Continuum modeling of myxobacteria clustering

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\textbf{Abstract.} In this paper we develop a continuum theory of clustering in ensembles of self-propelled inelastically colliding rods with applications to collective dynamics of common gliding bacteria \textit{Myxococcus xanthus}. A multi-phase hydrodynamic model that couples densities of oriented and isotropic phases is described. This model is used for the analysis of an instability that leads to spontaneous formation of directionally moving dense clusters within initially dilute isotropic ‘gas’ of myxobacteria. Numerical simulations of this model...
confirm the existence of stationary dense moving clusters and also elucidate the properties of their collisions. The results are shown to be in a qualitative agreement with experiments.

Online supplementary data available from stacks.iop.org/NJP/15/035029/mmedia

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1. Introduction

Interacting self-propelled particles are known to engage in non-trivial forms of collective behavior. Examples of such behaviors abound in biology and include flocking of birds, schooling of fish and herding of animals, as well as self-organization of various microorganisms [1]. Mechanisms of interaction among ‘biological particles’ can be rather complicated and include a variety of chemical or visual signaling. However, numerical simulations, theoretical analysis and laboratory experiments with swimming microorganisms, molecular motors/actin filaments and synthetic self-propelled particles show that often even purely mechanical interactions (for example, steric repulsion, binary collisions or long-range hydrodynamic forces) are sufficient to account for coherent states in groups of interacting self-propelled particles [2–12].

One interesting example of coordinated behavior of bacteria is presented by the myxobacteria *Myxococcus xanthus*, a widespread species of bacteria found in cultivated soils. The myxobacteria employ two different types of motility (A-motility, slime secretion from their trailing poles and S-motility, retraction of type IV pili from their leading poles), to glide over solid surfaces along their axes. Myxobacteria have shapes similar to flexible spherocylinders about 0.5 µm wide and 5–10 µm long and move with typical speeds of 0.025–0.1 µm s⁻¹. Every few minutes they reverse their direction of motion [13–15]. When starved for nutrients, myxobacteria enter a new developmental phase in which they move toward certain central loci and form multi-cellular cavernous fruiting bodies [16], in close analogy to slime mold development [17]. Communication among myxobacteria under starvation involves both long range (A-signaling) and contact (C-signaling) interaction [18]. Under favorable growth conditions, myxobacteria near the edge of a swarm often form dense packs of bacteria gliding together [18].

In the recent paper Peruani *et al* [19] demonstrated that a mutant strain of myxobacteria (SA2407) which only had contact interaction (no S-motility) and did not perform direction
reversals, nonetheless exhibited formation of clusters similar to those of self-propelled rods studied previously theoretically and numerically [20, 21]. Peruani et al [19] analyzed statistics of cluster size distribution and found a transition at a certain critical cell density $\eta \sim 0.17$ at which the distribution acquires a power law with exponent close to 0.9. At larger densities, the cluster size distribution forms a peak at large sizes indicating formation of large clusters only limited by the system size.

Several mathematical and computational models of the myxobacteria life cycle have been developed [2, 4, 22]. The most detailed description is based on direct simulations of individual organisms as self-propelled flexible rods [22, 23]. Much insight can also be gained from representation of bacteria in the form of solid self-propelled rods with apolar inelastic interactions [20, 21, 23] or even point-like self-propelled particles with nematic interaction rules [3]. Theoretical modeling approaches include the mean-field theory for studying cluster-size distribution introduced in [20] as well as hydrodynamic models for ‘active fluids’ with nematic interactions [24–26] that can be used to describe the dynamics of myxobacteria in a dilute state. However, the latter description cannot account for the most interesting regime when finite-size dense clusters coexist with the dilute phase.

In this paper we further advance the continuum modeling of myxobacterial colonies motivated by our recent experimental observations with myxobacteria. In these experiments, colonies of myxobacteria Myxococcus xanthus were grown under normal conditions on CTT (Casitone-Tris) agar plates, and then transferred on top of thin (0.2–0.5 mm) agar layers inside hermetically sealed microchambers (the microchamber was a modification to the chamber presented in [27]). The high-resolution time-lapse images (1200×1200 pixels) were acquired by a digital camera attached to a microscope with oil-immersion objectives. The images were recorded with time intervals of 5 or 10 s over a time period of several hours. Several images demonstrating collisions of individual bacteria and small clusters formed by Myxococcus xanthus are shown in figure 1 (see also supplementary movies 1 and 2, available from stacks.iop.org/NJP/15/035029/mmedia). Bacteria and clusters generally do not glide along straight lines because bacteria prefer to follow slime tracks left by other bacteria. However, one can identify major scenarios of collisions between the clusters depending on the initial angle. Figures 1(a)–(c) illustrate two types of collisions of individual bacteria. In the case where the collision angle is acute, the bacteria become nearly collinear and stay together after collision. In the case where the angle is obtuse, the two bacteria become anti-parallel. Similar dynamics are observed in collisions of small clusters (figures 1(d)–(i)), two co-propagating clusters typically merge after collision, but bacteria in two counter-propagating clusters are able to penetrating through the opposing clusters). Furthermore, one can see that large clusters coexist with small clusters and individual bacteria. Evidently, this coexistence is a result of a dynamical balance between merging of clusters and individual bacteria and their splitting off due to random fluctuations, or, possibly, encountering of diverging slime tracks. Since bacteria tend to follow the slime tracks, diverging slime track may result in a breakup of the entire cluster.

