ELSEVIER
Physica A 306 (2002) 262–269
PHYSICA A
www.elsevier.com/locate/physa

Statistical hydrodynamics of ordered suspensions of self-propelled particles: waves, giant number fluctuations and instabilities

R. Aditi Simha, Sriram Ramaswamy*

Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560 012, India

Abstract

General principles of symmetry and conservation are used to construct the hydrodynamic equations for orientationally ordered suspensions of self-propelled particles (SPPs). Without knowledge of the microscopic origins of the ordering or the mechanisms of self-propulsion, we are able to make a number of striking, testable predictions for the properties of these nonequilibrium phases of matter. These include: novel wavelike excitations in vectorially ordered suspensions; the *absolute* instability of *nematic* SPP suspensions at long wavelengths; the *convective* instability of low-Reynolds-number vector-ordered suspensions; and giant number fluctuations in vector-ordered SPP suspensions. © 2002 Published by Elsevier Science B.V.

PACS: 87.10.+e

1. Introduction and results

1.1. Motivation

Groups of living organisms are frequently found to move coherently in a single direction [1,2]. Such examples of spontaneously broken rotation-invariance (and possibly translation-invariance [1]) in driven systems are important territory for the statistical mechanician to explore. The relevant "living" aspect of these organisms, for the

* Corresponding author.
E-mail addresses: aditi@physics.iisc.ernet.in (R.A. Simha), sriram@physics.iisc.ernet.in (S. Ramaswamy).
URL: http://physics.iisc.ernet.in/~sriram

0378-4371/02/$ - see front matter © 2002 Published by Elsevier Science B.V.
PII: S0378-4371(02)00503-4

purposes of this work, is not that they reproduce or have DNA, but that they metabolise, generating the energy to move without the action of an external force. They are thus *self-propelled particles* (hereafter SPPs). While SPPs are most naturally thought of as moving in a given direction, i.e., vector-like, Gruler [3] discusses a class of active, energy-dissipating amoeboid cells which are head–tail symmetric or *apolar* and hence have the symmetry of a nematic director. We shall call both types of particles SPPs, since both display internally generated motion. Similarly, two types of macroscopic uniaxial orientational order are possible in SPPs, namely, (i) a moving state, in which the order parameter is a *vector*, and (ii) a purely *nematic* state, with head–tail symmetry and hence no net motion. The ordered states formed by polar and apolar particles would be predisposed [1] to be vectorial and nematic "living liquid crystalline" [4] states, respectively. Many SPPs function [5–7] in a fluid medium, in which the hydrodynamic interaction between the particles plays an essential role; most studies of ordering phenomena in SPPs [1] have, however, ignored this interaction. We concentrate here on such SPP *suspensions*, rather than on SPPs on a substrate, to which the analysis of [1] should apply unaltered. Our interest here is in uncovering the essential *qualitative* ways in which such ordered, nonequilibrium suspensions differ from their *thermal equilibrium* analogues. Accordingly, this work (see also [8]) uses general arguments based on symmetries and conservation laws to construct the hydrodynamic equations of motion for ordered phases of collections of self-propelled particles suspended in a fluid medium. Our detailed analysis is for uniaxial orientational order, i.e., for vector- and nematic-ordered SPP suspensions, but the method generalises simply to other types of ordered states. The predictions we make can be tested in careful studies of video images of ordered phases of coherently swimming fish or bacteria (depending on the Reynolds-number range of interest), Stokesian or Lattice Boltzmann computer simulations, or perhaps experiments on suspensions of artificial SPPs.

1.2. Results

Our main results, obtained by linearising our equations of motion about a perfectly ordered state with no externally imposed orienting or flow fields, are as follows: SPP *suspensions* with *purely nematic* order, i.e., orientationally ordered but with no mean motion in any direction, are *always* linearly unstable to a coupled long-wavelength modulation of the axis of orientation and the hydrodynamic velocity field, with wavevector $\mathbf{q}$ oriented near 45° to the nematic axis. This instability is not *inevitable* in *vectorially ordered* suspensions; i.e., parameter ranges of nonzero extent can always be found such that it is averted. Vector-ordered SPP suspensions display novel propagating modes as a result of the coupling of hydrodynamic flow with distortions in the ordering axis and the concentration. Defining θ to be the angle between the wavevector and the

[1] One could in principle imagine purely nematic phases made of paired-up, oppositely directed polar particles, or vector phases made of V-shaped pairings of apolar particles.

