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Fluctuations of rotational and translational degrees of freedom in an interacting active dumbbell system

Leticia F. Cugliandolo [a], Giuseppe Gonnella [b,*], Antonio Suma [c]

[a] Sorbonne Universités, Université Pierre et Marie Curie – Paris VI, Laboratoire de Physique Théorique et Hautes Énergies, 4 Place Jussieu, 75252 Paris Cedex 05, France
[b] Dipartimento di Fisica, Università di Bari and INFN, Sezione di Bari, via Amendola 173, Bari I-70126, Italy
[c] SISSA – Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, Trieste 34136, Italy

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ABSTRACT

We study the dynamical properties of a two-dimensional ensemble of self-propelled dumbbells with only repulsive interactions. After summarizing the behavior of the translational and rotational mean-square displacements in the homogeneous phase that we established in a previous study, we analyze their fluctuations. We study the dependence of the probability distribution functions in terms of the Péclet number, describing the relative role of active forces and thermal fluctuations, and of particle density.

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1. Introduction

Active matter is characterized by the continuous partial conversion of internal energy into work. Some examples, at different scales, are the cytoskeleton, bacterial colonies, algae suspensions, bird flocks and schools of fish. Self-propelled units can also be artificially realized in the laboratory in different ways, for example, by surface treatment of colloidal particles [1,2]. All these systems live, or function, in conditions far from thermodynamic equilibrium and pose challenging questions to non-equilibrium statistical mechanics. Active matter exhibits non-trivial collective properties that have no analog in passive materials such as large scale coherent motion in the absence of any attractive interaction and a phase separation into an aggregate and a gas-like phase. Several review articles are devoted to this rapidly developing field of research [3–13].

The diffusive properties in these systems are of particular interest. A number of experimental and numerical studies addressed how the diffusive properties are affected by self-propulsion and the density of the suspension; some focused on the dynamics of *passive tracers* immersed in the active bath [14], others focused instead on the mean-square displacement of the *active particles* themselves [15–18].

An interesting model of active matter is one in which the active components have the elongated shape of many natural swimmers. A first study of the phase diagram of such a system with active dumbbells molecules [19] appeared in [20,21]. The analysis of effective temperature ideas [22], and the averaged rotational and translational mean-square displacements were presented in [23] and [24], respectively, for a two-dimensional system.

In this paper we recall some of the results in these publications and we extend the analysis to the fluctuations of translational and rotational degrees of freedom. In Section 2 the dumbbell model is very briefly explained. In Section 3 the numerical results for the translational and rotational fluctuations in the interacting active system are presented. A discussion will complete the paper in Section 4.

2. The model

We briefly present the model and the parameters used in the simulations. More details can be found in [23,24]. The

* Corresponding author. Tel.: +39 080 5442435; fax: +39 080 5442470.
E-mail addresses: leticia@lpthe.jussieu.fr (L.F. Cugliandolo), gonnella@ba.infn.it (G. Gonnella), antonio.suma@gmail.com (A. Suma).

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dumbbells are diatomic molecules formed by two spherical colloids, elastically linked together *via* the finite extensible non-linear elastic force

$$\mathbf{F}_{\rm fene} = -\frac{k\mathbf{r}}{1-(r^2/r_0^2)}, \tag{1}$$

with $k > 0$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ the vector linking the centers of the spherical colloids, with diameter $\sigma_{\rm d}$ and mass $m_{\rm d}$. An additional Weeks–Chandler–Anderson potential,

$$V_{\rm wca}(r) = \begin{cases} V_{\rm LJ}(r) - V_{\rm LJ}(r_c) & r < r_c \\ 0 & r > r_c \end{cases}$$

with

$$V_{\rm LJ}(r) = 4\epsilon\left[\left(\frac{\sigma_{\rm d}}{r}\right)^{12} - \left(\frac{\sigma_{\rm d}}{r}\right)^{6}\right], \tag{2}$$

where ε is an energy scale and r_c is the minimum of the Lennard–Jones potential, $r_c = 2^{1/6}\sigma_{\rm d}$, is added to ensure that the colloids in the same molecule do not overlap. The active forces are polar and act along the main molecular axis $\hat{\mathbf{n}}$, are constant in modulus but follow the molecules' rotations, and are the same for the two spheres belonging to the same molecule,

$$\mathbf{F}_{\rm act} = F_{\rm act}\,\hat{\mathbf{n}}. \tag{3}$$

$\mathbf{F}_{\rm act}$ is directed from the ith colloid (tail) to the i + 1th colloid (head). The active forces are applied to all molecules in the sample during all their dynamic evolution. We take the interaction between the spheres in different dumbbells to be purely repulsive.