These observations have demonstrated that upon either acute or obtuse collision, myxobacteria acquire nearly identical nematic orientation, thus rendering the collisions in angular space completely inelastic. At low density of particles, such interactions can be studied using kinetic equation for the angular probability distribution of particles where the collision integral only takes into account pair-wise interactions of particles leading to their ‘instantaneous’ change of orientation as a result of collision. We used this approach earlier to describe polar alignment of microtubules via molecular motors [28, 29] or of swimming...
Figure 1. Illustrations of collisions between individual bacteria and clusters of *Myxococcus xanthus*. (a)–(c) Collisions of individual bacteria. Top left corner: three bacteria moving in the same general direction become nearly collinear. Bottom right corner: two counter-propagating myxobacteria become anti-parallel. (d)–(f) Collision of two small clusters moving towards each other. (g)–(i) Merging of two clusters moving in nearly the same direction (shown in red) and their collision with a cluster moving in the opposite direction (shown in green). See also supplementary movies 1 and 2 (available from stacks.iop.org/NJP/15/035029/mmedia) illustrating dynamics of cluster collisions.

In a recent paper [30] a qualitatively similar approach to study nematic alignment of self-propelled rods based on a correspondingly generalized Vicsek model was used. The solution of that model yielded a variety of non-trivial dense localized band solutions (both stationary and dynamic) embedded in a low-density ‘gas’ of non-aligned rods. These solutions are qualitatively similar to the clusters of myxobacteria. For completeness, in the supplementary
material (available from stacks.iop.org/NJP/15/035029/mmedia) we introduce and analyze the simplified kinetic model of the dilute population of self-propelled particles undergoing totally inelastic nematic pair-wise collisions. In addition to the nematic alignment and random angular fluctuations already introduced in [30], we take into account direction reversals, but we ignore the interaction between bacteria via chemical signaling and slime tracks formation. At sufficient density of bacteria, this kinetic model exhibits a symmetry breaking instability that in the nonlinear regime eventually leads to formation of highly ordered dense nematic clusters of myxobacteria, however the critical density for the nematic ordering instability of an isotropic state is higher than the for the polar case with equal interaction strength.

As mentioned above, the experiments point at the coexistence of two phases in colonies of myxobacteria: dense, almost close-packed highly-aligned clusters and dilute nearly isotropic ‘gas’ phase. Based on this observation, in this paper we propose a multi-phase one-dimensional (1D) hydrodynamic model that couples densities of oriented dense and isotropic dilute phases. This model describes a sub-critical transition that leads to formation and growth of highly-localized directionally-moving dense packs from small perturbations in initially dilute isotropic ‘gas’ of myxobacteria. Our numerical investigation of this model also elucidated collisions of dense clusters and formation of stationary dense moving clusters (solitons). Colliding clusters may either permeate through each other or coalesce depending on their angle of collision. We also generalize our multi-phase model to the quasi-two-dimensional (2D) case, which allowed us to describe oblique collisions of self-propelled dense clusters of myxobacteria.

2. One-dimensional field model for dense and dilute phases

Experiments with myxobacteria show that at intermediate densities of cells, dense oriented clusters coexist with isolated cells. Since bacteria within the dense clusters are nearly close-packed, one cannot directly apply the kinetic description, see supplementary material, which is based on the assumption of binary collisions among the cells. An alternative approach is to describe the dense and dilute phases as separate but coupled fields. Such two-phase approach was pioneered for interacting elongated particles in [31–33], however in that work the particles were not self-propelled along their orientation. In this section, we introduce a similar approach to the description of myxobacteria in the clustering regime. Guided by the experiments, we make a simplifying assumption that locally the dense phase is only bi-directional, i.e. cells only oriented and move with velocity \( c \) in two opposite directions \( \phi_+ \) and \( \phi_- = \phi_+ + \pi \). Additionally, we assume that the dilute phase is isotropic. In other words, the probability distribution function is taken to have the following form

\[
P(r, \phi, t) = \rho_+ \delta(\phi - \phi_+) + \rho_- \delta(\phi - \phi_-) + \rho_g,
\]

where \( \rho_\pm \) are the concentrations of aligned particles with the orientations \( \phi_+ \) and \( \phi_- = \phi_+ + \pi \), and \( \rho_g \) is the concentration of isotropic state. This simplification will allow us to cast a model in the form of partial differential equations instead of integro-differential ones as in the kinetic theory (supplementary material and [31–33]). Generally, all variables \( \rho_\pm, \phi_\pm, \rho_g \) can be functions of space and time. However, in this section we make an additional simplifying assumption that clustered cells are moving only along one preferred direction (which, e.g., can be enforced by the geometry of the system or a slime track), so we can take \( \phi_- = \phi_+ + \pi = 0 \) without loss of generality. The equations for the three densities can be written in the following form.
general form:

\[ \partial_t \rho_+ + c \partial_x \rho_+ = \partial_x J_+ + \alpha (\rho_+ + \rho_-) \rho_+ - \mu \rho_+ (\rho_m - \rho_+ - \rho_-) + \beta (\rho_- - \rho_+), \]  
\[ \partial_t \rho_- - c \partial_x \rho_- = \partial_x J_- + \alpha (\rho_+ + \rho_-) \rho_- - \mu \rho_- (\rho_m - \rho_+ - \rho_-) + \beta (\rho_+ - \rho_-), \]  
\[ \partial_t \rho_g = D_g \partial_x^2 \rho_g - 2\alpha (\rho_+ + \rho_-) \rho_g + \mu (\rho_+ + \rho_-) (\rho_m - \rho_+ - \rho_-) \nu. \]  

