}^{2\pi} f(\theta, x, t) \, d\theta \); \( \langle \ldots \rangle_x = \int_{R} \ldots \, dx_2 \, dx_3 \ldots \, dx_n \) denotes the integration over all positions, \( n - 1 \) particles can assume within the interaction circle; \( \langle \ldots \rangle_{\tilde{\theta}} = \int_{-\pi}^{\pi} \ldots \, d\tilde{\theta}_2 \, d\tilde{\theta}_3 \ldots \, d\tilde{\theta}_n \) is the average over the pre-collisional angles of all particles in the interaction circle except particle 1. Here, particle 1 is assumed to be the focal particle. It is fixed at position \( x \) and particles 2, 3, \ldots, \( n \) are supposed to be its neighbors. Of course, this is not the only possibility but since the particles are identical, all particle permutations give the same contribution and are already taken into account by the combinatorial factor \( 1/(n-1)! \). It is interesting to note that this combinatorial factor together with the exponential \( e^{-M_R} \) describes a Poisson distribution of the particle locations. The Poissonian character of these fluctuations was not put in by hand – it rather is a consequence of the Molecular Chaos approximation and the definition of \( f(\theta, x) \) as the ensemble average of the microscopic phase space density. That means, the density fluctuations of an ideal gas are already implicitly contained in Eq. (6). Therefore, one has to be very careful with inserting additional noise terms to construct fluctuating kinetic equations, something which is quite popular for other systems, \([43,44,45]\). Note, that the exponential prefactor \( \exp(-M) \) is only obtained in the thermodynamic limit, \( N \rightarrow \infty \). In realistic active particle systems, \( N \) is not that large. However, even for finite \( N \) a version of Eq. (10) can be derived where the Poisson distribution is replaced by a binomial factor \( [10] \) in order to better describe agent-based simulations with small \( N \).
4 Phase diagram and hydrodynamic equations

4.1 Calculating the phase diagram

For stationary and spatially homogeneous solutions, the mean-field kinetic equation turns into a nonlinear Fredholm integral equation of the second kind,

\[ f(\theta) = \sum_{n=1}^{N} \int_{-\pi}^{\pi} w_n(\xi) \frac{A^{n-1} e^{-M}}{(n-1)!} \times \left( \prod_{i=1}^{n} \int_{-\pi}^{\pi} f(\tilde{\theta}_i) d\tilde{\theta}_i \right) \delta[\theta - \xi - \Phi_1(\tilde{\theta}_1, \ldots, \tilde{\theta}_n)] \]  

(11)

where \( A = \pi R^2 \) is the area of the collision circle and the average particle number in this circle, \( M = A \rho_0 \) is proportional to the particle number density \( \rho_0 \). It is easy to see that the constant distribution \( f_0 = \rho_0 / (2\pi) \) that describes a disordered state is a solution for all possible noise distributions. Ordered solutions \( f(\theta) \neq \text{constant} \) with nonvanishing polar order can be determined numerically and bifurcate continuously from the disordered solution. For the noise distribution defined in Eq. (8) one finds that the critical noise below which the ordered state exists follows from the condition \( \Lambda = 1 \), where

\[ \Lambda = 4 \eta \sin \left( \frac{\eta}{2} \right) e^{-M} \sum_{n=1}^{N} \frac{n^2 M^{n-1}}{n!} I(n) \]

\[ I(n) = \frac{1}{(2\pi)^n} \int_{0}^{2\pi} d\theta_1 \ldots \int_{0}^{2\pi} d\theta_n \cos \theta_1 \cos \Phi_1(\theta_1, \ldots, \theta_n) \]

(12)

Here, \( \Phi_1 \) is the average angle defined in Eq. (2). The integral \( I(n) \) and similar integrals were evaluated analytically for \( n \leq 3 \) and numerically for \( n \leq 10 \). In addition, asymptotic expressions for \( n \to \infty \) are known [23,24]. For values \( n > 10 \) an interpolation between the known integrals at low \( n \) and the asymptotic results was used.

Analyzing the condition \( \Lambda = 1 \) in the low density limit \( M \ll 1 \), using \( I(1) = 1/2 \) and \( I(2) = 1/\pi \), leads to an explicit expression for \( \eta_C \),

\[ \eta_C = \sqrt{48M \left( \frac{2}{\pi} - \frac{1}{2} \right) + O(M)}, \]

(13)

In the opposite limit of infinite density, \( \eta_C \) goes to \( 2\pi \). For the behavior at intermediate densities, see Ref. [23]. Close to the bifurcation, that is at \( \eta_c - \eta \ll 1 \), an analytical solution of Eq. (11) in terms of angular Fourier modes can be obtained and, as expected, one finds that the order parameter of the state of collective motion follows the mean-field scaling \( \Omega \sim (\eta_c - \eta)^{1/2} \). It turns out [30,31,24], that the homogeneous ordered state just near \( \eta_C \) is linearly unstable to long wavelength fluctuations, at least for large mean free path, \( v_0 \tau / R \gg 1 \). These perturbations turn into steep soliton-like waves [11]. Direct simulations of Eq. (9) demonstrate that these waves show hysteresis and turn the flocking transition into a discontinuous phase transition [6]. Recently, Thueroff et al. [7] observed similar wave behavior by directly simulating the Boltzmann equation proposed by Bertin et al. [30,31]. Since the PSA approach is only valid at large mfp and a Boltzmann approach is in practice never valid near the transition as shown in Sect. 5 it is not clear yet whether the same soliton-scenario applies also at the highly correlated regime of small mfp, \( v_0 \tau / R \ll 1 \). In this low velocity regime, see for example Fig. 1 of Ref. [5], isolated flocks were observed rather than the straight, boundary-spanning density waves of the high velocity regime, shown in Figs. 4 and 5 of Ref. [5].
4.2 Deriving hydrodynamic equations

