Generalized hydrodynamics of active polar suspensions

Dibyendu Mandal,1 Katherine Klymko,2 and Kranti K. Mandadapu3,4

1Department of Physics, University of California, Berkeley, CA 94720, U.S.A.
2Department of Chemistry, University of California, Berkeley, CA 94720, U.S.A.
3Department of Chemical and Biomolecular Engineering, University of California, Berkeley, CA 94720, U.S.A.
4Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, U.S.A.

(Dated: March 5, 2018)

We utilize a generalized Irving-Kirkwood procedure to derive the hydrodynamic equations of an active matter suspension with internal structure and driven by internal torque. The internal structure and torque of the active Brownian particles give rise to a balance law for internal angular momentum density, making the hydrodynamic description a polar theory of continuum mechanics. We derive exact microscopic expressions for the stress tensor, couple stress tensor, internal energy density, and heat flux vector. Unlike passive matter, the symmetry of the stress tensor is broken explicitly due to active internal torque and the antisymmetric component drives the internal angular momentum density. These results provide a molecular basis to understand the transport characteristics and collectively provide a strategy to develop the theory of linear irreversible thermodynamics of active matter.

Systems composed of self-activating units are called active matter [1,6,7]. Active matter systems exhibit interesting emergent behavior such as enhanced tracer diffusion, giant number fluctuations, motility induced phase separation (MIPS), spontaneous emergence of rectification, collective motion, odd viscosity, and topological localization. Active matter systems are abundant in the biological domain, ranging from the cytoplasmic fluid and bacterial colonies to flocks of birds and herds of animals. On the technological side, they provide a viable candidate for the development of colloidal programmable matter.

Active matter systems offer an opportunity to revisit the notions of statistical mechanics and condensed matter physics from a fresh nonequilibrium perspective. The concept of pressure has recently received particular emphasis. For example, (osmotic) pressure of active matter physics from a fresh nonequilibrium perspective. The original Irving-Kirkwood procedure was developed for passive, point particles, without any internal rotational degree of freedom. Our work can be considered to be a generalization of the procedure to structured (polar) fluids. Furthermore, we have discovered the existence of asymmetric stress tensor for ADPs, which is absent in passive and even self-propelled active Brownian suspensions (such as ABP suspensions). We have also suggested a potential experimental realization of our results.

An ADP colloidal “molecule” $i$ is composed of two “atoms” $(i,1)$ and $(i,2)$, as shown in Fig. 1(a). The mass, position, and momentum of the atom $(i,\alpha)$ are denoted by $m_i^\alpha$, $x_i^\alpha$, and $p_i^\alpha$, respectively. The interaction force on $(i,\alpha)$ from $(j,\beta)$ is denoted by $F_{ij}^{\alpha\beta} = -\partial u_{ij}(x_i^\alpha, x_j^\beta)/\partial x_i^\alpha$ for some two-body potential energy $u_{ij}(x_i^\alpha, x_j^\beta)$ [88]. We assume $u_{ij}(x_i^\alpha, x_j^\beta) = u_{ij}(|x_i^\alpha - x_j^\beta|)$. The ADPs are assumed to be suspended in a stationary solution. Due to their asymmetric interactions with the surrounding fluid, the ADPs are subjected to an internal torque as shown...
in Fig. 1(a) with the active forces $f_1 = -f_2$. We assume that the active forces are always perpendicular to the line joining the two atoms of an ADP molecule [89]. A possible realization of ADPs involves the setup of Ref. [40] where a colloidal sphere has a protruding hematite cube that can catalyze the decomposition of hydrogen peroxide in the presence of blue light. An ADP can be created by tethering together two colloidal spheres with their hematite protrusions in opposite directions, as shown in Fig. 1(b). Because the ADPs are inside a solution, they feel the thermal Langevin forces as well, a drag force $-\zeta p_\alpha^i / m_\alpha^i$, for drag coefficient $\zeta$, and a Gaussian white noise force, $\sqrt{2k_B T} \xi^\alpha_i$, with $\langle \xi^\alpha_i \rangle = 0$ and $\langle \xi^\alpha_i(t) \xi^\beta_j(t') \rangle = \delta_{ij} \delta_{\alpha\beta} \delta(t-t')$ for Kronecker deltas $\delta_{ij}$ and $\delta_{\alpha\beta}$ and Dirac delta function $\delta(t-t')$. Here $k_B$ is the Boltzmann constant and $T$ is the temperature of the solution. The equations of motion are

$$\dot{x}^\alpha_i = p^\alpha_i / m_\alpha^i, \quad \dot{p}^\alpha_i = \sum_{j} F^\alpha_{ij} + f^\alpha_i + f^\alpha_{i,\text{Th}},$$