Here \( J_\pm \) are the mass fluxes for each phase \( \rho_\pm \) correspondingly,

\[ J_\pm = -\rho_\pm \partial_x p + \epsilon \partial_x \rho_\pm. \]  

The first term in this expression describes the contribution to the mass flux due to the pressure \( (p) \) gradient arising from hard-core repulsion between the cells in the dense phase. The specific form of this term is not important, as long as the pressure increases with density and diverges at certain critical (close-packed) density \( \rho_m \). One possible phenomenological choice for the pressure is \( p = p_0/\left(\rho_m - \rho_+ - \rho_-\right) \) (we neglect in this expression the density of gas phase). In the following we will take \( p_0 = 1 \) for the sake of simplicity. The second term describes the diffusion flux of each component with the translational diffusion coefficient. While we expect translational diffusion to be weak in the dense phase \( (\epsilon \ll 1) \), we introduce this term for regularization of equations (2)–(4) for \( \rho_\pm \to 0 \) \( (\text{for } \epsilon = 0 \text{ equations (2) and (3) may develop infinite density gradients}) \).

The first term in the rhs of equation (4) describes translational diffusion in the dilute (gas) phase due to fluctuations in the direction of motion of individual particles. The corresponding diffusion coefficient \( D_g \approx 2c^2/D_r \), where \( D_r \) is rotational diffusion of a bacterium [34]. The terms \( \sim \alpha \) in equations (2)–(4) describe alignment of bacteria from the gas phase along the nematic direction upon their collision with the dense phase cells. The terms \( \sim \mu \) describe the inverse process of returning nematicaligned cells back into the gas phase (scattering). In principle, these terms can be derived from the kinetic equation which becomes formally valid for \( \rho_\pm \to 0 \). Thus, \( \alpha - \mu \) corresponds to the growth rate of second harmonics \( \lambda_2 \), see equation (13) in supplementary material (available from stacks.iop.org/NJP/15/035029/mmmedia). However, in the densely packed state this process should cease, thus we model it by introducing a fitting parameter \( \nu \gg 1 \), so the scattering rapidly disappears as the oriented phase density approaches \( \rho_m \). The terms \( \sim \beta \) in equations (2) and (3) describe spontaneous orientation reversals. Since the reversal occur between two dense phases \( \rho_\pm \), there is no contribution from the reversals to equation (4) for the gas phase. Note that our equations (2)–(4) are different from the phenomenological balance equations for free and bound self-aligning objects studied in [33].

It is convenient to re-write equations (2)–(4) for the variables \( U = \rho_+ + \rho_- \) (total density of the nematic phase) and \( W = \rho_+ - \rho_- \) (net polarization). Then equations (2)–(4) assume the form

\[ \partial_t U + c \partial_x W = \partial_x \left( \frac{1}{\rho_m - U} + \epsilon \partial_x U \right) + 2\alpha U \rho_g - \mu U (\rho_m - U) \nu, \]  
\[ \partial_t W + c \partial_x U = \partial_x \left( \frac{1}{\rho_m - U} + \epsilon \partial_x W \right) - \mu W (\rho_m - U) \nu - 2\beta W, \]  
\[ \partial_t \rho_g = D_g \partial_x^2 \rho_g - 2\alpha U \rho_g + \mu U (\rho_m - U) \nu. \]  

For completeness, we can also write the analogous model for the polar interaction between the colliding particles. The only difference between this model and the apolar interaction...
model (2)–(4) is in the alignment term \(\sim \alpha\) and the absence of the reversal term. The polar case only requires two equations for the single dense phase \(\rho\) and the gas phase \(\rho_g\)

\[
\begin{align*}
\partial_t \rho + c \partial_x \rho &= \partial_x \left( \rho \frac{\partial_x \rho}{\rho_m - \rho} + \epsilon \partial_x \rho \right) + \alpha \rho \rho_g - \mu \rho (\rho_m - \rho) \nu, \\
\partial_t \rho_g &= D_g \partial_x^2 \rho_g - \alpha \rho \rho_g + \mu \rho (\rho_m - \rho) \nu.
\end{align*}
\]  

(7)

\[\partial_t \rho + c \partial_x \rho = \partial_x \left( \rho \frac{\partial_x \rho}{\rho_m - \rho} + \epsilon \partial_x \rho \right) + \alpha \rho \rho_g - \mu \rho (\rho_m - \rho) \nu, \]

\[\partial_t \rho_g = D_g \partial_x^2 \rho_g - \alpha \rho \rho_g + \mu \rho (\rho_m - \rho) \nu. \]

2.1. Linear stability of the homogeneous nematic state

Equations (6) admit a symmetric uniform solution with \(W = 0, U = U_0 = \text{const}\). In the steady state, the gas density is \(\rho_g = \rho_\text{g} = \mu(\rho_m - U_0)^\nu/2\alpha\). Then, using the total mass conservation \(U_0 + \rho_g = \rho_0\), we obtain nonlinear equation \(\rho_0 - U_0 = \mu(\rho_m - U_0)^\nu/2\alpha\). Note that for large enough \(\nu\) this equation may possess multiple solutions in some range of \(\rho_0\), indicating discontinuous transition from the pure gas state \((U_0 = 0)\) to a symmetric state with non-zero oriented phase \((U_0 > 0)\) as the total density of bacteria \(\rho_0\) increases.