The Chapman-Enskog expansion (CE) from 1916 is one of the standard techniques to extract macroscopic behavior from kinetic equations [16]. It can be seen as an elaborate expansion in small gradients of hydrodynamic fields. Its key assumption is that after a few collisions that involve rapid changes of the distribution function $f$, the system reaches a “hydrodynamic state” where local equilibrium is achieved and where $f$ can be expressed as a functional of the slow hydrodynamic variables [9]. This means, $f$ is expected to depend on space and time only indirectly through those hydrodynamic fields. The hydrodynamic variables are just the lowest velocity moments of $f$, for example, density $\rho$ and momentum density $w$ are given by

$$\rho(x, t) = \int_{-\pi}^{\pi} f(x, \theta, t) \, d\theta$$
$$w(x, t) = \rho u = \int_{-\pi}^{\pi} v(\theta) \, f(x, \theta, t) \, d\theta$$  (14)

The Chapman-Enskog assumption can be rephrased as the claim that knowledge of just the first few moments of $f$ is sufficient to describe the system on large length and time scales. Since $f$ is uniquely defined by all its moments, this assumption would be justified if either all higher moments are negligibly small or that they are “enslaved” to the lower moments, meaning that they could be expressed as functionals of the lower moments.

Applying CE to the Vicsek model is tricky because the only true and nontrivial hydrodynamic field is the density $\rho(x, t)$. This is because momentum is typically not conserved by the collision rule, Eq. (3), and energy is trivially conserved since the particle speed is constant. However, at the order-disorder threshold the interplay between angular noise and alignment leads to momentum conservation in an averaged sense. Mathematically, this can be seen in the evolution equation for momentum density, Eq. (18), a Navier-Stokes-like equation, which has a gain/loss term that vanishes at the threshold. Therefore, in the VM, I will treat momentum density as a pseudo-hydrodynamic mode. Since we are mostly interested in the behavior near the threshold, we should have a separate equation for this variable; that is exactly what Toner and Tu [10] postulated – one equation for the density and one for the momentum density.

The Chapman-Enskog expansion takes the local stationary state as a reference state and expands around it in powers of the hydrodynamic gradients. To systematically account for these gradients a dimensionless ordering parameter $\epsilon$ is introduced, which is set to unity at the end of the calculation. The physical meaning of this parameter is that it assumed to be proportional to the Knudsen number, e.g. the ratio of the mean free path to the length scale over which hydrodynamic fields change considerably. The CE procedure starts with a Taylor expansion of the l.h.s of Eq. (9) around $(\theta, x, t)$. The spatial gradients that occur are scaled as $\partial_{\theta} \rightarrow \epsilon \partial_{\theta}$, and multiple time scales $t_i$ are introduced in the temporal gradients. For the VM, the following scaling that respects the physics of the microscopic collisions was chosen,

$$\partial_t = \partial_{t_0} + \epsilon \partial_{t_1} + \epsilon^2 \partial_{t_2} \ldots$$  (15)

This sequence differs from the usual set of equations for models with momentum conservation [52,53] because of the fast time scale $t_0$ which is not multiplied by a power of $\epsilon$ and contributes time derivatives of all orders. However, expansions that contain all powers of $\partial_{t_0}$ can be conveniently summed up by the time evolution operator

$$T = \exp (\tau \partial_{t_0})$$  (16)
which shifts the time-argument of a function by the discrete time step $\tau$, $T \circ f(t) = f(t + \tau) + O(\epsilon)$.

The next step in the CE is to expand the distribution function $f$ and the collision integral $C$, e.g. the right hand side of Eq. (9), in powers of $\epsilon$,

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \ldots$$

$$C = C_0 + \epsilon C_1 + \epsilon^2 C_2 + \ldots \tag{17}$$

Inserting this into Eqs. (9) [10], and collecting terms of the same order in $\epsilon$, yields a hierarchy of evolution equations for the $f_i$. Due to the absence of momentum conservation and Galilean invariance this set of equations is very different from the usual one. It is not a priori evident whether the scaling ansatz for the time derivatives is correct. However, it turns out that this choice avoids any inconsistencies if additionally the expansion of the distribution function $f$ is identified as an angular Fourier series with $f_n(x, \theta, t) = \rho(x, t)/2\pi$ and, for $n > 0$, $f_n(x, \theta, t) = |a_n(x, t) \cos (n\theta) + b_n(x, t) \sin (n\theta)|/\pi n^0$.

The goal is to find a hydrodynamic description of the first two moments of $f$, namely the particle density and the macroscopic momentum density. Inserting the Fourier representation of $f$ into the definition of these moments, Eqs. (12), shows that the coefficients for the first order contribution $f_1$ are given by the momentum density, $a_1 = w_x$ and $b_1 = w_y$. Multiplying the hierarchy of evolution equations by powers of the microscopic velocity vector $v = (v_x, v_y) = v_0(\cos \theta, \sin \theta)$ and integrating over $\theta$ gives a set of equations for the time development of the density and the moment $a_i$ and $b_i$. These equations still depend on higher order moments. To significantly simplify the closure of this hierarchy of moment equations, the analysis is restricted to the vicinity of the threshold where $\Lambda$, defined in eq. (12), is close to one. Specifically, I assume the scaling, $1 - \Lambda = O(\epsilon^2)$. This allows me to express the time evolution of the moments of the higher order distribution functions $f_2$ and $f_3$ in terms of gradients of the hydrodynamic fields. This means these functions depend only implicitly through their functional dependence on $f_0$ and $f_1$. Thus, at order $O(\epsilon^3)$ and near the flocking threshold, I found that the moments $f_2$ and $f_3$ are enslaved to $f_0$ and $f_1$, whereas even higher functions such as $f_4$ can be neglected at this order. This results in a consistent closure of the hydrodynamic equations and leads to two hydrodynamic equations with a larger number of terms than postulated [10] or derived by other authors [21]. The question that come to mind is, what would happen if the system is further away from the threshold where $1 - \Lambda$ is not small? It is possible that two hydrodynamic equations will not be sufficient anymore. Equations for higher order (non-hydrodynamic) moments might be needed or a description in more convenient variables might be more useful.