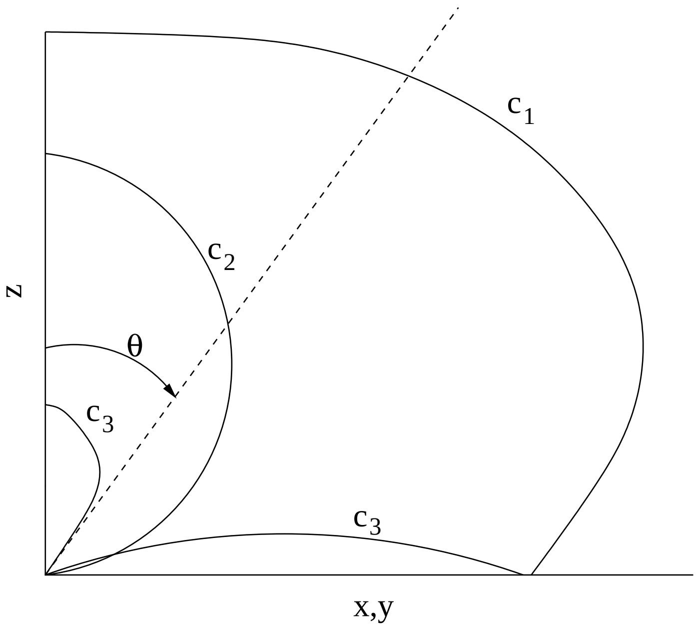

Fig. 1. The three speeds $c_{1,2,3}$ of the splay-concentration waves for wavevectors oriented at an angle θ to the z-axis are given by the radial distances of the curves from the origin (a schematic sketch).

ordering direction, we find: (i) a pair of bend-twist waves with waves peeds

$$c_{bt}(\theta) = (v_1 \pm v_2)\cos\theta\,, \tag{1}$$

where v_1 and v_2 are phenomenological constants of order the SPP drift speed v_0, and (ii) three splay-concentration waves whose speeds c_i for $i = 1$ to 3 are more simply understood from Fig. 1 than from an equation. The above wavespeeds are of course calculated at lowest order in wavenumber, neglecting viscous damping which arises at the next order. This is acceptable for schools of small fish, i.e., small enough to keep the Reynolds number from reaching the turbulent range and yet large enough that viscosity does not dominate totally. Experiments on *bacterial* suspensions are, however, likely to be in the *Stokesian* limit $Re \ll qa \ll 1$, where $Re = v_0 a/\nu$ is the Reynolds number of an SPP of size a in a fluid with kinematic viscosity ν. In that regime we find, remarkably, that a vector-ordered suspension *always* suffers an instability related to that mentioned above for nematic suspensions. In the vector case, however, the instability is *convective*: the mode propagates, with a speed $\sim v_0$, as it grows. For θ near $\pi/4$ its frequency

$$\omega \sim -iB\cos 2\theta \pm \text{ const.} \times q\,, \tag{2}$$

implying an instability just above or just below $\theta = \pi/4$, depending on the sign of the phenomenological constant $B \sim v_0^2/\nu$. Lastly, we predict that the relative variance $(\langle N^2\rangle - \langle N\rangle^2)/\langle N\rangle$ should diverge as $N^{2/3}$ as the number of particles $N \to \infty$, in vector-ordered SPP suspensions, whereas the same quantity in thermal equilibrium liquid crystalline phases would approach a finite constant.

Some of the above findings are generalisations of behaviours already predicted [1] for SPPs on a substrate, i.e., ignoring hydrodynamic fluid flow. The bend-twist waves and the instabilities are, however, unique to SPP *suspensions* and are should therefore be of particular interest to experimenters. Our results are robust because they arise not from microscopic modelling of a particular class of SPPs but from coarse-grained equations of motions which should be obeyed by any SPP mesophase with a given type of order. Let us now show briefly how these equations arise.