Linearizing equations (6) near this symmetric (pure nematic) uniform steady state, \(U = U_0 + u, W = w\), with small spatially periodic perturbations \(u, w \sim \exp(\lambda t + ikx)\) (setting \(\epsilon = 0\) and \(\rho_m = 1\) for simplicity), we can compute three eigenvalues \(\lambda_{1,2,3}\). For \(k = 0\), these eigenvalues are given by simple expressions \(\lambda_1 = 0, \lambda_2 = -2\beta - \mu(1 - U_0)^\nu\) and \(\lambda_3 = U_0(\mu\nu(1 - U_0)^{\nu-1} - 2\alpha)\). It is easy to see that the second eigenvalue is always negative, and the third eigenvalue also becomes negative for sufficiently large \(\nu\). In contrast, uniform gas state \(U_0 = 0, \rho_g = \rho_0\) is unstable for \(\rho_g = \rho_0 > \mu\rho_m/2\alpha\). Since for \(\nu \gg 1\) the term \((1 - U_0)^\nu-1\) is small, the dense phase is stable if the gas is unstable.

We can also find the long-wave limit of the critical eigenvalue \(\lambda_1\) for small but finite \(k\). The explicit calculation yields (see the appendix for details)

\[
\lambda_1 = \frac{1}{2\alpha - \mu(1 - U_0)^{\nu-1}} \left( \nu \mu(1 - U_0)^{\nu-1} D_g - 2\alpha D_s - \frac{2\alpha c^2}{2\beta + \mu(1 - U_0)^\nu} \right) k^2 + O(k^4). 
\]

(8)

Here \(D_s = U_0/(1 - U_0)^2\). As we have seen above, the spatially-uniform homogeneous symmetric (pure nematic) state is stable at \(k = 0\) if \(2\alpha > \mu(1 - U_0)^{\nu-1}\). According to equation (8), it could become unstable for small but finite \(k\) if the gas diffusion \(D_g\) was large enough, i.e

\[
D_g > \frac{2\alpha D_s + \frac{2\alpha c^2}{2\beta + \mu(1 - U_0)^\nu}}{\nu \mu(1 - U_0)^{\nu-1}}. 
\]

(9)

However, since we assume that \(\nu \gg 1\) (in the rest of the paper we use \(\nu = 8\), \((1 - U_0)^\nu \to 0\) and so this instability would require unphysically large diffusion constant \(D_g\).

2.2. Localized solutions

Despite the linear stability of the uniform dense phase, the numerical simulations show rich spatiotemporal dynamics of the coupled gas and dense phase system equations (2)–(4) or equations (6). For example, small but finite initial perturbations of the oriented phase within the gas phase in the regime slightly below the instability threshold eventually grow, leading to the emergence of multiple counter-propagating domains of the dense phase. Eventually a single self-sustained localized solution emerges that is a 1D analogue of a cluster (see figures 2(a) and (b)). These fixed-shape propagating pulses can be obtained either by direct numerical
Figure 2. (a), (b) Instability of a uniform gas state with small but finite random perturbations of the two counter-propagating dense phases, and the emergence of counter-propagating pulses of dense phase in a 1D domain of length 500 with periodic boundary conditions. Eventually, a single pulse wins. (c), (d) Interaction of two opposite pulses in a 1D domain of length 400 with periodic boundary condition, where again one pulse eventually dies and another wins. Panels (a) and (c) show densities of the oriented phases and (b) and (d) show the gas density. Parameters are: $\alpha = 0.2$, $\beta = 0.0002$, $\mu = 0.1$, $D_g = 10$, $\epsilon = 0.1$. In panels (a) and (c) field $\rho^+$ is shown in red and $\rho^-$ in blue. In panels (b), (d) intensity of $\rho_g$ changes from black (0) to yellow (max).

Simulations of the full 1D model (6) or by searching for stationary solutions of equations (6) in a co-moving frame using shooting-matching method. The corresponding stationary solutions are shown in figure 3(a) for the nematic case and figure 3(c) for the polar case. As can be expected from the mass conservation, the gas concentration far away from the front and rear of the pulse are equal $\rho_g(x \rightarrow -\infty) = \rho_g(x \rightarrow +\infty) = \rho^0_g$. In the nematic case, the pulse is a localized bound state of two sub-fields $\rho^+$ and $\rho^-$ with opposing polar orientations, because the dense phase orients incoming gas particles in either of the two directions equally and also there are also spontaneous orientation reversals. Cells oriented against the direction of motion of the pulse quickly leave it through the back and form a tail of the opposite oriented phase (see the red line in figure 3(a)), whereas particles moving in the same direction as the pulse, remain within it for a long time. It is also interesting to note that the pulse velocity is a monotonously increasing function of its mass $M = \int_{-\infty}^{\infty} (\rho^+ + \rho^-) \, dx$, see figures 3(b). However, its dependence
Figure 3. (a) The profile of the dense phase pulse for the case of nematic interaction (2)–(4) with parameters $\alpha = 0.2$, $\beta = 0.0002$, $\mu = 0.1$, $D_g = 10$, $\epsilon = 0.1$; (b) mass $M$ and velocity $V$ of the pulse as functions of the gas density. Panels (c) and (d) display analogous results for the polar interaction model, parameters $\alpha = 0.2$, $\mu = 0.1$, $D_g = 10$, $\epsilon = 0.1$, equation (7). Pulses move from left to right.