All equations are rescaled by expressing time in units of $\tau$ and distances in units of the mfp, $\tau v_0$, which also makes $\rho$ and $w$ dimensionless. After tedious calculations one obtains the continuity equation $\partial_t \rho + \partial_i w, w = 0$, and an equation for the momentum density,

$$\partial_t w + \nabla \cdot \mathbf{H} = -b \nabla \rho + (A - 1) w + Q_1 \cdot w + Q_2 \cdot \nabla \rho \tag{18}$$

with $b = (3 - \Lambda)/4$. The momentum flux tensor $\mathbf{H}$ and the tensors $Q_1$, $Q_2$,

$$\mathbf{H} = \sum_{i=1}^{5} h_i \Omega_i \quad Q_1 = \sum_{i=1}^{5} q_i \Omega_i \quad Q_2 = \sum_{i=1}^{5} k_i \Omega_i \tag{19}$$
are given in terms of five symmetric traceless tensors $\Omega_i$,

\begin{align*}
\Omega_{1,\alpha\beta} &= \partial_\alpha w_\beta + \partial_\beta w_\alpha - \delta_{\alpha\beta} \partial_\gamma w_\gamma \\
\Omega_{2,\alpha\beta} &= 2\partial_\alpha \partial_\beta \rho - \delta_{\alpha\beta} \partial_\gamma^2 \rho \\
\Omega_{3,\alpha\beta} &= 2w_\alpha \partial_\beta \rho - \delta_{\alpha\beta} w^2 \\
\Omega_{4,\alpha\beta} &= w_\alpha \partial_\beta \rho + w_\beta \partial_\alpha \rho - \delta_{\alpha\beta} w_\gamma \partial_\gamma \rho \\
\Omega_{5,\alpha\beta} &= 2(\partial_\alpha \rho)(\partial_\beta \rho) - \delta_{\alpha\beta} (\partial_\gamma)^2 ,
\end{align*}

which are all of order $O(\epsilon^2)$. The tensor $\Omega_1$ is the viscous stress tensor of a two-dimensional fluid. The transport coefficients $h_i$, $k_i$ and $q_i$ were explicitly obtained in the limit of large mfp, $\tau v_0 \gg R$, mainly for simplicity but also because the PSA approach is not expected to be reliable at low mfp. The detailed expressions are given in Ref. [23]. They are valid at arbitrary density and depend on $v_0 \tau/R$, $\eta$ and $M$. The concerns expressed in Ref. [56] on the complexity of these expressions are only partially justified because the occurring sums and angular integrals can be quite accurately evaluated using a Mathematica® script and the interpolation technique mentioned in the discussion of Eq. (12).

Expressing the Navier-Stokes-like equation, Eq. (18), in terms of tensors and vectors makes it easier to see that all terms are rotationally invariant. This is because once one has verified that all the $\Omega_i$ transform like tensors, the products of these quantities with vector like $\nabla \rho$ or $w$ also transform like vectors and thus are rotationally invariant. One also sees now explicitly that the loss-term that is linear in $w$ has the prefactor $\Lambda - 1$ and therefore vanishes at the threshold. That means at the threshold, macroscopic momentum is approximately conserved.

Comparing Eq. (18) with the equations postulated in Ref. [10] and amended by Toner [14] there seems to be additional terms that are not included in the Toner-Tu theory. For example, analyzing the $x$-component of Eq. (18) one finds a contribution $w_x(\partial_x^2 \rho - \partial_y^2 \rho) + 2w_y \partial_x \partial_y \rho$ in tensor $Q_1$ which originates from the tensor $\Omega_2$. This term is relevant for the linear stability of the ordered state. No term in Eq. (1) of Ref. [14] is able to reproduce this expression, even if one assumes that the coefficients in that equation depend on density. Because these novel terms have not been systematically analyzed yet, it is not clear whether they change anything in the main conclusions of the Toner-Tu theory.

A recent derivation of hydrodynamic equations by Großmann et al. [32] for active Brownian particles leads to similar terms. By assigning a power of $\epsilon$ to every gradient and to every occurrence of the momentum density, $w_\sim \epsilon$, one can write down all possible products of $\rho$, $w$ and its gradients that are at most of order $O(\epsilon^3)$. It appears that Eq. (18) contains all possible, rotationally invariant terms of this type (assuming that the coefficients of the terms are density-dependent). Therefore, I believe that models with the same symmetries as the VM such as the metric-free model of Refs. [47,48,24] will lead to hydrodynamic equation with the same terms just with different coefficients.

### 4.3 Validity of the hydrodynamic equations

So far, a direct term-by-term verification of the hydrodynamic equations, Eq. (18), is lacking. However, a number of indirect consistency tests were successfully completed. One of them was the numerical solution of the kinetic equation, Eq. (9), in large systems [6]. This test, at least, probes the kinetic foundation from which the hydrodynamic description was derived but, of course, cannot prove the validity of the hydrodynamic equations. The shape and speed of the solitons observed in these runs...
agreed within a few percent with agent-based simulations of the VM, at $\tau v_0/R \gg 1$. To check the hydrodynamic equations, we have also performed a linear stability analysis of both the hydrodynamic equation, Eq. (18), in Ref. [23], and the kinetic equation, see Ref. [24]. Since the hydrodynamic equations are only supposed to be valid close to the threshold and the analysis of the kinetic equation was done in the binary collision approximation, we chose $\eta_C - \eta \ll 1$ and $M \ll 1$ where both approaches should be valid. In this limit, the dispersion relations for a small longitudinal perturbation of the ordered state, agreed quantitatively with each other [46]. Finally, the numerical solution of the hydrodynamic equation by a finite-difference scheme showed a linear instability of the ordered phase once the system size exceeds a certain length. A length of similar size above which spatial inhomogeneities occurred was found in simulations of the kinetic equation.