2. The model

2.1. Constructing the equations of motion

Our aim in this section is to construct equations of motion which are to SPP mesophases what the equations of, say, [9,10] are to thermal equilibrium liquid crystals. The general principles governing their construction are a natural, nonequilibrium generalisation of those stated in Ref. [11]: (i) Use only those variables ("conserved" and "broken-symmetry" [11]) which relax or oscillate at a rate which vanishes as the wavenumber goes to zero; these are the "slow modes" or "hydrodynamic variables" of the problem and provide a complete description of the dynamics of the system at asymptotically large length- and time-scales. (ii) Rule out from the equations of motion only those terms *explicitly forbidden* by symmetry or conservation laws. (iii) Work to leading orders in a gradient expansion. That's all. Since our systems are in nonequilibrium steady states, we may not demand that forces arise from a free-energy functional, nor may we relate the various phenomenological coefficients to each other or to the strengths of noise sources in our model, except perhaps on grounds of purely *geometrical* symmetry.

The slow modes [2] are, therefore, the fluctuations $\delta c(\mathbf{r}, t)$ in the local concentration $c(\mathbf{r}, t)$ of SPPs about its mean c_0, the total momentum density $\mathbf{g}(\mathbf{r},\mathrm{t})$ of solute plus solvent, and the broken-symmetry modes which we describe below. We treat the mass density ρ of the suspension as constant since the SPPs swim exceedingly slowly. The hydrodynamic velocity field $\mathbf{u} \equiv \mathbf{g}/\rho$ therefore satisfies $\nabla \cdot \mathbf{u} = 0$.

We consider two kinds of uniaxial order, along the $\hat{\mathbf{z}}$ direction: *nematic*, invariant under $\hat{\mathbf{z}} \to -\hat{\mathbf{z}}$, and *vectorial*, where $\hat{\mathbf{z}}$ and $-\hat{\mathbf{z}}$ are inequivalent. The transverse xy directions are labelled $\perp$. The nematic order parameter [9,10] is a traceless symmetric 2nd-rank tensor $\mathbf{Q}(\mathbf{r}, t)$ [$= Q_0\,\mathrm{diag}(-1, -1, 2)$ on average when diagonalised in the ordered phase], and the vector order parameter is simply the drift velocity vector $\mathbf{v}(\mathbf{r}, \mathbf{t})$ [$= (0, 0, v_0)$ on average in the ordered phase] of the SPPs *relative to the fluid*. The broken-symmetry modes in both these phases are the deviations $\delta\mathbf{n}_\perp$ of a

[2] Ignoring the energy density as well as any nutrient fields, and working on timescales on which birth and death of SPPs can be neglected.

unit vector field $\hat{\mathbf{n}}$ (the local axis of orientation) with mean value $(0,0,1)$. The order parameters are related to $\delta\mathbf{n}_\perp$ by $Q_{\perp z} = Q_{z\perp} = Q_0\delta\mathbf{n}_\perp$; $\mathbf{v}_\perp = v_0\delta\mathbf{n}_\perp$.

Having assembled the hydrodynamic variables, we now construct the equations of motion, *linearized* about a perfectly ordered state, to *lowest* order in a gradient expansion. This won't tell us the damping rates of the propagating modes, but it will give us their *speeds*, which are of primary interest to us here. We shall discuss the role of viscosities and diffusivities later. It is most convenient to discuss the case of a vector-ordered phase of SPPs first, and then take up the nematic as a limiting case. We present the equations without deriving them, and then explain the physical origin of the terms therein. To leading order in gradients, the broken-symmetry field $\delta\mathbf{n}_\perp$ obeys

$$(\partial_t + \lambda_1 v_0 \partial_z)\delta\mathbf{n}_\perp = \tfrac{1}{2}(\gamma_2 + 1)\partial_z \mathbf{u}_\perp + \tfrac{1}{2}(\gamma_2 - 1)\nabla_\perp u_z - \sigma_1 \nabla_\perp \delta c + O(\nabla\nabla) + \text{ nonlin. terms}\,. \tag{3}$$

The lack of $z \to -z$ symmetry is apparent in the advection term on the left-hand side of (3), as well as in the σ term, which is a nonequilibrium "osmotic pressure", arising since $\delta\mathbf{n}_\perp$ is a velocity. The "flow-alignment" [9,10] terms involving the phenomenological parameters $\gamma_2 \pm 1$ are standard in nematic hydrodynamics, and play a central role in our story.