on the asymptotic gas concentration $\rho_g^0$ in non-monotonic: in a certain range of $\rho_g^0$ two different solutions exist for the same $\rho_g^0$. For each set of the parameters there is also a minimal mass of the pulse. Similar dependence occurs also for the polar case described by equations (7). Both the pulse shape and its velocity dependence on the total mass have similar trends as in the nematic case, see figures 3(c) and (d). The overall picture of localized solutions and their evolution is qualitatively similar to the situation described by the Ginzburg–Landau type equation for polar particles derived near the threshold of orientational instability [30, 35]. Note that in both polar and nematic cases the speed of the pulse is slightly higher than the speed of an individual bacterium $c$. While it may appear counter-intuitive, it is a consequence of the following mechanism: the moving cluster absorbs particles from the gas phase on the leading front and ejects them at the rear. Thus, due to deposition of particles from the gas, the pulse can move faster than individual bacteria. We also studied numerically the interaction of two pulses traveling in the opposite directions. Our simulations show that this configuration is unstable, and eventually one pulse always wins, while the other decays (see figures 2(c) and (d)).
3. Multi-phase field model in the two-dimensional case

In this section we generalize the 1D description and introduce a 2D continuum model for the dynamics of self-propelled particles. In the polar case, as in the previous section we have equations for the gas density \( \rho_g(r, t) \) and the dense (aligned) phase density \( \rho(r, t) \), however now the orientation of bacteria in the dense phase is not fixed by the geometry of the system. Accordingly, we introduce the auxiliary orientation field variable \( \tau(r, t) \). We construct it in such a way that this vector field is everywhere parallel to the director field \( n \), however to avoid degeneracies, we do not require \( \tau \) to have a unit length, furthermore, we construct the equation for \( \tau \) such that \( |\tau| \to 0 \) as the density of the aligned phase vanishes. The set of equations for these variables can be written as

\[
\begin{align*}
\partial_t \rho &+ c \nabla (\tau \rho) = \nabla \left( \rho \nabla \frac{1}{\rho_m - \rho} + \epsilon \nabla \rho \right) + \alpha \rho \rho_g - \mu \rho (\rho_m - \rho)^\nu, \\
\partial_t \rho_g &= D_g \nabla^2 \rho_g - \alpha \rho \rho_g + \mu \rho (\rho_m - \rho)^\nu, \\
\partial_t \tau &+ c \tau \nabla \tau = D_\tau \nabla^2 \tau + A(\rho(|\tau|^2)\tau).
\end{align*}
\]

The first two equations are straightforward generalizations of the 1D equations (7). The equation for \( \tau \) has the form of the Ginzburg–Landau equation, so the magnitude of the director is a function of local density. As stated above, we assume that \( h(\rho) \) is a monotonous function satisfying the following conditions: \( h < 0 \) if \( \rho = 0 \), and it quickly approaches 1 as \( \rho \) becomes non-zero. We also choose large \( A \) to enforce quick convergence of the magnitude of \( \tau \) to its equilibrium value. Thus, when \( \rho \to 0 \), field \( \tau \) indeed decays to zero, but for non-zero \( \rho \), \( |\tau| \) rapidly approaches 1. The dynamics described by equations (10)–(12) are not very sensitive to a specific choice of the function \( h(\rho) \). In our simulations we used \( h(\rho) = 1.1 \tanh(20\rho) - 0.1 \).

Equation (12) also incorporates spatial diffusion \( D_\tau \rho \nabla^2 \tau \) of the director field (that provides polar alignment of neighboring cells, the factor of \( \rho \) is due to alignment of particles by binary collisions, compare [28]) and its convective transport by the cells themselves, \( c \tau \nabla \tau \). In the dilute regime these terms can be derived from the kinetic theory, see equation (1) in supplementary material (available from stacks.iop.org/NJP/15/035029/mmedia). Here we postulate phenomenologically that they are valid in the dense regime as well.

Equations (10)–(12) were solved in a periodic 2D domain using implicit finite-difference method. The results for head-on collisions of two localized initial perturbations (‘blobs’) are shown in figures 4(a)–(d). As we see from the figure, the blobs propagate toward each other, collide and jam (since this polar model only deals with one orientation field in a given spatial location, and so does not allow inter-penetration of clusters). Then, after some time, a single blob traveling in the transversal direction is formed. The resulting direction of cluster propagation is determined by the initial conditions. For slightly different initial conditions we also observed that the head-on colliding blobs can produce two blobs traveling in the opposite directions.