A well-known issue is the possible divergence of higher order Chapman-Enskog and similar gradient expansions [20]. The most famous example is that in regular gases an expansion to second order gives the stable Navier-Stokes equation but going to the next order leads to the Burnett equation that turns out to be unstable [19]. For the VM, a similar problem seems to occur. The numerical solution of Eq. (18) correctly shows a linear long wavelength instability once the system size exceed a critical length at slightly smaller noise than the threshold noise [23]. However, in contrast to agent-based simulations and direct simulations of the kinetic equation, these perturbations never settle but keep growing, e.g. are nonlinearly unstable. This means, the hydrodynamic equations, Eqs. (18)-(20), whose coefficients were all derived from the microscopic rules, were unable to reproduce stable, inhomogeneous solutions. Some researchers handle this problem by inserting one or more higher order nonlinearities phenomenologically to control this behavior [51], others perform a tedious summation to all orders [20,22] or use non-perturbative techniques similar to the Schwinger-Dyson equation [21]. However, the latter techniques, while very promising, might only be feasible for simpler systems than the VM. Such summations of higher order gradients and nonlinearities can well lead to nonlocal hydrodynamics [22]. A pragmatic solution was presented in Ref. [6] where, instead of dealing with complicated gradient expansions, the non-local kinetic equation (9) was solved on the computer as is. This amounts to an implicit summation of gradient terms to all orders.

Another idea is to go to the next higher order, $O(\epsilon^4)$, in the CE, in the hope that the new nonlinearities behave “nicer” and regularize the instability but this would be very tedious, the number of terms would become huge, and in the end, the extended equation might even be more unstable. In Ref. [59] it was hypothesized that the nonlinear instability of Eq. (18) might be due to an incorrect closure of the moment hierarchy. While this has not been completely ruled out yet for most kinetic theories of active matter, I think that similar to the Burnett-equation one should rather expect a higher order gradient expansion of a kinetic equation to diverge at some point. I tend to believe that if such an expansion would be fully stable at all wavelengths and perturbation sizes, it must be a very lucky case.

5 Binary escape time and the failure of Boltzmann approaches

The Boltzmann equation is the most common kinetic equation for regular gases, and became also quite popular in active matter research [30,41,47,58]. The success of the Boltzmann approach for regular matter is based on its accuracy at low densities. The derivation of the Boltzmann equation involves a number of assumptions, the most important ones being the Molecular Chaos assumption and the binary collision assumption, e.g. the neglect of collisions involving more than two particles. It is
Fig. 1. The binary escape time $\tau_0$ measured in Monte-Carlo simulations as a function of the threshold density $M_C = M(\eta_C)$ for different time steps $\Delta t$, averaged over $10^6$ runs. The noise $\eta$ is set equal to the mean-field critical noise given in Eq. (13). The solid black line is the time between collisions for a regular gas, $\tau_{coll} = l_{coll}/v_0$, see Eq. (4). Parameters: $R = 1$, $v_0 = 1$.

an important question whether these crucial assumptions also hold in active matter systems. Recently, the validity of the Molecular Chaos assumption (MC) for a realistic active colloidal system has been critically assessed in Ref. [8]. Indicators of molecular chaos were also investigated for the topological Vicsek-model [24]. Here, I would like to focus on the binary collision assumption.

Lowering the density reduces the probability of non-binary collisions in regular gases with short-ranged repulsion. This is because at low density the range of interaction $R$ is much smaller than the average distance between particles $l_D \sim 1/\sqrt{\rho}$. According to Eq. (4) this leads to $R \ll l_D \ll \tau_{coll}$ where $\tau_{coll}$ is the average distance a molecule travels until it collides with another one. This disparity in length scales translates to the relevant time scales: The typical time a particle is engaged in an interaction, $\tau_0 \approx R/v$, where $v$ is the thermal speed, is much smaller than the time between collisions, $\tau_{coll}$. This makes it very unlikely that a particle meets two or more other ones in its action radius within a short time interval of order $\tau_0$. This scenario changes for attractive interactions, particles could capture each other and orbit around one another. The alignment interactions of the VM, Eq. (3), can also have such a capturing effect at low noise because particles move almost in parallel after a collision and have a tendency to stay together, effectively prolonging the collision time $\tau_0$. If $\tau_0$ is large, the likelihood of a third particle to join an ongoing binary encounter increases and three-particle interactions might become non-negligible.

As a first step to check the validity of the binary collision assumption, I measure the collision time $\tau_0$ for the binary alignment interactions of the VM by Monte Carlo simulations. These simulations involve only two particles which are initially placed at distance $r = R - 2\lambda \xi$ where $\xi$ is a random number equally distributed in the interval $(0, 1]$ and $\lambda = v_0 \tau$. This range of $r$ covers all possible positions two particles with $\lambda/R < 1$ can have after they have entered into each other’s action circle for the first time. Then, the initial flying directions, $\theta_1$ and $\theta_2$ are chosen randomly, and define the velocities of the particles. To check the consistency of the initial conditions,
the particles are traced back to their previous positions $x_{i,\text{old}} = x_i - \tau v_i$. If $d_{12} = |x_{2,\text{old}} - x_{1,\text{old}}|$ is smaller than the interaction radius $R$, the particles were not at the very beginning of a binary encounter. In this case, the initial condition is discarded and a new set of positions and velocities is chosen until the condition $d_{12} \geq R$ is met. Then, the two particles evolve according to the collision and streaming rules of the VM, see Eqs. (1,3), until their distance $d_{12}$ exceeds again the collision radius. The time until this happens is the duration of a collision and will also be called binary escape time. These measurement are repeated for different noises $\eta$ and different time steps, and are ensemble-averaged over many random initial conditions.