The suspension as a whole (SPP + fluid) is subject to no external forces. Thus, the generalised Navier–Stokes equation for an SPP suspension follows from the condition of momentum conservation $\partial_t g_i = -\nabla_j \sigma_{ij}$, and the stress tensor σ_{ij} contains, apart from the terms already present in any fluid, a shear stress $\sigma_{ij}^{(p)} \propto c_0[n_i n_j - (1/3)\delta_{ij}]$. This term, which is unique to self-propelling systems, is not forbidden by any symmetry, but is nonetheless ruled out in *thermal equilibrium* nematics because it cannot be obtained via Poisson brackets [12] from a free-energy functional. The usual [9,10] nematic elastic torques, which do follow from such a functional, are of higher order in gradients than $\sigma_{ij}^{(p)}$ and therefore do not feature in our analysis. The form of $\sigma_{ij}^{(p)}$ can also be obtained [8,13] by considering the force density associated with a single SPP. Incorporating σ_{ij}^{p} in the momentum equation, and imposing incompressibility, we see after some straightforward algebra that the hydrodynamic velocity field $\mathbf{u}_\mathbf{q}$ at wavevector $\mathbf{q}$ obeys

$$\frac{\partial \mathbf{u}_\perp}{\partial t} = -iw_0\left(\mathbf{I} - 2\,\frac{\mathbf{q}_\perp\mathbf{q}_\perp}{q^2}\right)\cdot\delta\mathbf{n}_\perp - i\,\frac{q_z^2}{q^2}\,\alpha(\mathbf{q}_\perp\delta c)\,, \tag{4}$$

where $\mathbf{I}$ is the unit tensor, and several phenomenological parameters have been introduced. The anisotropic "pressure" (α) term and and the force density proportional to the curvature $q_z\delta\mathbf{n}_\perp$ are both fundamentally nonequilibrium effects.

Conservation of the number of SPPs implies

$$(\partial_t + iv_0 q_z)\;\delta c + ic_0 v_0 \mathbf{q}_\perp\cdot\delta\mathbf{n}_\perp = 0\,; \tag{5}$$

the concentration changes by advection by the mean drift v_0 or by a divergence in the local SPP velocity. Coupling to the hydrodynamic velocity field does not enter here in a linearised description, since $\mathbf{u}$ is divergence-free.

2.2. Mode structure: waves and instabilities

With equations in hand, we can now study the dynamic mode structure, that is, the dispersion relation between frequency ω and wavevector $\mathbf{q}$, with particular attention to those features which distinguish it qualitatively from that which obtains [1] if fluid flow is ignored. The analysis is straightforward, and we describe it only briefly.

Bend and twist ($\nabla \times \mathbf{n}_\perp$) of the axis of orientation couple to vorticity ($\nabla \times \mathbf{u}_\perp$) in the fluid flow, as can be seen by taking the curl of (3) and (4). This results in propagating *bend-twist waves* with speeds given by Eq. (1). Without hydrodynamic flow, these degrees of freedom would relax in a purely diffusive manner. [3]

If instead we take the *divergence* of (3) and (4) we see that splay ($\nabla \cdot \mathbf{n}_\perp$), in-plane expansion ($\nabla \cdot \mathbf{u}_\perp$) and concentration fluctuations δc combine to yield three wavelike eigenmodes whose speeds as a function of direction are illustrated schematically in Fig. 1. In the simplifying limit $\sigma_1 = \alpha = 0$, they can be seen as the coupled dynamics of splay and in-plane expansion, accompanied by simple advection of the concentration by the mean drift.