If only one small blob is formed initially in the system, it will absorb the gas and grow, mostly extending in the transversal direction, and gradually evolve into a quasi-1D pulse. However the growth process is very slow, and in a finite system it eventually may stop due to depletion of the gas phase.

Note that equations (10)–(12) for \( \rho, \tau \) appear similar to the hydrodynamic model by Toner and Tu [36] that were derived from the kinetic theory near the threshold of flocking instability. However, there is an important difference: since our model phenomenologically describes the
Figure 4. Numerical simulations of the 2D models with parameters $\alpha = 0.1$, $\mu = 0.1$, $\epsilon = 0.08$, $D_\tau = 8$, $D_g = 10$, $A = 20$, in the 2D periodic domain of 400 units, $800 \times 800$ mesh points, and initial conditions in the form of two colliding polar 'blobs'. (a)–(d) Polar model (10), (12), almost head-on collision, spots form a shock, then merge and travel together down, see supplementary movie 3 (available from stacks.iop.org/NJP/15/035029/mmedia); (e)–(i) Apolar model (13), (15), nearly head-on collision, spots go through each other almost undisturbed, see supplementary movie 4. The parameters: $\alpha = 0.2$, $\mu = 0.1$, $\beta = 10^{-4}$, $D_\tau = 16$, $D_g = 10$, $\epsilon = 0.08$, $A = 50$, $\gamma = 1$, $h(\rho) = 1.2\tanh(20\rho) - 0.2$, $\nu = 8$. In panels (e)–(i) field $\rho_+$ is shown in red and $\rho_-$ is shown in blue.

clustering regime far from the threshold, the orientation field $\tau$ is not a true hydrodynamic velocity, and so the equation for $\tau$ does not contain a pressure-like term $\nabla \rho$. Indeed, in our model all bacteria within the cluster have the same orientation, and a pressure gradient cannot locally change it by rotating the bacteria. Consequently, the resulting dynamics exhibited by equations (10)–(12) are different from that described by the Toner and Tu-like models for the suspensions of swimming bacteria Bacillus subtilis. Equations (10)–(12) do not exhibit a variety of turbulent-like states observed in experiments [37, 38].

Now we turn to the apolar case. In this case, we need to introduce three scalar fields, gas $\rho_g$, and two oriented dense fields, with densities $\rho_{\pm}(\mathbf{r}, t)$, $\rho_{\mp}(\mathbf{r}, t)$, plus two auxiliary orientation field variables $\tau_{\pm}(\mathbf{r}, t)$ corresponding to the densities $\rho_{\pm}$. However, unlike the polar case, we have to limit ourselves by the quasi-1D case, when $\tau_{\pm}$ are confined to a narrow sector along a selected direction (which we can associate with $x$-axis for definiteness) everywhere within the 2D plane. Fully 2D nematic case cannot be treated in this framework since in the general case, there will be no clear distinction between ‘+’ and ‘−’ fields. The equations for the three densities in the apolar case are again similar to those in the 1D case

$$
\partial_t \rho_{\pm} + c \nabla (\tau_{\pm} \rho_{\pm}) = \nabla \left( \epsilon \nabla \rho_{\pm} \pm \rho_{\pm} \nabla \frac{1}{\rho_m - \rho_+ - \rho_-} \right) + \alpha (\rho_+ + \rho_-) \rho_g + \beta (\rho_+ \mp \rho_-) - \mu \rho_{\pm} (\rho_m - \rho_+ - \rho_-)^\nu ,
$$

$$
\partial_t \rho_g = D_g \nabla^2 \rho_g - \alpha (\rho_+ + \rho_-) \rho_g + \mu (\rho_+ + \rho_-) (\rho_m - \rho_+ - \rho_-)^\nu .
$$

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The equations for the two auxiliary vector orientation fields \( \tau_\pm \) in the quasi-1D case read

\[
\partial_t \tau_\pm + c \tau_\pm \nabla \tau_\pm = D_\tau \rho_\pm \nabla^2 \tau_\pm + A(h(\rho_\pm) - |\tau_\pm|^2) \tau_\pm - \gamma_0 \rho_\pm (\tau_+ + \tau_-). \tag{15}
\]

Unlike equation (12), the rhs of equation (15) has an additional coupling term \( \sim \gamma_0 \). This term enforces antiparallel alignment between the two fields due to nematic interaction between counter-propagating particles; it is easy to see that it leads to the exponential decay of \( \tau_+ + \tau_- \), i.e. it favors anti-parallel alignment of \( \tau_\pm \). The rate of this mutual alignment is proportional to the density of the ‘opposite’ phase.

We investigated interactions of cluster within equations (13)–(15) numerically, see figure 4. For the nearly head-on collision, figures 4(e)–(i), we observed penetration of clusters through each other, similar to the 1D case. Similar to the polar case, the blobs slowly grow and extend in the transverse direction.

In addition to moving blobs equations (13) and (14) admit a one-parametric family of transversal quasi-1D solutions in which nematic order is confined to a narrow band and vector \( \tau \) is oriented along the dense band with local density \( \rho_+ = \rho_- \) surrounded by a homogeneous disordered ‘gas’. Bands were observed in particle simulation of the Vicsek model with nematic alignment [3] and derived analytically in the continuum limit [30] valid near the threshold of nematic transition.