Since kinetic theories for active particles are designed to describe the order-disorder transition and the state of collective motion, the noise $\eta$ has to be close to the threshold noise $\eta_C$ for any interesting application. Therefore, in order to estimate $\tau_0$ near the flocking threshold, I map the noise used in the simulations to the rescaled density $M = \pi R^2 \rho$ using the mean-field expression, Eq. (13), for the threshold noise $\eta_C$. The average binary escape time $\tau_0$ is plotted as a function of $M = M(\eta_C)$ in Fig. 1. As seen in this figure, $\tau_0$ converges for time steps $\Delta t \lesssim 0.01 R/v_0$. The main result is that, for small $M$, the escape time scales as $\tau_0 \sim M^{-\nu}$ with an exponent $\nu = 1$, assuming the particular mapping between density and noise, $\eta = \eta_C \sim \sqrt{M}$. For comparison, the time between collisions in a regular gas, $\tau_{\text{coll}} = l_{\text{coll}}/v_0 \sim M^{-1}$, is also plotted. While isolated particles in the VM do not go on straight lines like in regular gases but undergo a correlated random-walk due to self-interactions, I still expect a similar scaling of $\tau_{\text{coll}}$ with $M$. For small densities $M \leq 0.1$, both times seem to be very close to each other and actually seem to follow nearly the same scaling with density. One has to keep in mind that the observed $\tau_0$ likely overestimates the duration of a binary collision in the VM because the Monte Carlo procedure assumes that particle velocities are completely uncorrelated before they enter each others action circle and only get strongly correlated while engaged in the collision. This leaves out situations where particles that have just left each other re collide again while their directions did not have enough time to become very different from each other. Nevertheless, my numerical results suggest that the ratio of $\tau_0$ and $\tau_{\text{coll}}$ remains of order one or at least goes down very slowly with decreasing density. This would mean, that contrary to regular gases the binary collision assumption does not become valid at small densities.

To check this conjecture in a more direct way, I perform agent-based simulations of the VM with $N = 6000$ particles near the flocking threshold in the disordered phase and measure the fraction of particles $p_n$ that are engaged in a $n$-particle interaction. These fractions are time-averaged over very long runs. For example, $p_2$ tells me the probability that a particle is part of a two-particle cluster. Similarly, $p_3$ is the probability that a particle is interacting with exactly two others in the collision step. These probabilities are normalized as $\sum_{n=1}^{N} p_n = 1$. For an ideal gas and $N \rightarrow \infty$, the probabilities are Poissonian and are given by,

$$ p_n^{\text{id}} = e^{-M} \frac{M^{n-1}}{(n-1)!} \quad (21) $$

In Fig. 2 the ratio $p_3/p_2$ as a measure of the importance of three-particle collisions is plotted as a function of density for fixed $\Gamma = \pi v_0 / R = 0.03$. This value of $\Gamma$ is the one suggested in Vicsek’s original paper [4]. In addition, the quantity

$$ S = \sum_{n=3}^{N} p_n = 1 - (p_1 + p_2) \quad (22) $$

is shown as a measure of all interactions neglected by the binary collision assumption. It gives the fraction of all particles that are interacting with at least two others at
Fig. 2. Agent-based simulations of the probability ratios $p_3/p_2$, $p_4/p_3$, and the probability for non-binary interactions, $S = 1 - (p_1 + p_2)$, versus density $M$ at fixed time step $\tau = 0.03$. The noise $\eta$ is set equal to the mean-field prediction $\eta_C(M)$ from Eq. (13). Parameters: $R = v_0 = 1$, $N = 6000$, up to $7.3 \times 10^6$ time steps.

Fig. 3. Agent-based simulations of the probability ratios $p_3/p_2$, $p_4/p_3$, and the probability for non-binary interactions, $S = 1 - (p_1 + p_2)$, versus $\varepsilon = R/\tau v_0$ at fixed density $M = 0.1$ and $\eta = 1.1\eta_C$. Other parameters are the same as in Fig. 2. The values at $\varepsilon = 0$ are not from simulations but from Eqs. (21, 22).
once. The ideal gas predictions are \( p_3^d/p_2^d = M/2 \) and \( S^d = M^2 + O(M^3) \). Fig. 2 shows that the observed quantities are much larger than these predictions even at the lowest density of \( M = 0.01 \). This lowest density corresponds to \( \rho = 0.0032 \) in the terminology of Refs. [4,5,41], and thus is two to three orders of magnitude smaller than typical densities used by these authors. However, even at this low density one sees that \( p_3/p_2 \) and \( S \) are of order one and, therefore, more than one order of magnitude larger than the ideal gas predictions. At larger density these quantities become even larger. While the asymptotic behavior for \( M \to 0 \) is not completely clear, one can still conclude that for \( M \geq 0.01 \) at least 42\% of all particles are engaged in a non-binary interaction and that the fraction of particles involved in three-particle collisions is only a factor \( \geq 0.67 \) smaller than the ones undergoing binary interactions. This means that for all practical purposes (e.g. realistic densities above \( M = 0.01 \)) the binary collision assumption is not valid in the continuous time VM near the flocking threshold in both the ordered and disordered phases [12]. As a consequence any Boltzmann approach applied to the VM close to the threshold cannot be expected to be quantitatively correct because it fails to correctly describe what about half of the particles do. My results suggest that the reason for this failure is the alignment interaction that leads to a huge increase of the collision time \( \tau_0 \) at small densities.

In the discrete-time VM, the divergence of the collision time for \( M \to 0 \), is strongly reduced by the small ratio \( \varepsilon = R/\lambda \); the alignment interactions cannot keep particles together for too long. Instead, particles just jump away from each other after only a few microscopic interactions. To verify this behavior, in Fig. 5 the quantities \( p_3/p_2 \) and \( S \) are shown for small \( \varepsilon \) in the disordered phase near the flocking threshold. For \( \varepsilon \leq 0.2 \) only a few percent of the particles are involved in non-binary interactions. The binary collision assumption becomes exact for \( \varepsilon \to 0 \) and \( M \to 0 \). Note, that the data points at \( \varepsilon = 0 \) were not obtained by extrapolation but by using the ideal gas predictions, Eqs. (21, 22). The fact, that these predictions fit perfectly into this plot with agent-based numerical data, is an additional consistency check of the simulation. This plot can also be used to judge the quality of the Molecular Chaos (MC) approximation. Agreement of \( S \) and \( p_3/p_2 \) with the ideal gas predictions, that is the data points at \( \varepsilon = 0 \) in Fig. 3 are taken as indicator of the validity of MC. For \( M = 0.1 \) one sees that \( p_3/p_2 \) has already doubled at \( \varepsilon = 0.2 \). Thus, the PSA approach which relies on MC but not on binary interactions, is expected to be accurate for \( \varepsilon \geq 5R \). This is consistent with earlier results on the metric-free VM [24].