(1)

with $f^\alpha_{i,\text{Th}} = -\zeta p^\alpha_i / m_\alpha^i + \sqrt{2k_B T} \xi^\alpha_i$. Here and in what follows, $(\ast) = d(\ast)/dt$ denotes the total time derivative. In the current setup, we have assumed that all the body force comes from the solvent. The situation can be generalized in a straightforward way to include other body forces, such as self-propulsive (convective) forces (as in ABPs [15]) and gravity.

A key element in our discussions is a coarse-graining function $\Delta(x - x^0) \equiv \Delta^\alpha$, which is a unimodal function concentrated about $x^0_\alpha$, and whose effect is to replace the particle $(i, \alpha)$ by a smeared density distribution with equal total mass [90]. This helps us make a transition from the microscopic particulate picture to a continuous hydrodynamic picture, as illustrated in Fig. 2. This is different from considering an average over several repetitions of the dynamics with different initial conditions and noise realizations. Fluctuations from the initial conditions and noise realizations are still present in our picture, albeit in a smeared and less pronounced manner [91]. In the following, we do not consider any specific form for $\Delta^\alpha$, other than the following property, $\partial \Delta^\alpha / \partial x^\alpha_i = -\partial \Delta^\alpha / \partial x^\alpha_j$, which implies $\Delta^\alpha$ is a function of just the difference $x - x^0$ [92]. Based on the coarse graining function $\Delta^\alpha$, we can introduce local densities for mass ($\rho$), momentum ($\rho v$), angular momentum ($\rho \mathbf{L}$), and energy ($\rho e$):

$$\rho\{1, v, L, e\} = \sum_i \{m_\alpha^i, p^\alpha_i, x^\alpha_i \times p^\alpha_i, e^\alpha_i\} \Delta^\alpha_i$$

(2)

with energy per particle $e^\alpha_i = (1/2) \sum_{\beta} [m^\beta_i (v^\beta_i)^2 + \sum_{j} u_2(x^\beta_j, x^\beta_i)]$ [93].

We now use the expressions in Eq. (2) to derive the balance equations for local densities. We assume that the point of observation is moving with the barycentric velocity $v(x, t)$, introduced in Eq. (2) (Lagrangian point of view). This is equivalent to assuming that $\mathbf{x}$ itself is a function of time with $\dot{\mathbf{x}} = v(\mathbf{x}(t), t)$ . The method to derive balance laws involves (i) differentiation of the densities defined in Eq. (2) with respect to time; (ii) usage of the equations of motion (Eq. (1)), the property $\partial \Delta^\alpha_i / \partial x^\alpha_j = -\partial \Delta^\alpha_i / \partial x^\alpha_j$, and $\dot{x} = v(\mathbf{x}(t), t)$; and (iii) utilization of tensor identities to express the resulting equations in forms considered in continuum mechanics [96, 65, 79], i.e., in terms of surface (divergence) and volumetric terms. The details are presented in [94].

For mass balance, we get the usual continuity equation, $\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0$. The linear momentum balance can be derived to be of the form

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \rho \mathbf{b},$$

(3)

where $\mathbf{T}$ is the stress tensor and $\mathbf{b}$ is the body force per unit mass. A pictorial definition of $\mathbf{T}$ based on continuum mechanics perspective is given in Fig. 2(a). Pressure is given by $p = -\text{Tr} (\mathbf{T})$. This mechanical notion of pressure is well defined in all fluids, equilibrium or not. For fluids in thermodynamic equilibrium, the me-
the forces and moments by infinitesimal moment $\Delta m$ and normal vector $n$. For any infinitesimal surface element with area $\Delta s$ and normal vector $n$, an infinitesimal force $\Delta f$ and an infinitesimal moment $\Delta m$ can be applied. Then, the stress tensor $T$ and the couple stress tensor $C$ are related to the forces and moments by $\lim_{\Delta s \to 0} \Delta f/\Delta s = T \cdot n$ and $\lim_{\Delta s \to 0} \Delta m/\Delta s = C \cdot n$, respectively [68]. Here, the dot product between a tensor and vector is equivalent to matrix multiplication. (b) An ADP can rotate about an instantaneous axis because of its internal structure and torque. This internal spin leads to an internal angular momentum.