Having discussed the propagating modes, let us turn next to the instabilities we mentioned in Section 1.2. The equations of motion for an SPP *nematic* suspension follow from (3)–(5) upon setting $v_0 = \sigma_1 = \alpha = 0$, i.e., restoring $z \to -z$ invariance. A little algebra then shows that the squares of the splay-concentration wavespeeds vanish for $\theta = \pi/4$, which means the speeds themselves are *imaginary* (signalling an instability) either just above or just below 45°, depending on the sign of some phenomenological parameters. Physically, this is because the $z \to -z$ symmetry means that a distortion with wavevector at exactly 45° does not know which way to go, so the $O(q^2)$ contribution to the squared frequency $\omega^2(\mathbf{q})$ vanishes at this angle. [4]

Beyond leading order in q, we must include viscous damping $\sim \nu q^2 \mathbf{u}$ in the momentum equation, director relaxation $D_n q^2 \delta \mathbf{n}_\perp$ in the equation for $\delta \mathbf{n}$, and particle diffusion $Dq^2 \delta c$ in the concentration equation, where ν is the kinematic viscosity of the suspension, and D_n and D are diffusivities for the director and the concentration respectively. For SPPs whose size a is more than a few μm, thermal Brownian motion should be negligible. D and D_n should then be dominantly of hydrodynamic origin: $D \sim D_n \sim v_0 a$, where v_0 is a typical speed of an SPP. We thus see that the real parts of the wave frequencies $\sim v_0 q \gg Dq^2 \sim D_n q^2$ for all q upto $1/a$, whereas viscous damping $\nu q^2 \gg v_0 q$ for $q \gg v_0/\nu$, i.e., for particle-scale Reynolds number $\mathrm{Re} \equiv v_0 a/\nu$, $\ll qa \ll 1$. While this regime is nonexistent for large, fast SPPs like fish, it is precisely the range of interest for experiments on bacteria [14,7,5]. For such low Reynolds number [15] we can take the velocity field $\mathbf{u}$, out to length scales $\sim a/\mathrm{Re}$, to be determined instantaneously by a balance between viscous and other (e.g., self-propulsive) stresses, i.e., we can replace the left-hand side of (4) by $\nu q^2 \mathbf{u}$. Eliminating $\mathbf{u}$ from (3) and

[3] This is strictly true only in a linearised description. When nonlinearities are included, as in Ref. [1], the mode would remain non-propagating, but with a dynamic exponent that can differ from 2.

[4] The conventional nematic-elastic torques, which enter at next order in q, will mitigate the instability beyond a crossover wavenumber q_*, which means that systems of size $L < q_*^{-1}$, will not show the instability [8,13].

(5) via (4) yields effective equations of motion for $\delta\mathbf{n}_\perp$ and δc. The coupled dynamics of splay and δc in this case leads to the unstable mode with growth rate as in Eq. (2). The constant B in (2) is independent of the *magnitude* of $\mathbf{q}$ as a result of the long-ranged Stokesian hydrodynamic interaction.

2.3. Number fluctuations

We turn next to the giant number fluctuations advertised at the start of this article. SPP suspensions fluctuate for three reasons: thermal Brownian motion (negligible for particles larger than a few microns), the chaos of moving, hydrodynamically interacting particles, and intrinsic fluctuations in the self-propelling activity of individual SPPs. We thus include (Gaussian) noise sources $\mathbf{f}_u$, f_c, and $\mathbf{f}_n$, delta-correlated in time, in the equations of motion for $\mathbf{u}$, c, and $\mathbf{n}$. For wavenumber $q \to 0$, the variances for $\mathbf{f}_u$ and f_c are $O(q^2)$ as a result of momentum and number conservation, while that for $\mathbf{f}_n$ is nonvanishing. With the noise and damping terms in place we can calculate the steady-state correlation functions of the various fields. Unsurprisingly for a broken symmetry field, we find that the variance of director fluctuations $\langle|\delta\mathbf{n}_\mathbf{q}|^2\rangle$ at wavenumber q grows as q^{-2} at small q. Remarkably, the variance $\langle|\delta c_\mathbf{q}|^2\rangle \sim q^{-2}$ as well. This means that the variance of the number N of particles, scaled by the mean, grows as $N^{2/3}$ in three dimensions, whereas it would be a constant in any thermal equilibrium system away from a critical point. This is a direct consequence of the nonequilibrium nature of SPP systems: a curvature in the director field produces a proportionate mass flow. The large director fluctuations lead immediately to giant number fluctuations. This effect was already predicted in the analysis of [1], which does not include the effects of hydrodynamic flow. It is reassuring to note that it survives when such flow is included.