To compare to the continuous-time VM, data for large \( \varepsilon \), more specifically for small time step \( \tau \), are shown in Fig. 4. Even if the product \( \tau_0 \) is further reduced from the value \( \lambda = 0.03 \) used in Ref. [4], \( p_3/p_2 \) and \( S \) keep rising slowly and thus invalidate the binary collision assumption even further. Computational limitations prevent me from investigating the limit \( \tau \to 0 \) in more detail. By monitoring the global polar order parameter, I made sure that all data in figures 2-4 are taken in the disordered phase.

Since all my results are for the VM which uses point-particles it would be interesting to see whether active matter models with more realistic interactions, for example models with additional short-range repulsion, show a similar failure of the Boltzmann approach near the threshold to collective motion.

6 Comparison to the Boltzmann model of Bertin et al.

6.1 Detailed mapping

Since the Boltzmann approach by Bertin, Droz and Gregoire (BDG) [30,31] looks similar to the kinetic equation (6), it is important to understand the differences. The
BDG approach is given by
\[
\left( \frac{\partial}{\partial t} + \mathbf{v}(\theta) \cdot \nabla \right) f(x, \theta, t) = I_{diff}[f] + I_{col}[f, f]
\] (23)
featuring the convective time derivative on the left hand side. The right hand side consists of the diffusion term
\[
I_{diff} = \lambda d \left\{ -f(x, \theta, t) + \int_{-\pi}^{\pi} d\tilde{\theta}_1 \int_{-\infty}^{\infty} d\xi w_1(\xi) \hat{\delta}[\theta - \xi - \tilde{\theta}_1] f(x, \tilde{\theta}_1, t) \right\}
\] (24)
and the binary collision term,
\[
I_{col} = 2Rv_0 \int_{-\infty}^{\infty} d\xi \int_{-\pi}^{\pi} d\tilde{\theta}_1 \int_{-\pi}^{\pi} d\tilde{\theta}_2 w_2(\xi) |\mathbf{e}(\tilde{\theta}_2) - \mathbf{e}(\tilde{\theta}_1)|
\times f(x, \tilde{\theta}_1, t) f(x, \tilde{\theta}_2, t) \left\{ \hat{\delta}[\theta - \xi - \Phi_1] - \hat{\delta}[\theta - \tilde{\theta}_1] \right\}
\] (25)
where I adapted the original notation to the one used for PSA. Obvious differences between Eqs. (23) and (9) are that BDG is a continuous time approach and only considers binary collisions whereas PSA has a discrete time step \(\tau\) and can handle collisions of an arbitrary number of partners. Assuming point particles, PSA can be applied to arbitrary density whereas a Boltzmann approach is always limited to the limit of vanishing density. If these were the only differences, in the limit of small density one would expect the phase diagram for stationary homogeneous states to be the same. This is not the case [23].

To pinpoint the fundamental difference between the models, let us perform the low density limit, \(M \ll 1\) of Eq. (10) and neglect terms with \(n > 1\), which describe genuine interactions of three and more particles. To ensure mass conservation, the prefactor \(\exp(-M)\) is replaced by \(1/(1 + M)\), see supplemental material of Ref. [6]. Because \(f\) does not depend on position, the integral over the position of particle 2 inside the collision circle can be performed. Dividing by \(\tau\) and adding \(-f(\theta, t)/\tau\) on both sides, Eq. (10) is rewritten such that the left hand side becomes the discrete time derivative. On the r.h.s. the following decomposition is performed
\[
-\frac{f(\theta)}{\tau} = -\frac{f(\theta) + Mf(\theta)}{\tau(1 + M)} = -\frac{f(\theta)}{\tau(1 + M)} - \frac{M}{\tau(1 + M)} \int_{-\pi}^{\pi} d\tilde{\theta}_2 f(\tilde{\theta}_2) f(\theta)
\] (26)

**Fig. 4.** Agent-based simulations of the probability ratios \(p_3/p_2\), \(p_4/p_3\), and the probability for non-binary interactions, \(S = 1 - (p_1 + p_2)\), versus time step \(\tau\) at density (a) \(M = 0.1\) and (b) \(M = 0.01\). Parameters: \(\eta = \eta_C\), for the rest of the parameters see Fig. 2.
that makes use of the equalities, $M = A\rho$ and $\int_{-\pi}^{\pi} d\tilde{\theta}_2 f(\tilde{\theta}_2) = \rho$. The first term in Eq. (26) adds a loss contribution to the self-diffusion term $I_1$; and the second term is incorporated into the binary collision term. Finally, one obtains for the spatially-homogeneous PSA approach at low densities,

$$\frac{f(\theta, t + \tau) - f(\theta, t)}{\tau} = I_1 + I_2$$

$$I_1 = \frac{1}{\tau(1 + M)} \left\{ - f(\tilde{\theta}_1, t) + \int_{-\pi}^{\pi} d\xi \int_{-\pi}^{\pi} d\tilde{\theta}_1 w_1(\xi) f(\tilde{\theta}_1, t) \delta(\theta - \xi - \tilde{\theta}_1) \right\}$$

$$I_2 = \frac{A}{\tau(1 + M)} \int_{-\pi}^{\pi} d\xi \int_{-\pi}^{\pi} d\tilde{\theta}_1 \int_{-\pi}^{\pi} d\tilde{\theta}_2 w_2(\xi)$$

$$\times f(\tilde{\theta}_1, t) f(\tilde{\theta}_2, t) \left\{ \delta(\theta - \xi - \Phi_1) - \delta(\theta - \tilde{\theta}_1) \right\}$$

(27)

where $f(\theta, x + \tau v, t + \tau)$ was replaced by $f(\theta, t + \tau)$ and the normalization $\int_{-\pi}^{\pi} d\xi w_n = 1$ was used. For stationary homogeneous states, the left hand sides of both kinetic equations vanish and we merely have to compare the collision integrals. The self-diffusion term $I_1$ of BDG becomes exactly equal to the corresponding term $I_1$ in Eq. (27) by choosing a self-diffusion frequency $\lambda_d = 1/\tau(1 + M)$.