Mechanical pressure coincides with the statistical mechanical definition of pressure derived from the partition function formalism [95, 96]. Exact microscopic expressions derived for $T$ and $b$ are given in Table I (second column), where we see that stress tensor $T$ is composed of three components – kinetic $T^K$, potential $T^P$, and active $T^A$ [97]. The kinetic part of the stress tensor $T^K$ includes contributions from the fluctuations of the velocity of particles with respect to the barycentric velocity $v$ [68]. The potential part $T^P$ contains contributions from the interactions between the particles from both intermolecular and harmonic spring interactions. The $T^K$ and $T^P$ parts of the stress tensor are common to any fluids as was originally derived by Irving and Kirkwood. However, as can be seen in Table I there exists a new contribution $T^A$ to the stress tensor that comes from the active forces on the dumbbell. This contribution is specific to active matter and differentiates the system from passive matter. In $T^P$ and $T^A$, we needed to introduce the Noll bond function $b_{ij}^a = \int_0^1 d\lambda \Delta(x - \lambda x_i + x_j^a)$ with $x_j^a = x_j^\alpha - x_j^{\alpha\beta} [76, 77, 79]$. While $T^K$ and $T^P$ are symmetric tensors, $T^A$ is not. This asymmetry in the stress tensor arises due to the active couples from the active forces $f_i^\alpha$, which break the microscopic rotational symmetry at the level of particle dynamics [99]. The existence of asymmetric stress tensor in ADP suspensions is one of the central findings of this Letter. This asymmetry is absent in passive and active self-propelled (convective) suspensions [100].

The balance equation for angular momentum can be derived to be of the form

$$\rho \ddot{L} = \nabla \cdot C + \rho G + A + x \times \rho b + x \times (\nabla \cdot T),$$

(4)

where $C$ is the total couple stress tensor, $G$ is the body couple per unit mass, and $A$ is the antisymmetric component of the stress tensor, $A_i = \epsilon_{ijk} T_{jk}$, where $\epsilon_{ijk}$ is the Levi-Civita symbol. A geometric definition of $C$, from a purely continuum mechanics point of view, is illustrated in Fig. 3(a). Exact microscopic expressions for $C$ and $G$ are given in Table I (third column). As with the stress tensor $T$, the couple stress tensor $C$ is composed of three components – kinetic $C^K$, potential $C^P$, and active $C^A$ – with similar origins [101]. As can be seen from the expressions in Table I all the components of $C$ are given by the moments of the forces acting on the atoms with respect to the center $x$ of the coarse-graining volume. These terms are analogous to the terms in the stress tensor $T$, with moments replacing the forces. The microscopic derivation of the balance of angular momentum was not considered by Irving and Kirkwood. Our work can be seen as a generalization of their work to structured particles with internal torques. The couple stress tensor $C$ for passive matter is often negligible because the relaxation time of the couple stresses is generally small compared to the observation timescale [66]. Therefore, the change of angular momentum is ignored leading to the conclusion that the stress tensor is symmetric [102]. In the case of ADPs, $C^A$ results from the internal torque and is not negligible. In this case the angular momentum effects cannot be ignored, the stress tensor is not symmetric, and there is a possibility for coupled linear and angular momentum phenomena [34, 72]. The body couple $G$ comes from the moments of body forces $f_i^\alpha, T^\alpha$ and $f_i^\alpha$ with respect to $x$. It is interesting to see that the torque from the active forces $f_i^\alpha$ contributes to both the surface term $C$ and the body term $G$. The last two terms on the right of Eq. (4) denote the moments induced by the body forces and the surface forces with respect to the origin in the laboratory frame [103].