Stationary bands can be found from equations (13) and (14) by seeking a solution in the form \( \rho_+(x, y, t) = \rho_-(x, y, t) = U(y)/2 \) and \( \rho_g(x, y, t) = \rho_g(y) \). With constant unit vectors \( \tau_\pm \) oriented along the \( x \)-axis equation (15) are trivially satisfied. Summing up equations (13), after integration we obtain algebraic relation between \( \rho_g \) and \( U = \rho_+ + \rho_- \) (for simplicity we set \( \epsilon \to 0 \)):

\[
\rho_g = \rho^0_g - \frac{1}{D_g} \left( \frac{U}{(1-U)} + \log(1-U) \right), \tag{16}
\]

where \( \rho^0_g = \text{const} \) is the asymptotic value of gas density far from the band. Substituting \( \rho_\pm \) from equations (16) to (13), after summing them up and multiplying by \( (U \partial_y U)/(1-U)^2 \), we obtain an additional first integral in the form

\[
\left( \frac{U \partial_y U}{(1-U)^2} \right)^2 + F(U) = 0, \tag{17}
\]

where \( F(U) \) is an explicit but rather cumbersome function of \( U \). The band solution can be found by integrating numerically equation (17), a typical solution is shown in figure 5.

The bands exist for the gas densities \( \rho^0_g \) that are significantly smaller than the critical density of the isotropic state instability \( \rho_g = \mu/2\alpha \). In contrast to exponentially localized bands in the Ginzburg–Landau type model of [30], due to a nonlinear diffusion \( \sim \partial_y (U \partial_y (1/(1-u))) \), the bands in equations (13) and (14) for \( \epsilon = 0 \) have finite support: function \( U \) is exactly zero outside the band. The mass of the band \( M = \int_{-\infty}^{\infty} U dy \) depends on the asymptotic value of the gas density \( \rho^0_g \), see inset to figure 5. The stability properties of these bands are likely different from that of solutions [30].
Figure 5. Band solution of the 2D model equations (13), (14) with parameters \(\alpha = 0.2, \mu = 0.1, \epsilon = 0, D_s = 10, \rho_g^0 = 0.032\). Inset: mass of the band \(M = \int_{-\infty}^{\infty} U \, dy\) as function of \(\rho_g^0\).

4. Conclusions

In this work we introduced a continuum multi-phase model for description of collective motion of myxobacteria both within clusters and in the dilute ‘gas’ phase. The phases are driven by the hydrodynamic pressure and diffusion and coupled by exchange terms due to nematic or polar alignment (gas ‘condensation’ on clusters), escape (‘evaporation’), and direction reversals. Continuum field models have been derived previously by expanding the kinetic equation near the threshold of the symmetry-breaking instability of an isotropic state [28–30, 35], however they cannot handle the regime far away from the initial instability when dense clusters begin to form. Our phenomenological multi-phase model is thus complementary to these near-threshold hydrodynamic models and extends them to the situations when the clusters have almost closed-packed density similar to the one observed in experiments. This model successfully describes a sub-critical transition that leads to formation and growth of highly-localized dense packs of bacteria (pulses) from initially isotropic gas. Despite the underlying nematic alignment mechanism, the pulses have a dominant polar component, and move directionally. This polar orientation within a pulse is formed spontaneously because bacteria with opposite polarity leave the pulse quickly. Our analysis shows that the pulses move with the speed slightly exceeding speed of individual bacterium, a prediction that needs to be validated by experiments.

There is a number of limitations inherent to our phenomenological modeling approach. Without knowledge of the actual equations of state, we postulated simple analytical expressions for the pressure developed within a dense phase as well as the nonlinear rates of alignment and scattering. It would be of interest to derive these expressions from first principles or deduce them from experimental data. Our 2D model in the nematic case is only applicable in quasi-1D settings when clusters can propagate in two clearly separable directions imposed, for example,
by the geometry of the system. The complete description of the fully-2D case is still an open problem. We also neglected a number of other complicated factors that affect the dynamics of real myxobacteria, such as C-signaling, the chemotactic effects of slime tracks and realistic direction-reversal dynamics of individual bacteria. (For details about nonlinear diffusion model of self-propelled rods reversing with specific frequency see [39].) We anticipate that these factors can be taken into consideration within our general modeling approach. The interaction with slime tracks can be incorporated on the level of continuum description by introducing an additional field of slime concentration. The reversal dynamics can be more realistically described by introducing some memory effects in the reversal rate kernel. And finally, random fluctuations can be included into the model in order to study breakup of clusters, the effect observed experimentally [19].