3. Experiments and future prospects

All the effects we have predicted are testable in laboratory experiments. The wavespeeds are expected to be of order the drift speed of an SPP (from microns to centimetres per second, from bacteria to fish), and can thus be measured easily. The growth rate of the convectively unstable mode in Stokesian vector-ordered SPP suspensions, say for bacteria (where velocities are ~ 10 μm/s, size $a \sim$ μm), should be about 0.1 s^{-1} if the viscosity is taken to be that of water. Although this is slow, careful experiments performed on a timescale of tens of minutes should see it. We urge experimenters to carry out such tests of our predictions.

Our current [8,13] and future research on these exciting systems will focus on: the complete nonlinear equations of motion of with noise, to look for singular renormalisations of the speeds and dampings of the modes, and of the scaling of number fluctuations; the interaction of SPPs with imposed flow fields; the nature of phase transitions to the isotropic and other phases; the behaviour of topological defects in these systems; the behaviour of *isotropic* SPP suspensions, to understand the observations of Ref. [6]; and SPP nematics on a substrate [16].

Acknowledgements

SR thanks the Aspen Center for Physics for support while part of this work was done.

References

[1] J. Toner, Y. Tu, Phys. Rev. E 58 (1998) 4828 and references cited therein.
[2] T. Vicsek, Phys. Rev. Lett. 75 (1995) 1226;
A. Czirok, H.E. Stanley, T. Vicsek, J. Phys. A 30 (1997) 1375.
[3] H. Gruler, U. Dewald, M. Eberhardt, Eur. Phys. J. B 11 (1999) 187;
R. Kemkemer, D. Kling, D. Kaufmann, H. Gruler, Eur. Phys. J. E 1 (2000) 215.
[4] H. Gruler, M. Schienbein, K. Franke, A. deBoisfleury-Chevance, Mol. Cryst. Liq. Cryst. 260 (1995) 565–574 (appear to have been the first to use this term).
[5] T.J. Pedley, J.O. Kessler, Annu. Rev. Fluid Mech. 24 (1992) 313 (discusses aspects of the hydrodynamics of swimming microorganisms).
[6] X.-L. Wu, A. Libchaber, Phys. Rev. Lett. 84 (2000) 3017 (studies the dynamics of a disordered bacterial suspension in a fluid film).
[7] H.C. Berg, Phys. Today 53 (2000) 24.
[8] R.A. Simha, S. Ramaswamy, cond-mat/0108301, Phys. Rev. Lett. (2001), submitted for publication.
[9] P.G. de Gennes, J. Prost, The Physics of Liquid Crystals, Clarendon Press, Oxford, 1995.
[10] S. Chandrasekhar, Liquid Crystals, Cambridge University Press, Cambridge, 1992.
[11] P.C. Martin, O. Parodi, P.S. Pershan, Phys. Rev. A 6 (1972) 2401.
[12] I.E. Dzyaloshinskii, G.E. Volovik, Ann. Phys. (NY) 125 (1980) 67.
[13] R.A. Simha, S. Ramaswamy, in preparation.
[14] E.M. Purcell, Proc. Natl. Acad. Sci. USA 94 (1997) 11307.
[15] J. Happel, H. Brenner, Low Reynolds Number Hydrodynamics, Martinus Nijhoff, Dordrecht, 1986.
[16] S. Ramaswamy, R.A. Simha, J. Toner, in preparation.