The ADPs can have internal rotations or spin because of their internal structure and torque as illustrated in Fig. 3(b) [104]. Because of internal rotations, we can define the quantities internal angular momentum density $\rho M(x, t)$, moment of inertia density $I(x, t)$, and local angular velocity $\omega(x, t)$

$$\rho \ddot{M} = \rho L - \rho x \times v, \quad I = \sum_{i_a} T^i_{i_a} \Delta_{i_a}^i, \quad I \omega = \rho M$$

(5)

where $\rho x \times v$ is the moment of momentum of the continuum point $x$, $I^i_{i_a} = m_i^\alpha (\dot{x}_i^\alpha - x_i^\alpha)^2 I - m_i^\alpha (\dot{x}_i^\alpha - x_i^\alpha) \otimes (\dot{x}_i^\alpha - x_i^\alpha)$, and $I$ is the identity matrix. Note that the local angular velocity in Eq. (3) depends on the coordinate system because of the definition of moment of inertia. Therefore, all the results that include $\omega$ should be interpreted accordingly. The balance equation for the internal angular momentum can be derived to be [61, 62, 78]

$$\dot{\rho} M = \nabla \cdot C + \rho G + A,$$

(6)

which states that the internal angular momentum density is driven by the local surface and volume couples, and the antisymmetric portion of the stress tensor. This
is Cauchy’s second law of motion, a generalization of Euler’s equation for rigid body rotation to deformable bodies [88]. The relevance of internal angular momentum density for material properties was first pointed out by Cosserats and then revived by H. Grad, and Dahler and Schriven, among others [61, 88]. Our work shows that active suspensions provide a timely illustration of these ideas.

The kinetic energy density of the system at the hydrodynamic level is composed of the translational part $\rho v^2/2$ and the rotational part $(\mathbf{\Omega} \cdot \mathbf{\Omega})/2$. Accordingly, we define the internal energy density $\rho e$ by

$$\rho e = \rho c - \frac{1}{2} \rho v^2 - \frac{1}{2} (\mathbf{\Omega} \cdot \mathbf{\Omega})$$

(7a)

$$= \frac{1}{2} \sum_{i \alpha} \left[ m_{i \alpha} (v_{i \alpha} - \bar{v}_{i \alpha})^2 + \sum_{j \beta} u_{ij} (x_{i \beta} - x_{j \beta}) \right] \Delta_{i \alpha}$$

(7b)

$$\equiv \sum_{i \alpha} \epsilon_{i \alpha} \Delta_{i \alpha},$$

(7c)

where $\rho c$ is the total energy density defined in Eq. (2), and $\bar{v}_{i \alpha} = \mathbf{v} + \mathbf{\Omega} \times (x_{i \alpha} - x)$ is the rigid body like convective velocity of any particle $(i, \alpha)$. The internal energy per particle $\epsilon_{i \alpha}$ is therefore composed of inter-particle potential energies and the “thermal” energy of particles coming from the fluctuations in velocity with respect to the locally comoving and corotating frame, $v_{i \alpha} - \bar{v}_{i \alpha}$. Note that in a simple (nonpolar) fluid the thermal energy is defined only with respect to the comoving frame because the internal rotations are absent. To write down the balance equation for both total and internal energy density, we need the balance equation for moment of inertia density, which can be derived to be of the form

$$\dot{I} + \mathbf{I} \cdot (\nabla \cdot \mathbf{v}) = \nabla \cdot \sum_{i \alpha} \mathbf{I}_{i \alpha} \otimes (\mathbf{v} - \bar{v}_{i \alpha}) \Delta_{i \alpha} \equiv \nabla \cdot \mathbf{Y},$$

(8)

where $\mathbf{Y}$ (defined in the second relation) is a third order tensor that corresponds to the flux of moment of inertia. The balance of moment of inertia exists simply due to the exchange of ADPs through the neighborhood of the macroscopic point $x$.