Putting these ingredients together, the dynamic equations are

$$\begin{aligned} m_{\rm d}\ddot{\mathbf{r}}_i(t) &= -\gamma\dot{\mathbf{r}}_i(t) + \mathbf{F}_{\rm fene}(\mathbf{r}_{i,i+1}) \\ &\quad + \boldsymbol{\eta}_i - \sum_{\substack{j=0\\ j\neq i}}^{2N} \frac{\partial V_{\rm wca}^{ij}}{\partial r_{ij}}\frac{\mathbf{r}_{ij}}{r_{ij}} + \mathbf{F}_{{\rm act}\,i}, \\ m_{\rm d}\ddot{\mathbf{r}}_{i+1}(t) &= -\gamma\dot{\mathbf{r}}_{i+1}(t) - \mathbf{F}_{\rm fene}(\mathbf{r}_{i,i+1}) \\ &\quad + \boldsymbol{\eta}_{i+1} - \sum_{\substack{j=0\\ j\neq i+1}}^{2N} \frac{\partial V_{\rm wca}^{i+1,j}}{\partial r_{i+1,j}}\frac{\mathbf{r}_{i+1,j}}{r_{i+1,j}} + \mathbf{F}_{{\rm act}\,i} \end{aligned} \tag{4}$$

with $i = 1, 3, \dots 2N-1$, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} = |\mathbf{r}_{ij}|$ and $V_{\rm wca}^{ij} \equiv V_{\rm wca}(r_{ij})$ with $V_{\rm wca}$ defined in Eq. (2).

The coupling to the thermal bath at temperature T is modeled in the manner of Langevin, with γ the friction coefficient and η a Gaussian random noise with zero mean, $\langle\eta_{ia}(t)\rangle = 0$, and

$$\langle\eta_{ia}(t)\eta_{jb}(t')\rangle = 2\gamma k_B T\delta_{ij}\delta_{ab}\delta(t-t'), \tag{5}$$

with k_B the Boltzmann constant. a and b label the coordinates in d dimensional space. An effective rotational motion is generated by the random torque due to the white noise acting independently on the two beads.

The surface fraction is

$$\phi = N\,\frac{S_{\rm d}}{S} \tag{6}$$

with $S_{\rm d} = \pi\sigma_{\rm d}^2/2$ the area occupied by an individual dumbbell in $d = 2$, S the total area of the box and N their total number. The spring is supposed to be massless and void of surface. We impose periodic boundary conditions on the two directions.

The Péclet number, Pe, is a dimensionless ratio between the advective transport rate and the diffusive transport rate. For particle flow one defines it as $\mathrm{Pe} = Lv/D$, with L a typical length, v a typical velocity, and D a typical diffusion constant. We choose $L \to \sigma_{\rm d}$, $v \to F_{\rm act}/\gamma$ and $D \to D_{\rm cm}^{\rm pd} = k_BT/(2\gamma)$ of the passive dumbbell to be derived below; then,

$$Pe = \frac{2\sigma_{\rm d}F_{\rm act}}{k_BT}. \tag{7}$$

The active Reynolds number $Re_{\rm act} = m_{\rm d}F_{\rm act}/(\sigma_{\rm d}\gamma^2)$ is defined in analogy with the hydrodynamic Reynolds number.

3. Single dumbbell dynamics

The averaged single dumbbell motion can be derived analytically under the hypothesis that $r \approx \sigma_{\rm d}$. Details on the calculations can be found in [23,24]. Here, we simply summarize the main results. Within this approximation, at absolute times and time-differences that are longer than the inertial time-scale $t_I = m_{\rm d}/\gamma$, not taking into account its periodic character, the angle θ between the dumbbell's main molecular axis and an axis fixed to the laboratory is a Gaussian random variable with mean $\langle\theta\rangle = \theta_0$ that diffuses according to

$$\langle\theta^2\rangle = \theta_0^2 + 2D_Rt \tag{8}$$

with θ_0 the initial angle, t the time-delay, and the angular diffusion constant

$$D_R = \frac{2k_BT}{\gamma\sigma_{\rm d}^2}. \tag{9}$$

Averaging over the initial angles, taken from a flat distribution around $\theta_0 = 0$, yields $\langle\theta\rangle = 0$ and, in the long times limit, $\langle\theta^2\rangle \to 2D_Rt$. In the absence of interactions, the angular displacements, $\Delta\theta$ between two times that are longer than t_I is also Gaussian distributed. If one imposes the periodicity of the angles in the interval $[-\pi, \pi]$ the angular distribution remains flat.

The translational mean-square displacement is ballistic in the limit $t \ll t_I$, and crosses over to a very rich behavior beyond this time-scale,

$$\langle\triangle\mathbf{r}_{\rm cm}^2\rangle(t) = 4D_{\rm cm}^{\rm pd}\,t + \left(\frac{F_{\rm act}}{\gamma}\right)^2\frac{2}{D_R}\left(t - \frac{1-e^{-D_Rt}}{D_R}\right), \tag{10}$$

where

$$D_{\rm cm}^{\rm pd} = \frac{k_BT}{2\gamma} \tag{11}$$

is the diffusion constant in the passive limit, $\mathbf{F}_{\rm act} = 0$, see [23]. This equation presents several time scales and limits. For $t_I \ll t \ll t_a = D_R^{-1}$ one finds

$$\langle\triangle\mathbf{r}_{\rm cm}^2\rangle = 4D_{\rm cm}^{\rm pd}\,t + \left(\frac{F_{\rm act}}{\gamma}\right)^2 t^2, \tag{12}$$

that can still be split into the passive diffusive limit $\langle\triangle\mathbf{r}_{\rm cm}^2\rangle = 4D_{\rm cm}^{\rm pd}\,t$ for $t_I \ll t < t^* \ll t_a$, and a ballistic regime $\langle\triangle\mathbf{r}_{\rm cm}^2\rangle = (F_{\rm act}/\gamma)^2\,t^2$ for $t^* < t \ll t_a$, where the time scale t^* is

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