The main difference between BDG's and PSA's collision operators is now evident: The binary collision frequencies, that is the prefactors of the terms $I_2$ and $I_{coll}$, do not agree. PSA’s collision frequency is proportional to $1/\tau$ and to the area of the collision circle, $A$, but independent of the velocity $v_0$ and the angles of the involved particles. The underlying physics is the one of the Vicsek model with finite time step $\tau$: particles are assumed to be invisible to each other during streaming and only collide once they have reached their final location. This means when in “flight” they might have very close encounters with other particles, e.g. go through each others action circles but do not interact until the end of the streaming step. If, for example, the time step $\tau$ is reduced by a factor of ten, the particles make ten times more “stops” during the same physical time. Hence, the likelihood of an interaction increases by a factor of ten, and the collision frequency increases accordingly to $w_{coll} \sim 1/\tau$.

The physical picture behind the collision frequency of BDG is different; it describes the interaction rule of BDG’s binary collision model: when two particles get closer than a threshold distance, a binary interaction occurs, as outlined in the sentence “In addition, binary collisions occur when the distance between two particles becomes less than $d_0$ ...” of Ref. [30]. Since this model has a continuous time evolution, during a fixed time $T$, the focal particle engages in an interaction with every particle that crosses its path. Thus, unlike in the VM, particles are never invisible to each other. Mathematically, in the intuitive derivation of the Boltzmann equation, this behavior is described by a collision cylinder (or collision rectangle in 2D) of length $v_{rel} \delta t$ and width $2R$ with $v_{rel} = v_2 - v_1$ and an infinitesimal time interval $\delta t$. Particle 2 has to be in this collision cylinder in order to collide with the focal particle between time $t$ and $t + \delta t$. This leads to a collision frequency proportional to $v_0$, because the faster the particles move the bigger is their chance to run into other particles during a fixed time interval.

Let’s contrast this behavior with the one of the VM in the extreme limits of vanishing and infinite particle speed $v_0$. For $v_0 = 0$ and moderate to large density, there will be particles with overlapping collision circles. Even though they cannot move, according to the rules of the VM, they will still engage in the alignment interaction. The PSA approach has a nonzero collision frequency even for zero speed and does describe this. However, no binary collisions occur in the BDG kinetic equation at $v_0 = 0$. This is actually common behavior for Boltzmann-like equations, because they
are all derived in the limit of vanishing density, where the likelihood of overlaps goes to zero and no collisions can happen. To accommodate overlaps one would have to derive higher order density corrections to the Boltzmann equation. In contrast, the PSA approach naturally deals with overlaps. In the other limit of \( v_0 \to \infty \), the collision frequency of BDG diverges because the focal particle runs into an infinite number of particles during its travel. In the VM and in PSA, \( r_{\text{coll}} \) remains finite. It does not matter how many particles the focal particle passes during flight; it just becomes “visible” to others at its final location.

One could be tempted to reconcile both kinetic approaches by saying “The BDG model might not correspond to the VM but couldn’t it just be the Boltzmann theory for a different microscopic model with continuous time dynamics?” There is several issues with this view.

First, in the traditional derivation of the Boltzmann equation by Grad, Kirkwood, Bogolyubov from the BBGKY-hierarchy, a coarse-graining over distances of order \( R \) and times of order \( \tau_0 \), the average duration of a collision, has to be performed and the information about two-particle encounters only enters the Boltzmann equation in a statistical statement, namely the scattering cross section in the collision integral and not through the direct interaction force, or in our case, the direct alignment rule, Eq. (3). In this statistical Boltzmann-sense, a collision is registered as soon as two particles enter each other’s action spheres and finished if their distance is larger than the interaction range. The coarse graining means that the Boltzmann equation cannot resolve these details and only cares about in what state particles enter the sphere and how they come out again. This is necessary because the molecular chaos assumption which assumes that particles are statistically independent, can only be justified before the particles enter the action sphere. Once they are inside, during their encounter they become increasingly correlated. To avoid confusion, we have to distinguish between what is usually called a “collision” in the literature about the Vicsek-model and a coarse-grained collision in the spirit of the Boltzmann equation. The former is just a single application of the instantaneous alignment rule, Eq. (3), and will be called microscopic collision, whereas the latter can involve many subsequent streaming and microscopic interaction events. In chapter 5 it was shown that the duration \( \tau_0 \) of a collision in the Boltzmann-sense can be very long in the continuous-time VM.

In the PSA approach, this complication does not occur as long as the discrete time step is much larger than \( R/v_0 \). Then, there is only one single microscopic collision in the interaction sphere and particles immediately leave the sphere. Thus, one collision in Boltzmann’s definition corresponds to one collision step of the VM and the duration \( \tau_0 \) is of order \( \tau \). In other words, under the condition, \( \tau \gg R/v_0 \), the difference between Vlasov-like and Boltzmann-like theories vanishes.

However, for the continuous time VM, during one Boltzmann-collision many of the microscopic streaming and interaction events occur. This means, in a Boltzmann equation for this microscopic model, the scattering cross section and not the collision kernel \( w_2(\xi) \delta(\theta - \Phi_1 - \xi_1) \) for a single interaction should occur.

This is not how the BDG kinetic equation looks like. One could argue, “Well, let’s fix it, let’s keep Eq. (3) as the microscopic interaction and let’s determine the cross section”. While this could be done at least numerically, the problem outlined in chapter 5 remains: For all interesting applications, that is close to or inside the ordered phase, and even at very small densities, approximately half or more of all particles are engaged in non-binary interactions. Thus, in my opinion, there is no chance to set up a reliable Boltzmann approach for the continuous-time VM.
6.2 Discussion

To summarize,

(1) I believe any Boltzmann approach for the Vicsek model with small discrete time step, $\tau < R/v_0$, is invalid near the flocking threshold. This is in part due to the violation of the binary collision assumption and happens even in dilute systems, $0.01 \leq M \leq 0.1$, and in the disordered phase. Only deep in the disordered phase, far away from the threshold, a valid Boltzmann equation could be set up but that is not interesting. Here, the term “Boltzmann approach” refers to a description solely based on the one-particle distribution function $f(\theta, x, t)$, which only considers spatially-local single and binary collisions.