Using Eq. (8) and the definitions of the stress and couple stress tensors as well as the body forces and torques in Table I, the balance equation for total energy can be derived to be

$$\dot{\rho e} = -\nabla \cdot \mathbf{J}_q + \nabla \cdot (\mathbf{T}^T \mathbf{v}) + \nabla \cdot (\mathbf{C}^T \mathbf{\Omega}) + \rho (\mathbf{b} \cdot \mathbf{v} + \mathbf{G} \cdot \mathbf{\Omega})$$

(9)

The second and third terms in Eq. (9) are the rates of work done by the stress and couple stress tensors, respectively. Similarly, the fourth and fifth terms, respectively, are the rates of work done by the body forces and couples. The sixth term (containing $\mathbf{Y}$) is kinematic in nature, arising out of the diffusive transport of moment of inertia. The last term, $\Lambda$ (given in the following), is a source of heat by body forces and appears as a result of the “thermal” fluctuations of the velocities, the thermal forces $\epsilon_{i \alpha} \mathbf{f}_{i \alpha \Omega}$, and the work done by the active torques on the ADP as a whole. The term $\Lambda$ may be understood as an extension of the concept of heat in the stochastic energetics framework to flowing extended systems. We have

$$\Lambda = \sum_{i \alpha} \left[ (v_{i \alpha} - \bar{v}_{i \alpha}) \cdot \mathbf{f}_{i \alpha \Omega} + (\bar{v}_{i \alpha} - \bar{v}_{i \Omega}) \cdot \mathbf{f}_{i \alpha} \right] \Delta_{i \alpha}$$

Finally, the balance equation for internal energy can be derived as

$$\dot{\rho e} = -\nabla \cdot \mathbf{J}_q + \mathbf{T} : \nabla \mathbf{v} + \mathbf{C} : \nabla \mathbf{\Omega} - \mathbf{A} : \mathbf{\Omega}$$

$$-\frac{1}{2} \mathbf{Y} : (\nabla (\mathbf{\Omega} \otimes \mathbf{\Omega})) + \Lambda,$$

(11)

where we have used the notations $(\nabla \mathbf{g})_{ij} = (\partial / \partial x_j) g_{ij}$ for any vector $\mathbf{g}$ and $\mathbf{B} : \mathbf{D} = \sum_{i \beta} B_{i \beta} D_{i \alpha}$ for any two second rank tensors $\mathbf{A}$ and $\mathbf{B}$. It is interesting to note that the antisymmetric portion of the stress tensor $A$
contributes to work done on the system by coupling with local angular velocity $\omega$. Equation (11) can be interpreted as the first law of thermodynamics where the first term on the right denotes heat flow and the rest denotes work. The equations in this Letter can be considered a development towards the stochastic thermodynamics of continuous media for active matter systems.

The authors would like to thank Frédéric van Wijland, Steve Granick, Michael Hagan, David Limmer, Robert Jack, Michael R. DeWeese, and Panayiotis Papadopoulos for useful discussions. KKM acknowledges support from a National Institutes of Health Grant R01-GM110066. He is also supported by Director, Office of Science, Office of Basic Energy Sciences, Chemical Sciences Division, of the U. S. Department of Energy under contract No. DE-AC02-05CH11231. DM acknowledges support from the U.S. Department of Energy under contract No. DE-AC02-05CH1123. DM acknowledges support from the U.S. Army Research Laboratory and the U. S. Army Research Office under contract W911NF-13-1-0390. KK acknowledges support from an NSF Graduate Research Fellowship.

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In the accompanying paper, we have $T^p = T^V + T^S$. The symbol $\otimes$ in these expressions indicates the dyadic product, i.e., the products $a \otimes b$ of any two vectors $a$ and $b$ is a second order tensor with elements $a_i b_j$. Note that, in general, the dyadic product does not yield a symmetric tensor, i.e., $a \otimes b \neq b \otimes a$.

This is not the thermal part of the velocity, which we define after Eq. 1.

In other words, the dynamics of the ADPs is nonHamiltonian in nature.

We assume only pairwise radial interactions.

In the accompanying paper, we have $C^p = C^V + C^S$.

Note that systems modeled by three-body potentials, such as Stillinger-Weber potentials (PhD Thesis, K. K. Mandadapu) can contribute three-body terms to the stress tensor, which break the symmetry. Such terms can affect the balance of angular momentum through the term $A$.

Note that the divergence of a second order tensor is defined as $(\nabla \cdot S)_i = \sum_j (\partial / \partial x_j) S_{ij}$.

This is how our study differs from – it does not consider internal rotation or torque. They have considered self-propulsion only. Also, they have used dissipative particle dynamics, as opposed to the Langevin dynamics considered here.

In the accompanying paper we have $J^p_0 = J^V_0 + J^S_0$.

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