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Appendix

Here we consider a long-wave limit of the critical eigenvalue \( \lambda_1 \) for small but finite \( k \to 0 \). We set for simplicity \( \epsilon = 0 \). Linearized near \( U = U_0, V = 0, \rho_g = \bar{\rho}_g \) equations (6) assume the form

\[
\begin{align*}
\lambda u + i c k w &= -D_s k^2 u + 2 \alpha u \bar{\rho}_g + 2 \alpha U_0 \rho_g - \mu (1 - U_0)^v u + \nu U_0 (1 - U_0)^{v-1} u, \\
\lambda w + i c k u &= -\mu w (1 - U_0)^v - 2 \beta w, \\
\lambda \rho_g &= -D_g k^2 \rho_g - 2 \alpha U_0 \rho_g + \mu (1 - U_0)^v u - \nu U_0 (1 - U_0)^{v-1} u. 
\end{align*}
\]

These equations can be further simplified by substituting the expression for the steady state \( \bar{\rho}_g = \mu (1 - U_0)^v / (2 \alpha) \):

\[
\begin{align*}
\lambda u + i c k w &= -D_s k^2 u + 2 \alpha U_0 \rho_g + \mu \nu U_0 (1 - U_0)^{v-1} u, \\
\lambda w + i c k u &= -\mu w (1 - U_0)^v - 2 \beta w, \\
\lambda \rho_g &= -D_g k^2 \rho_g - 2 \alpha U_0 \rho_g - \mu \nu U_0 (1 - U_0)^{v-1} u. 
\end{align*}
\]

Here \( D_s = U_0 / (1 - U_0)^2 \).

Further simplification is possible for the critical eigenvalue \( \lambda_1 \) assuming that \( \lambda = \lambda_1(k) \sim k^2 \). Then we can exclude \( w \) from the second equation, i.e substitute \( w = -i c k u / (\mu (1 - U_0)^v + 2 \beta) \) into the first equation

\[
\begin{align*}
\lambda u + \frac{c^2 k^2 u}{\mu (1 - U_0)^v + 2 \beta} &= -D_s k^2 u + 2 \alpha U_0 \rho_g + \mu \nu U_0 (1 - U_0)^{v-1} u, \\
\lambda \rho_g &= -D_g k^2 \rho_g - 2 \alpha U_0 \rho_g - \mu \nu U_0 (1 - U_0)^{v-1} u. 
\end{align*}
\]
Expanding for small $k$, we obtain

$$\lambda_1 = \frac{1}{2\alpha - \mu v(1 - U_0)v^{-1}} \left( v\mu (1 - U_0)^{v-1} D_s - 2\alpha D_s - \frac{2\alpha c^2}{2\beta + \mu (1 - U_0)v} \right) k^2 + O(k^4).$$

References

[1] Krause J and Ruxton G 2002 *Living in Groups* (Oxford: Oxford University Press)
[2] Stevens A 2000 *SIAM J. Appl. Math.* 172–82
[3] Ginelli F, Peruani F, Bär M and Chaté H 2010 *Phys. Rev. Lett.* **104** 184502
[4] Wu Y, Jiang Y, Kaiser D and Alber M 2007 *PLoS Comput. Biol.* **3** e253
[5] Schaller V, Weber C, Semmrich C, Frey E and Bausch A 2010 *Nature Mater.* **10** 462–8
[6] Sokolov A, Aranson I S, Kessler J O and Goldstein R E 2007 *Phys. Rev. Lett.* **98** 158102
[7] Aranson I S, Sokolov A, Kessler J O and Goldstein R E 2007 *Phys. Rev. E* **75** 040901
[8] Drescher K, Dunkel J, Cisneros L H, Ganguly S and Goldstein R E 2011 *Proc. Natl Acad. Sci. USA* **108** 10940–5
[9] Saintillan D and Shelley M J 2008 *Phys. Rev. Lett.* **100** 178103
[10] Hernandez-Ortiz J P, Stoltz C G and Graham M D 2005 *Phys. Rev. Lett.* **95** 204501
[11] Deseigne J, Dauchot O and Chaté H 2010 *Phys. Rev. Lett.* **105** 98001
[12] Kaiser D 2004 *Annu. Rev. Microbiol.* **58** 75–98
[13] Kaiser D and Welch R 2004 *J. Bacteriol.* **186** 919–27
[14] Dworkin M 2007 *Microbe* **2** 18–24
[15] Harvey C W, Du H, Xu Z, Kaiser D, Aranson I S and Alber M 2012 *PLoS Comput. Biol.* **8** e1002850
[16] Ben-Jacob E, Cohen I and Levine H 2000 *Adv. Phys.* **49** 395–554
[17] Saintillan D and Shelley M J 2008 *Phys. Rev. Lett.* **100** 178103
[18] Edelstein-Keshet L and Ermentrout G 1990 *J. Math. Biol.* **29** 33–58
[19] Mogilner A, Edelstein-Keshet L and Ermentrout G 1990 *J. Math. Biol.* **29** 33–58
[20] Mogilner A and Edelstein-Keshet L 1995 *J. Math. Biol.* **33** 619–60
[21] Mogilner A and Edelstein-Keshet L 1996 *Physica D* **89** 346–67
[22] Peruani F and Morelli L 2007 *Phys. Rev. Lett.* **99** 10602
[23] Bertin E, Droz M and Grégoire G 2006 *Phys. Rev. E* **74** 022101
[24] Toner J and Tu Y 1998 *Phys. Rev. E* **58** 4828
[25] Sokolov A and Aranson I S 2012 *Phys. Rev. Lett.* **109** 248109
[26] Wensink H H, Dunkel J, Heidenreich S, Drescher K, Goldstein R E, Löwen H and Yeomans J M 2012 *Proc. Natl Acad. Sci. USA* **109** 14308
[27] Gejji R, Lushnikov P M and Alber M 2012 *Phys. Rev. E* **85** 021903

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