(2) The Boltzmann-inspired approach of BDG \cite{30} does neither correctly describe the continuous-time nor the discrete-time Vicsek model on the quantitative level because it seems to inconsistently mix a Boltzmann-like collision frequency with a Vlasov-like interaction kernel. However, on the plus side, it is easier to handle than the PSA approach and has delivered important qualitative results \cite{30,48,54}.

Adamant users of BDG might justify the interaction kernel $w_2(\xi) \delta[\theta - \xi - \Phi_1]$ as an already averaged mesoscopic cross section. However, this just leads to more questions such as, (i) what is the underlying microscopic interaction leading to this cross section, and is this interaction consistent with the physics of any real binary collision, and (ii) would this interaction violate the validity of the Boltzmann approach? My guess is, that even if one can reverse-engineer the underlying microscopic rule, the same will happen that was found in chapter 5: near the flocking threshold the collisions (defined in the Boltzmann-spirit) will take too long, thus leading to clusters with three and more particles even if the overall density is low.

One might wonder why Ref. \cite{31} reported decent agreement between the BDG theory and agent-based simulations of the discrete time VM. I believe this was coincidence because for fixed $R$ and $\lambda_d$ there is one value of the velocity $v_0$ where the collision integrals of both models approximately agree. The condition is $R^2 = 2R(\|v_1 - v_2\|)/\lambda_d \approx 2Rv_0/\lambda_d$. If this is fulfilled, the ratios $I_1/I_2$ and $I_d/I_{\text{col}}$ that determine the phase diagram of stationary, homogeneous solutions at low density, are approximately the same. As shown in Fig. 1 of Ref. \cite{31} large discrepancies can occur if one chooses other velocities or higher densities.

Another question that comes to mind is: if one were to send the time step $\tau$ to an infinitesimal value in the VM, one would recover the continuous time VM, and, formally, one could also write down the PSA approach for such a small time step. The two theories would then attempt to describe the same system, how come they still look different? The first part of the answer is: the PSA approach simply ceases to be valid if the time step violates the condition $v_0\tau/R \gg 1$. Second, the BDG kinetic equation is inconsistent with the microscopic collision rules, Eq. (3), of the VM. This is because a Boltzmann-equation in the traditional sense contains statistical information in form of a scattering cross section and not the scattering kernel of a single alignment interaction. This scattering cross section is the result of many streaming and alignment steps, that take place during the collision time interval $\tau_0$, see chapter 5. Third, the PSA approach resolves the microscopic time scale like the Vlasov-equation, whereas a Boltzmann approach works on a coarse-grained manifold, and therefore should look different.

While the PSA approach delivers quantitative agreement for $v_0\tau/R = 1/\varepsilon \gg 1$ and arbitrary density, one might still be tempted to dismiss it because of its unphysical feature that particles can “tunnel” through each other during streaming. I see this is as the price one has to pay to obtain a kinetic theory that is valid near the flocking threshold. Furthermore, this approach is just the zeroth order contribution in the expansion parameter $\varepsilon = R/v_0\tau$ of a more general theory for the VM. The next
correction in $\varepsilon$, which contains clustering effects and goes beyond Molecular Chaos, will be presented elsewhere, [46].

7 Summary

In this discussion & debate paper, a recent kinetic approach for active particles is reviewed. For simplicity, I focus on the Vicsek-model (VM) as a paradigm of active matter. The kinetic theory approach is named “Phase Space Approach” (PSA) because it is based on an exact Chapman-Kolmogorov equation in phase space. It is designed to handle discrete time dynamics and multi-particle interactions that are given by collision rules and are not required to follow from a Hamiltonian. The discrete time step of the VM-algorithm is utilized to turn the molecular chaos assumption into a controlled and tunable approximation. This approximation is used to obtain a nonlocal mean-field theory for the one-particle distribution function.

Hydrodynamic equations for the PSA approach are derived by means of a third-order Chapman-Enskog expansion using a non-traditional scaling of the temporal derivatives. The equations are compared to the Toner-Tu theory of polar active matter. New terms, that seem to be absent in the Toner-Tu theory, are emphasized. Common convergence problems of Chapman-Enskog and similar gradient expansions are pointed out and possible remedies are discussed.

The average duration $\tau_0$ of a collision of two particles that follow Vicsek’s alignment rule is measured in Monte Carlo simulations. It is found that this time scales with nearly the same power of the density than the mean free time between collisions, $\tau_{coll}$. Thus, if density is decreased, the ratio $\tau_0/\tau_{coll}$ does not go quickly to zero as in regular gases. This suggests that the binary collision approximation – a key ingredient of a Boltzmann approach – is not even valid in dilute systems because collisions take so long that typically other particles join ongoing binary encounters.

This hypothesis is confirmed by agent-based simulations of the standard VM. In these simulations, the fraction of particles that are engaged in non-binary interactions is recorded and turns out to be quite large. Therefore, Boltzmann approaches are not suitable for quantitative descriptions of the continuous-time VM near the transition to collective motion.

The Boltzmann approach of Bertin et al. (BDG), [30,31] is critically assessed and compared term-by-term to the PSA approach. I find that even at small densities and in homogeneous systems there is a significant difference between PSA and BDG: the collision frequencies of the binary collision terms depend on different physical parameters. I present arguments to substantiate my opinion that the approach of Refs. [30,31] is not a consistent description of a VM-like microscopic model and thus not able to produce quantitatively correct results for the VM in any limit. I also argue that it is not worth to make it consistent because of the general problems of Boltzmann approaches for systems with alignment interactions.

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